A Computer-Based Decision Tool for Prioritizing the Reduction of Airborne Chemical Emissions from Canadian Oil Refineries Using Estimated Health Impacts

by

Stephanie Gower

A thesis
presented to the University of Waterloo
in fulfilment of the
thesis requirement for the degree of
Doctor of Philosophy
in
Health Studies and Gerontology

Waterloo, Ontario, Canada, 2007

AUTHOR'S DECLARATION FOR ELECTRONIC SUBMISSION OF A THESIS

I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.
I understand that my thesis may be made electronically available to the public.

Abstract

Petroleum refineries emit a variety of airborne substances which may be harmful to human health. HEIDI II (Health Effects Indicators Decision Index II) is a computer-based decision analysis tool which assesses airborne emissions from Canada's oil refineries for reduction, based on ordinal ranking of estimated health impacts. The model was designed by a project team within NERAM (Network for Environmental Risk Assessment and Management) and assembled with significant stakeholder consultation. HEIDI II is publicly available as a deterministic Excel-based tool which ranks 31 air pollutants based on predicted disease incidence or estimated DALYS (disability adjusted life years). The model includes calculations to account for average annual emissions, ambient concentrations, stack height, meteorology/dispersion, photodegradation, and the population distribution around each refinery. Different formulations of continuous dose-response functions were applied to nonthreshold-acting air toxics, threshold-acting air toxics, and nonthreshold-acting CACs (criteria air contaminants). An updated probabilistic version of HEIDI II was developed using Matlab code to account for parameter uncertainty and identify key leverage variables. Sensitivity analyses indicate that parameter uncertainty in the model variables for annual emissions and for concentration-response/toxicological slopes have the greatest leverage on predicted health impacts. Scenario analyses suggest that the geographic distribution of population density around a refinery site is an important predictor of total health impact. Several ranking metrics (predicted case incidence, simple DALY, and complex DALY) and ordinal ranking approaches (deterministic model, average from Monte Carlo simulation, test of stochastic dominance) were used to identify priority substances for reduction; the results were similar in each case. The predicted impacts of primary and secondary particulate matter (PM) consistently outweighed those of the air toxics. Nickel, PAH (polycyclic aromatic hydrocarbons), BTEX (benzene, toluene, ethylbenzene and xylene), sulphuric acid, and vanadium were consistently identified as priority air toxics at refineries where they were reported emissions. For many substances, the difference in rank order is indeterminate when parametric uncertainty and variability are considered.

Acknowledgments

Many thanks to Dr. Stephen McColl, my advisor, who provided invaluable advice and support and pointed me in the right direction more times than I can count. He spent hours staring at graphs, discussing HEIDI, and finding the bugs – usually by questioning weird results. He is not only knowledgeable about almost everything biological, risk-related, and public-health related, but is always extremely supportive of me and has been a friend and a mentor throughout my time at Waterloo.

My committee has also been very helpful. John Hicks provided valuable guidance on how the dispersion modeling actually works and important advice on how to operationalize it in HEIDI. Kevin Brand challenged me to think hard about the meaning of the variables and functions used in the model and kept a sharp eye out for statistical problems, errors in interpretation, and even notation mistakes.

I would like to thank NERAM and in particular John Shortreed, Lorraine Craig, Steve McColl and John Hicks for bringing me into the HEIDI project in the first place and showing me how a great team can work together on a complex project. The members of the NFPRER Prioritization Subgroup provided valuable insights during development of the deterministic version of HEIDI II - which continues to make me think about the purpose of HEIDI II. CCME and the NFPRER supported the initial development of HEIDI II.

The support of my friends and family has been amazing. In particular, Daniela Friedman Dave Hammond, and Caroline Silverman, are brilliant colleagues. The Grovers have been my champions since we met. The support of my sister and my Dad – soon we'll *all* be doctors! – has been invaluable. Mom, I miss you and know you would have been really proud.

Most of all, thank you, Patrick – you always believe in me.

Table of Contents

ABSTRACT III

ACKNOWLEDGMENTS IV

TABLE OF CONTENTS V

LIST OF TABLES VIII

LIST OF FIGURES X

1 PART 1: INTRODUCTION, BACKGROUND, AND METHODS 1

1.1 INTRODUCTION 1
1.2 BACKGROUND 2
1.2.1 HEIDI IS BORN 2
1.2.2 MODEL DEVELOPMENT: HEIDI II INTRODUCTION 4
1.2.3 MODEL EVALUATION 11
1.2.4 PURPOSE AND OBJECTIVES 18
1.2.5 RATIONALE 19
1.3 DISCLAIMER 20
1.4 METHODS 21
1.4.1 DEVELOPMENT, TESTING, AND VALIDATION 21
1.4.2 MODEL DEVELOPMENT: PROBABILISTIC ADAPTATION OF HEIDI II. 26
1.4.3 MODEL PREDICTIONS (UNCERTAINTY ANALYSIS RESULTS) 34
1.4.4 RANKS AT THE HYPOTHETICAL REFINERY 34
1.4.5 FURTHER ANALYSIS 35

2 PART 2: RESULTS 38

2.1 MODEL VALIDATION AND ANALYSIS 38
2.1.1 BASIC VALIDATION 38
2.1.2 SENSITIVITY ANALYSIS 38
2.1.3 LOCAL SENSITIVITY ANALYSIS RESULTS 40
2.1.4 GLOBAL SENSITIVITY ANALYSIS RESULTS 80
2.1.5 GENERAL CONCLUSIONS ABOUT VARIABLES THAT ARE AND ARE NOT IMPORTANT 86
2.1.6 DISCUSSION 88
2.2 MODEL/ANALYTICAL FINDINGS 91
2.2.1 INTRODUCTION 91
2.2.2 PREDICTED CASE INCIDENCE AT THE HYPOTHETICAL WORST-CASE REFINERY 92
2.2.3 PREDICTED CASE INCIDENCE AT ACTUAL REFINERIES IN CANADA 100
2.2.4 HEIDI II AS A RANKING TOOL 104
2.2.5 DISCUSSION 116
2.3 FURTHER ANALYSIS – WHAT ELSE CAN HEIDI II DO OR TELL US? 124
2.3.1 IMPACT EQUIVALENTS 124

2.3.2 SEVERAL REFINERIES IN ONE AREA 126
2.3.3 USING OTHER MODELS TO PREDICT PRIORITIES FOR PETROLEUM EMISSIONS 129
2.3.4 APPLYING HEIDI II IN OTHER CONTEXTS 134
2.3.5 DISCUSSION 139

3 PART 3: DISCUSSION 141

3.1 MODEL PREDICTIONS 141
3.1.1 EMISSIONS REDUCTION 143
3.1.2 PROBABILITY DISTRIBUTIONS FOR MODEL VARIABLES 145
3.1.3 CHARACTERIZING PM EXPOSURE-RESPONSE 145
3.1.4 MODEL STRUCTURE AND INTERESTING QUESTIONS OF VALUATION, EQUALITY, FAIRNESS, AND ETHICS 146
3.2 LIMITATIONS 148
3.2.1 STACK HEIGHTS 148
3.2.2 GEOGRAPHIC ZONES SELECTED FOR EVALUATION 149
3.2.3 USE OF ANNUAL EMISSIONS DATA 150
3.2.4 EXPOSURE MODEL 152
3.2.5 DOSE-RESPONSE MODELS 152
3.2.6 SENSITIVITY ANALYSIS 154
3.2.7 VALUATION 155
3.3 USE OF HEIDI II 156
3.3.1 HEIDI II IN A NEW POLITICAL CONTEXT? 158
3.4 RECOMMENDATIONS AND FUTURE RESEARCH 159

4 CONCLUSIONS 160

REFERENCES 161

APPENDIX A: COMMON PROBABILITY DISTRIBUTIONS 169

APPENDIX B: VARIABLES LIST AND DESCRIPTION (HEIDI II DETERMINISTIC) 170

APPENDIX C: VARIABLES LIST AND DESCRIPTION 176

C1 USER-DEFINED PARAMETERS 176
C2 PARAMETERS BUILT INTO HEIDI 178

APPENDIX D – ANNUAL EMISSIONS DATA EXTRACTED FROM NPRI 212

APPENDIX E – SECONDARY PM CONCENTRATIONS 219

APPENDIX F – NIST DATA FOR CALCULATION OF ATMOSPHERIC OH VALUES 229

APPENDIX G – BACKGROUND CONCENTRATIONS USED IN HEIDI II 232

APPENDIX H – PARAMETRIC BACKGROUND CONCENTRATIONS 236

APPENDIX I: PROPORTION OF PREDICTED INCIDENCE BELOW THE *DE MINIMIS* RISK LEVEL FOR SUBSTANCES EMITTED FROM INDIVIDUAL REFINERIES 237

APPENDIX J: PREDICTED CASE INCIDENCE AND RATES FOR CLASS 3 SUBSTANCES AT EACH OF CANADA'S REFINERIES 251

GLOSSARY 256

List of Tables

Table 1: List of the 20 Canadian refineries included in HEIDI 3
Table 2: Steps for conducting a sensitivity analysis 13
Table 3: Criteria and methods used for testing and validation of HEIDI II 24
Table 4: The major contribution to variability for inputs used in HEIDI II directs the interpretation of the sensitivity analysis results 28
Table 5: Results and comments arising from basic validation efforts 39
Table 6: Sensitivity of predicted incidence to k and OH 42
Table 7: The sensitivity of predicted incidence to uncertainty in the C-R values used 44
Table 8: Sensitivity of predicted incidence to fluctuations in annual emissions. 46
Table 9: Sensitivity of predicted incidence to fluctuations in ambient concentrations. 47
Table 10: Predicted case incidence from Vanadium exposure using alternative inputs for C-R data 58
Table 11: Predicted case incidence from Nickel exposure using alternative inputs for Ni C-R data 58
Table 12: Predicted case incidence for PAH using alternative inputs for C-R data. 59
Table 13: Approximate number of predicted incident cases per million people at the hypothetical refinery for extreme values of background and C-R 61
Table 14: Percent change in predicted incidence at 25 km from the refinery for two photodegradation times 68
Table 15: Percent change in predicted incidence at 1 km from the refinery for two photodegradation times 68
Table 16: Predicted case incidence of leukemia from ethylene (class 1 substance) exposure at the worst-case refinery. 76
Table 17: Predicted case incidence from exposure to sulphuric acid and phenol, class 2 substances. 76
Table 18: Spearman (rank) correlation coefficients for inputs values and predicted incidence 81
Table 19: Correlation between age-group and outcome-specific specific annual average mortality coefficient values with predicted case incidence. 82
Table 20: Comparing how three different types of dose-response relationships affected the model output and behaviour 88
Table 21: Proportion of predicted case incidence above the 10^{-6} *de minimis* level for all class 1 and class 2 substances for the hypothetical worst-case refinery. 94
Table 22: Predicted case incidence for mortality, chronic bronchitis, asthma hospitalization and asthma ER visits for the hypothetical worst-case refinery. 99
Table 23: Class 1 and class 2 substances emitted from each refinery for which the proportion of predicted case incidence above the *de minimis* risk level was greater than zero. 101
Table 24: Predicted case incidence from exposure to primary and secondary PM at the Shell Montreal refinery and Shell Scotford refinery 103
Table 25: Predicted case incidence – annual rates per person at the Imperial Sarnia Refinery 104

Table 26: Comparing (within-class) ranks for substances using different ranking methods. 113
Table 27: Correlation coefficients between different ranking methods for within-class rankings. 114
Table 28: Comparing across-class ranks for substances using different ranking methods. 115
Table 29: Class 1: Benzene equivalents 124
Table 30: Class 2: Mercury equivalents 125
Table 31: Comparison of simple DALYs predicted for individual refineries in Sarnia. 127
Table 32: Predicted health impact at the hypothetical worst-case refinery as compared to the hypothetical Sarnia refinery. 127
Table 33: Predicted priority (within-class rankings) of health impact from emissions at the hypothetical worst-case refinery as compared to the composite Sarnia refinery. 128
Table 34: Rank order resulting from application of TRACI's characterization factors to class 1 substances at the hypothetical worst-case refinery. 130
Table 35: Rank order resulting from application of TRACI's characterization factors to class 2 substances at the hypothetical worst-case refinery 131
Table 36: Rank order resulting from application of TRACI's characterization factors to class 3 substances at the hypothetical worst-case refinery 132
Table 37: rank order resulting from application of TRACI's characterization factors across classes (omitting class 3, for which comparison of ranking is invalid) at the hypothetical worst-case refinery 133
Table 38: Tasks involved in adapting HEIDI II to another industrial context 135
Table 39: Stack heights for refineries in Canada as reported in the NPRI database for 2004 148

List of Figures

Figure 1: Geographic locations of Canada's 20 petroleum refineries 3
Figure 2: General Structure of HEIDI II model. 6
Figure 3: Example of a refinery (Chevron refinery, located in Burnaby, B.C.) and the 20 "zones" for which (a) ambient concentrations of each substance and (b) population at risk were determined. 8
Figure 4: Aspects of the model which must be considered in an integrative and ongoing way during development, testing and validation. 22
Figure 5: Basic Testing and Validation Approach for HEIDI II. 23
Figure 6: Sensitivity ratios for class 1. 49
Figure 7: Percent change in predicted case incidence with a one standard deviation change in input for class 1 substances 50
Figure 8: Sensitivity ratio for case incidence with one standard deviation increase in input values for selected class 2 substances. 53
Figure 9: Sensitivity Ratio for case incidence with one standard deviation decrease in input vlaues 54
Figure 10: Predicted case incidence for class 3 substances. 56
Figure 11: BTEX – predicted incidence across the range of values allowed for C-R and background. 62
Figure 12: BTEX – predicted incidence across the 20th percentile of values for C-R and background leading to highest predicted incidence. 63
Figure 13: Vanadium. Predicted incidence across the range of values allowed for C-R and background. 64
Figure 14: V – predicted incidence across the 20th percentile of values for C-R and background leading to highest predicted incidence. 65
Figure 15: Vanadium. Predicted incidence across the range of values allowed for C-R and Slope. 66
Figure 16: HEIDI II predicts that low stack heights deliver a much higher concentration to nearby locations, while intermediate stack heights deliver larger concentrations to intermediate distances. 70
Figure 17: The proportion of each substance remaining at any given location around the refinery depends on the degradation rate constant of the substance and the time available for photodegradation. 72
Figure 18: Ethylene (as oxide) (in the 1 km NE quadrant) is used as an example. 74
Figure 19: The interaction between stack height and photodegradation time. 75
Figure 20: Nickel, like all class 1 and class 2 substances, decreases in concentration with distance from the refinery. 78
Figure 21: Concentration of SOx increases with distance from the refinery, in contrast to all class 1 and 2 substances. 79
Figure 22: Sample scatterplot showing a strong linear relationship between C-R value and the predicted case incidence for 1,3-butadiene. 84
Figure 23: Sample scatterplot (for Mercury) showing the relationship typical of that observed between ED05 and predicted case incidence for class 2 substances. 84

Figure 24: There is a clear linear relationship between C-R value and predicted case incidence for all class 3 substances. 85
Figure 25: Cumulative probability distribution for predicted case incidence of lung cancer from Nickel (and compounds) at the hypothetical worst-case refinery. 93
Figure 26: Cumulative probability for predicted case incidence of each outcome associated with exposure to $PM_{2.5}$ from SO_x 96
Figure 27: Cumulative probability for predicted case incidence of each outcome associated with exposure to $PM_{2.5}$ from NO_x 97
Figure 28: Cumulative probability for predicted case incidence of each outcome associated with exposure to primary $PM_{2.5}$ 98
Figure 29: Distribution of population in each of 20 "quadrants" around the Imperial Sarnia Refinery 104
Figure 30: Probability that class 1 substances will be assigned a rank from 1-7 based on predicted incident cases. 105
Figure 31: Probability that class 2 substances will be assigned a rank from 1-10 based on predicted incident cases. 106
Figure 32: PM from SOx is always ranked as having the greatest impact on health effects based on predicted case incidence. 107
Figure 33: Cumulative probability for predicted case incidence of CNS neurotoxicity from BTEX, nasal irritation from Vanadium, and benign nasal tumors from sulphuric acid. 109
Figure 34: Applying DALY values to the predicted case incidence numbers changes the perception of which substance is "high priority". 110
Figure 35: Comparing probability distributions for predicted health impact across classes 111
Figure 36: Rankings for class 1 substances obtained from HEIDI II and TRACI correspond relatively well. 130
Figure 37: Rankings for class 2 substances obtained from HEIDI II and TRACI do not correspond well. 132
Figure 38: Frequency with which each class 1 substance achieved each possible rank during the Monte Carlo simulation. 137
Figure 39: Frequency with which each class 2 substance achieved each possible rank during the Monte Carlo simulation. 138
Figure 40: Frequency with which each class 3 substance achieved each possible rank during the Monte Carlo simulation. 138
Figure 41: Combined uncertainty and variability estimates for carcinogenesis in a population of 260 milion. 192

1 Part 1: Introduction, Background, and Methods

1.1 Introduction

Over the past decades, there has been recognition that many of the industries and products upon which our society depends may negatively affect the environment and human health. Although many industrial processes are essential, they may be associated with effects such as resource depletion, loss of wildlife habitat, and emission of toxic pollutants. Scientists, policymakers, and other stakeholders are making an effort to understand what the specific impacts are and to identify those with the greatest consequences. In Canada in 2003/2004, a unique national, multi-stakeholder effort was undertaken to identify the best ways to reduce airborne oil refinery emissions. One of the products of this process was HEIDI II (Health Effects Indicators Decision Index II) a computer-based tool designed to prioritize airborne emissions from Canadian petroleum refineries on the basis of estimated health impacts. HEIDI II was designed with extensive consultation with a multi-stakeholder committee which included representatives from government, industry, NGOs, and the academic community.

Currently, HEIDI II is available as a publicly available tool which uses deterministic values to rank groups of substances emitted from each of Canada's 20 oil refineries. The following project presents a new and updated version of HEIDI II: the model has now been extensively tested and validated, and incorporates knowledge about the uncertainty and variability associated with many of the model's inputs. A comparison of the distributions for predicted health impacts at Canadian refineries inform about priority substances for reduction in the face of uncertainty and hint at the range of potential risk which may be associated with each emission in each location. A comparison of various methods of ranking the probabilistic results confirms that the appropriate substances are being identified as high priority while allowing exploration of the implications of stochastic results for interpreting rank orders in general. The report also explores the possibility of adapting HEIDI II to other contexts, such as other industries, and emissions from several refineries simultaneously affecting one population.

1.2 Background

1.2.1 HEIDI is born

It is now universally recognized that poor air quality has adverse impacts on human health (Cohen, Anderson et al. 2004), and Canadians are becoming more concerned about the impact of industrial emissions (Corporate Research Associates Inc. 1997). One source of airborne pollutants is the petroleum refining industry. Currently, there are 18 petroleum refineries operating across Canada, some of which are located in highly populated areas (see Figure 1 and

Table 1)[1]. The types and amounts of emissions created by these refineries are publicly available through Canada's NPRI (National Pollutant Release Inventory) (Environment Canada 2005).

In 2001, the Canadian Petroleum Products Institute (CCPI), representing the refiners of Canada, approached provincial and federal departments of environment and energy with a proposal to establish and co-fund a new approach to reducing emissions from the petroleum refining sector. The NFPRER (National Framework for Petroleum Refinery Emissions Reductions) was conducted as a multi-stakeholder process with the ultimate goal of providing facility emissions caps for key pollutants and air toxics (McColl, Hicks et al. 2003; CCME (Canadian Council of Ministers of the Environment) 2005). One component of the framework required the formation of a Health Prioritization Subgroup.

The responsibilities of the Health Prioritization Subgroup included providing information on the health impacts of exposure to pollutants, either alone or as mixtures, making recommendations on addressing knowledge gaps, establishing a prioritized list of pollutants of concern, and participating in the development of principles and methods used by jurisdictions to establish performance-based facility emission caps that are protective of human health and the environment (McColl, Hicks et al. 2003; CCME (Canadian Council of Ministers of the Environment) 2005).

---

[1] At the project inception, 20 refineries were operating in Canada; two have since been closed down.

Figure 1: Geographic locations of Canada's 20 petroleum refineries

Table 1: List of the 20 Canadian refineries included in HEIDI

Canadian Refineries (Corporation and location)	
Chevron Canada Limited - Burnaby Refinery	Parkland Refining Ltd. - Bowden Refinery *(closed in 2001)*
Consumer's Co-operative Refineries Ltd./NewGrade Energy Inc., Regina	Petro-Canada - Edmonton Refinery
Husky Oil Operations Limited - Prince George Refinery	Petro-Canada - Mississauga Lubricant Center
Imperial Oil - Dartmouth Refinery	Petro-Canada - Raffinerie de Montreal
Imperial Oil - Nanticoke Refinery	Petro-Canada - Oakville Refinery *(closed in 2004)*
Imperial Oil - Sarnia Refinery Plan	Produits Shell Canada - Raffinerie de Montreal-est
Imperial Oil - Strathcona Refinery	Shell Canada Products - Sarnia Manufacturing Centre
Irving Oil Ltd. Refining – Saint John	Shell Canada Products - Shell Scotford Refinery
North Atlantic Refining - North Atlantic Refinery, Come-by-Chance	Sunoco Inc. - Sarnia Refinery
Nova Chemicals (Ltd.) - Nova Chemicals (Canada) Ltd., Corunna	Ultramar Ltee - Raffinerie St. Romuald

NERAM (the Network for Environmental Risk Assessment and Management) was engaged by the Health Prioritization Subgroup to provide a critical analysis of available prioritization schemes. In their extensive review, NERAM determined that a new tool would be needed to appropriately prioritize the refinery emissions, and developed a prototype of the tool, called HEIDI (Health Effects Indicators Decision Index) (McColl, Hicks et al. 2003).

As a prototype, HEIDI provided proof-of-concept, ranking six substances for four refinery scenarios (three "real" refineries plus a hypothetical "worst-case" refinery). The rankings were carried out for various levels of model complexity, and were used to identify an appropriate base-case for expansion into a comprehensive screening-level prioritization tool.

1.2.2 Model development: HEIDI II introduction

HEIDI II was designed by NERAM in consultation with the NFPRER Health Prioritization Subgroup as an expansion of the HEIDI 1 prototype (Model 4c) previously developed by NERAM in 2002-03 (McColl, Hicks et al. 2003) [2]. The level four prototype represented a model-based approach of relatively high complexity, and ranked substances using emission mass, toxicity weighting, physicochemical characteristics, and exposed population. The approach to model development was stakeholder-driven: throughout the development process all significant conceptual and methodological issues were reviewed on a periodic basis by the entire Health Effects Subgroup (HSP), or by delegated members of the HSP. The members of the NFPRER HSP included representatives from industry, NGOs, regulatory jurisdictions, and consultants. HEIDI II exists as a screening-level tool designed to assist policymakers in prioritizing reductions of air emissions from each Canadian petroleum refinery on the basis of estimated risk to human health.

Broadly, HEIDI II is a Microsoft Excel (Microsoft 2000) workbook[3] which produces facility-level rankings of the potential health impacts associated with three classes of air emissions: (1) non-threshold-acting air toxics (carcinogens), (2) threshold-

---

[2] The HEIDI I prototype explored five levels of complexity for prioritization ranking schemes.

[3] As a major requirement of HEIDI II was that it be completely transparent to potential users, it was created using Microsoft Excel software Microsoft (2000)., which is widely used and allows tracking of equations and data. Additionally, no elements of the program use visual basic code of any kind, as this was found to cause difficulties for users whose computer security settings are controlled by the larger organizations by whom they are employed.

acting air toxics (non-carcinogens), and (3) criteria air contaminants (CACs)[4] for each of the 20 refineries in Canada. As inputs to its calculations, HEIDI II considers the site-specific annual pollutant emission data, location-specific background (ambient) air concentrations, degradation properties of the emitted substances, substance-specific toxicity data for each emission, and site-specific population densities. HEIDI II predicts health impacts for three different health effects endpoint types: cancer, non-cancer illnesses, and cardiorespiratory illnesses and death, employing a specific concentration-response function for each class of health effects.

HEIDI II provides three sets of relative rankings of the estimated health impacts associated with the substances emitted from each facility, based on (i) predicted incidence of health effects, (ii) a simplified disability-adjusted life year (DALY) measure, and (iii) a more complex DALY measure. The DALYs represent summary measures of health impacts that allow for a comparative ranking of the incidence and severity of health effects within each of the three classes of air emissions (or across classes if desired by the user).

The following section provides a brief description of HEIDI II. For a more complete description of the input variables, data sources, and mathematical relationships between variables included in HEIDI II, please see Appendix B. Appendix C includes discussion of some of the limitations of the variable choices and justifications for their use. Decisions made about key parameters and a complete list of assumptions made during design of HEIDI along with the associated limitations and advantages are fully documented in the final technical report that accompanies the currently available version of the model (McColl, Gower et al. 2004).

1.2.2.1 A description of HEIDI II – the deterministic version

HEIDI II is best described as a modular tool (See Figure 2) that can be applied for any refinery in Canada.

---

[4] The term “criteria air contaminants” was defined by the US Clean Air Act amendments of 1970 and refers to ambient pollutants that are widespread and reasonably expected to present a danger to public health or welfare (National Research Council, 2004). Although “CAC” was initially an American term, its use is now widespread in Canada. Ontario provincial documents may also refer to “common air contaminants”

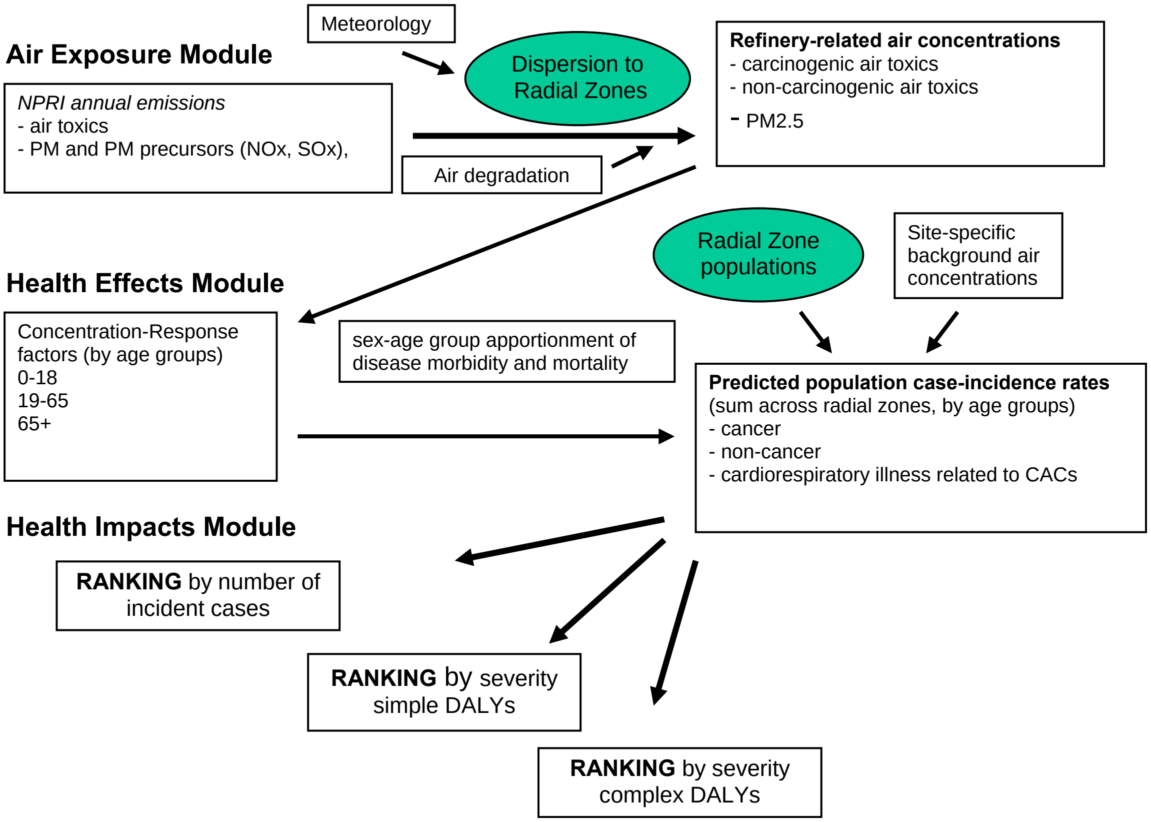


Figure 2: General Structure of HEIDI II model. Note modular structure, with three main modules: (i) Air exposure module, (ii) Health effects module, (iii) Health impacts module.

Substances included in HEIDI II

HEIDI II considers selected air pollutants that are reported annually to Environment Canada's National Pollutant Release Inventory (NPRI) database (Environment Canada 2005). HEIDI II assesses 29 air toxics including two mixtures: polycyclic aromatic hydrocarbons (PAHs), and BTEX (benzene, toluene, ethylene, and xylene). The air toxics were selected for inclusion in consultation with the CCME's NFPRER Health Prioritization Sub-group based on the following criteria: quantity of emissions reported in NPRI, CEPA-toxic substances, substances included on Health Canada Priority Substance List (PSL2), and PSL scores for toxicity, persistence and bioaccumulation.

The selection and characterization of the CACs was also accomplished in consultation with the Health Prioritization Sub-group. $PM_{2.5}$ (fine particulate matter) was assumed to be an indicator of overall ambient air quality, and the concentration-response functions chosen accounted for the health impacts of gaseous co-pollutants. PM_{10} and O_3 were not modeled HEIDI II in order to avoid "double-counting", although the authors recognized the importance of O_3 in particular for formation of photochemical smog.

Data used to develop model predictions (deterministic version of HEIDI II)

The HEIDI II tool is comprised of three modules:

(1) The **Air Exposure Module** uses a USEPA air dispersion computer model (AERMOD) to estimate ambient concentrations of carcinogenic and non-carcinogenic air toxics and particulate matter (PM) in the airshed impacted by each refinery. Specifically, air concentrations are estimated for 20 zones (defined by five radii, each subdivided into four geographical quadrants, within a 25 km boundary (See Figure 3)).

Refinery emissions data for the air toxics were retrieved from Environment Canada's NPRI database (2001) (Environment Canada 2005), and emissions of criteria air contaminant (CAC) emissions were drawn from 2001 data provided by Environment Canada in 2003 for the HEIDI I project. This CAC data was collected from CPPI member refineries and from publicly available information for non-CPPI refineries. HEIDI II also estimates in a simplified manner the formation of secondary particulate matter from PM precursors (NO_2 and SO_2) using conversion factors found in the research literature. The air pollutants are assumed to be emitted continuously at a constant average annual rate from a single stack in the centre of the refinery property. It is assumed that each substance is emitted at a constant rate over the period of one year. A generic meteorological profile representing southwestern Ontario is used as the default scenario, and the terrain is assumed to be flat, resulting in physical air distribution patterns being generic and not site-specific.

(2) The **Health Effects Module** estimates, for each refinery location, the predicted cancer incidence, systemic disease incidence, and cardiopulmonary disease incidence associated with the refinery's contribution to the ambient air concentration of each substance. Health effects are first estimated for each of 20 "zones" around each refinery (See Figure 3) and then summed to obtain a total estimate of the impact of the refinery's airborne emissions within 25 km of the facility.

To determine the population at risk, the Geographical Information System (GIS) software ArcMap (ESRI Inc. 1999-2002) was used to map site-specific population density profiles and Canadian age/sex distribution profiles extracted from 2001 Statistics Canada Census Data (Statistics Canada 2002). Environment Canada data for background air levels of pollutants from anthropogenic and natural sources collected in the vicinity of each of the refineries (Environment Canada 2003) was used to estimate the facilities' attributable contribution to ambient air concentrations above background levels at each location.

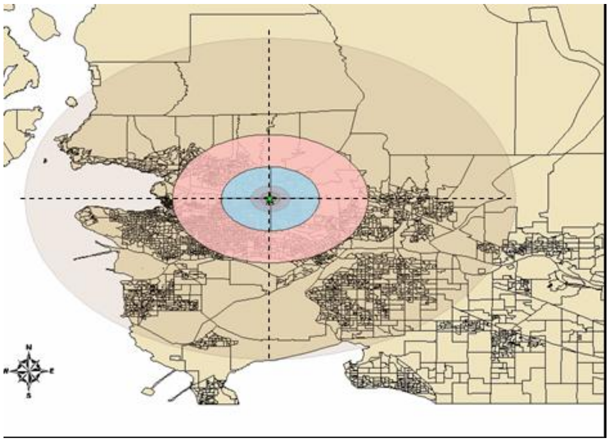


Figure 3: Example of a refinery (Chevron refinery, located in Burnaby, B.C.) and the 20 "zones" for which (a) ambient concentrations of each substance and (b) population at risk were determined. Underlying polygons represent census dissemination areas from which population density information was derived using ArcMAP software.

For estimating population health effects of air toxics, HEIDI II uses concentration-response parameter values based on standardized measures of concentration-response derived primarily from Health Canada source materials (Environmental Health Directorate Health Protection Branch 1996; Toxicology Excellence for Risk Assessment (TERA) & Concurrent Technologies Corporation 2004), or where Health Canada values are not available, from USEPA (Toxicology Excellence for Risk Assessment (TERA) & Concurrent Technologies Corporation 2004; U.S. Environmental Protection Agency 2004) or CalEPA sources (i.e., (California Air Resources Board 2005))(California Air Resources Board 2004). HEIDI II estimates chronic health effects associated with exposure to particulate matter (PM) based on the extensively peer-reviewed American Cancer Society (Pope, Thun et al. 1995) and Harvard Six-City chronic epidemiology studies (Dockery, Pope et al. 1993), or values from their reanalyses (Health Effects Institute 2000) where appropriate. In these and other studies, the population health impacts associated with chronic exposure to PM are estimated to be as large as or greater than those from acute exposure. However, HEIDI II likely underestimates the health effects associated with acute (daily) PM exposure to some extent. Although acute endpoints for CAC exposure (such as visits to the emergency room due to asthmatic episodes) arise from exacerbation of an underlying, chronic disorder in most cases, an assessment of other potential short-term effects of PM exposure is not included in HEIDI. HEIDI also does not characterize the acute effects of exposure to photochemical smog.

(3) The **Health Impacts Module** aggregates diverse health effects of varying severity using a common metric. Two variations of Disability Adjusted Life Years (DALYs) are applied for this purpose. In the first, a series of simplified DALYs is calculated based on an approach developed by ILSI which accounts for three basic levels of severity (Burke, Doull et al. 1996). The more complex form of DALYs, based on the World Health Organization's 'global burden of disease' approach (Murray and Lopez 1996), uses 140 illness categories representing fatal and non-fatal outcomes according to age, sex and other demographic factors.

The final output of HEIDI II is a priority ranking of those NPRI substances in order of preference for emissions reduction, according to either the predicted health effects case-incidence rates (which do not consider severity of health effects) or the predicted health impact DALYs (which attempt to take into account the severity of the health effect).

User-selected options

Several aspects of the HEIDI II program were designed to allow the user to set the scenario for analysis. The user-controlled options include stack height, hours of sunlight (which affects photodegradation) and an option to include substances in the ranking even if their emissions were reported as falling below the reporting guideline.

- Stack height - The default stack height is 30 metres, but HEIDI II can also perform rankings using stack heights of 5 metres or 15 metres.
- Photodegradation time - The default setting for photodegradation time (important for predicting the amount of decay that a given chemical will undergo) is 12 hours, but HEIDI II can also perform rankings using any photodegradation time from 0-24 hours (for Class I and Class II air toxics only).
- Refinery emissions reported to be zero[5] - Because many of the emissions fall below reporting guidelines set out by the NPRI, they are reported in the NPRI as being zero. In order to assess the rank order that might occur for substances if they are emitted at levels below the reporting guideline level, an alternate ranking scenario is available within the HEIDI II model. The user may choose a percentage value (1-99%) of the NPRI reporting threshold for substances that are reported in the NPRI as zero emissions. (The default setting for percent of the reporting threshold is 50%, if the user elects to include substances reported as zero emissions). With this scenario, **all** substances reported as being emitted at the zero level are evaluated at the same percent of their reporting guideline value (i.e, the user cannot select different percentages of the reporting guidelines for different substances).

Outputs created by HEIDI II

HEIDI provides the following three health impact ranking outputs for each facility:

1) Ranking of pollutants based on predicted number of annual incident cases of health effects. This ranking does not take into consideration differences between types of health effects i.e. temporary, chronic, and fatal conditions.
2) Ranking of pollutants based on simplified Disability Adjusted Life Years (DALYs) that provide a common measure for comparing the severity of different health endpoints (e.g. (i) irreversible/life-shortening, (ii) may be reversible, could be life-shortening, (iii) generally reversible, generally not life-threatening) across

---

[5] This scenario was later removed from the probabilistic version. As described in the Methods chapter, using a percentage of the reporting guideline did not appear to be a realistic approximation of possible emissions for these substances, since emissions documentation was frequently provided for many substances which were emitted at levels below these guidelines.

the three classes of air emissions. The DALY calculation is based on years of life lost due to death and loss of quality of life due to illness.

3) Ranking of pollutants based on more complex Disability Adjusted Life Years (DALYs) that consider type of cancer, type of systemic disease, or type of cardiopulmonary health effects.

Note that the predicted numbers of incident cases and predicted numbers of DALYs are useful only for purposes of making risk-related comparisons between chemicals and do not represent actual risk.

Application of HEIDI II results

The purpose of HEIDI II is to provide a screening-level risk-based ranking of refinery NPRI emissions, to help inform users in prioritizing emissions reductions at petroleum refinery emissions. Screening analysis models are purposefully based on simple models that will not underestimate exposure, and are used for identifying scenarios of concern (Cullen and Frey 1999). There are considerable uncertainties in the data inputs and modeling assumptions within each of the three HEIDI II modules, and care is advised when comparing health impacts between cancer, non-cancer effects, and the criteria air contaminants. The rankings rely on rough statistical estimates of predicted incidence rates for a variety of health endpoints of widely differing severity. As the technical report points out,

> *"The statistical models used to calculate priority rankings can provide useful guidance in relative terms by comparing estimated health impacts associated with annual emissions at the facility level, but they cannot adequately represent absolute estimates of health risk in the exposed populations."* (McColl, Gower et al. 2004)

1.2.3 Model Evaluation

Development, testing, and validation of models should occur in an integrated way (Saltelli, Tarantola et al. 2004), where results of model testing may influence decisions about model design. McKay (McKay 1988) suggests that model evaluation involves three main objectives: (i) exploration and investigation of model calculations, (ii) sensitivity analysis, and (iii) uncertainty analysis. Initially, this involves basic testing of the model to identify errors in its structure and inspecting the structure and results for validity. However, full evaluation of a model requires a structured method for testing models which allows for flexible analysis. Saltelli (Saltelli, Tarantola et al. 2004) sets out a specific framework for conducting sensitivity analyses (See Table 2). Applying these steps more broadly to include uncertainty analysis in the goals and methods of the analysis provides a useful framework on which to base model evaluation in general.

1.2.3.1 Sensitivity Analysis

Sensitivity analysis (SA) is used to determine to what degree model predictions are affected by variation in input values. The interpretation of SA varies depending on the reason for varying the input, including uncertainty, inherent variability, or manipulation by a modeler to represent alternate scenarios. SA identifies variables that matter to the model predictions; sources and ranges of variation for these variables ought to be well-characterized where possible. Using SA to test the upper and lower-bound estimates for uncertain or variable inputs can also identify cases where variation in input does not affect model predictions in a significant way. These variables can be characterized by point estimates without any loss of information, allowing development of models that maximize information in model output without introducing unnecessary model complexity. Testing various methods of representing data or relationships within the model allows comparison of various modeling approaches and can determine whether simple representations of ideas are adequate. SA is also useful in providing a sense of the range of possible outputs that might be observed across a variety of scenarios.

A common complaint regarding computer models is that, if manipulated in certain ways, they can be made to produce any output desired. According to Saltelli (Saltelli, Tarantola et al. 2004), sensitivity analysis can provide a valuable quality check and be carried out in a way that is unambiguous and defensible. She stresses the importance of defining the focus and setting for any sensitivity analysis that is carried out.

Best practice for sensitivity analysis suggests that models should create only relevant outputs that address the object of the analysis, and not be clouded by excess complexity and outputs. As well, patchy or piece-wise sensitivity analysis should be avoided. Finally, sensitivity analysis should be used in the process of model development (Saltelli, Tarantola et al. 2004).

Table 2: Steps for conducting a sensitivity analysis (Saltelli, Tarantola et al. 2004)

Step	Action
1	Establish the goal of the analysis and use it to define the form of the output function such that it answers your question. The question should be stated in a top-level form rather than in terms of the actual model output.
2	Decide which input factors should be included in the analysis. Trigger parameters (which sample across model structures) may be defined
3	Choose distribution functions for each of the input factors. These functions may derived from various sources: 1. literature 2. by fitting empirical distributions to empirical data 3. expert opinion 4. normal distributions truncated to avoid sampling outliers 5. in the case of triggers, weights may be applied to the different values of the triggers if prior information is available about the relative likelihood of possible model structures 6. correlation structures may be defined if appropriate
4	Choose a sensitivity analysis method based on: 1. the questions being addressed. (Is the issue a screening problem or is quantitative methodology required?) 2. the number of affordable model evaluations (if the number of input factors is high, either the method of Morris or grouping of factors may be required) 3. presence or absence of correlation structure between input factors (for screening, correlation can initially be dropped and subsequently reintroduced for the quantitative analysis of the few remaining important factors)
5	Generate input sample (follows from method chosen for the sensitivity analysis)
6	Evaluate the model on the generated sample and produce the output
7	Analyze the model outputs, draw conclusions, possibly start a new iteration of the analysis

Two broad types of sensitivity analysis include (i) a perturbative (or ‘local’) approach, which assesses the effect of varying one factor while all others are kept constant, typically by calculating partial derivatives, and (ii) a global approach, which evaluates the effect of the factor while all others are also varying (Saltelli 2002).

McKay suggests that the local approach can provide a complete description of importance (McKay 1988). He identifies two specific methods for assessing importance with local measures: (i) using partial rank correlation coefficients, to measure the degree of strength of association between input and output (after the spread in variable values has been normalized), and (ii) using regression coefficients to measure the intensity of the relationship; i.e., change in output per unit change in input. Both of these methods could be used to assess the relationship between any input variable and model predictions. Those with the strongest relationship would be deemed most important to predicting output.

Saltelli advocates use of the global approach (Saltelli 2002; Saltelli 2004) and identifies several focused settings for sensitivity analysis. In the “factors prioritization setting”, the objective is to determine the most important factor, where this is defined as being the one which, if its “true value” was known, would most reduce the variance in the model output. This method is used to identify priorities in research. The “factors fixing setting” is designed to simplify complex models through identification of non-influential factors whose values can be fixed anywhere within their range of uncertainty without significantly reducing the variance in output. In the “variance cutting setting”, the objective is to reduce the variance of the target function from its unconditional value to a lower pre-established threshold value. Finally, the “factors mapping setting” is used to determine which factors are responsible for creating output in a region of specific interest.

Variables, model parameters, or model formulations that are most responsive to changes in input are said to be more “sensitive”, and thus may play an important role in predicting outputs if they are naturally subject to variation or if they are highly uncertain. Thus, in the case of factors prioritization setting, sensitivity analysis is often also called “importance analysis”.

Sensitivity analysis may be particularly important in the context of a ranking model such as HEIDI II since small changes in sensitive input variables could dramatically alter the output ranking order. The interpretation and communication of the meaning of a rank order relative to its sensitivity to changes in input must be considered, where the meaning of an alteration in rank based on a subtle change in predicted impact should perhaps be differentiated from alterations in rank due to larger changes in predicted impact.

1.2.3.2 Uncertainty analysis

Modelers of health impacts acknowledge that use of point estimates to represent model parameters limits the value of model output, and are moving away from purely deterministic methods (Pennington, Norris et al. 2000). Various levels of uncertainty have been described (Gough 1997). These include (i) risk, which exists where the behaviour or character of the parameter or system is reasonably well-known, and distributions can be assigned, (ii) scientific uncertainty, where significant parameters have been identified, but their distributions are not known (iii) ignorance – about what is not known, and (iv) indeterminacy, where causal links, networks, and processes cannot be predicted.

Probabilistic analysis allows propagation of uncertainties in model estimates to yield quantitative information about both the range and relative likelihood of model predictions (Cullen and Frey 1999). Bailar and Bailar (Bailar and Bailar 1999) and others have identified various types of uncertainty that are relevant to modeling environmental health impacts, including parameter uncertainty, model uncertainty, and scenario uncertainty. Parameter uncertainty, which is associated with either a lack of knowledge about specific variables in the model, or inherent variability in the factors, is typically addressed using traditional statistical techniques such as calculation of standard deviations for each variable or Monte Carlo Simulation, which includes the probability of observing each value in the uncertain range calculated for the output (Morgan and Henrion 1990). These methods are well-established, and while they cannot reduce the uncertainty inherent in a given set of data, they allow appropriate description of the possible variation in outcome that could result from it. Model and scenario uncertainty are more difficult to assess. Model uncertainty refers to the construction of the model and how various elements are related to each other. An example of a gap in knowledge that creates model uncertainty is the controversy about whether linear, non-threshold models are sufficiently accurate to set conservative limits for exposure to carcinogens. Sensitivity analysis, in which changes in output are monitored as various input parameters (including functional relationships such as dose-response functions) are changed, is one method of assessing model uncertainty. It is also possible to include alternate formulations of a model in a simulation designed to assess the extent of uncertainty in outputs that could result from model uncertainty. Scenario uncertainty refers to the relevance of the model output, and may be partly addressed through formulation of alternative scenarios to see how well the model performs in a variety of related situations (Pruss, Corvalan et al. 2001). Some attempts have also been made to address scenario uncertainty through use of cultural theory, which distinguishes value systems which may be helpful in explaining peoples' attitudes (Hofstetter 1998; Goedkoop and Spriensma 1999). In general, current methods to address model and scenario uncertainty are inadequate, and disciplinary perspective can often colour how uncertainty is viewed and treated by scientists (Bailar and Bailar 1999). This may be important for communicating about how to use HEIDI II and how to interpret the results since users may include risk assessors, toxicologists, policy-makers, or interested members of the public.

Uncertainty analysis may be helpful in identifying key sources of uncertainty and variability that can focus future research activity (Cullen and Frey 1999). Dominici and Burnett confirm that providing uncertainty estimates for predictions relating air pollution to health effects is necessary to prioritize future research initiatives, and for more effective communication with regulators and the public (Dominici and Burnett 2003). Industrial representatives agree that uncertainties must be explicitly identified and communicated in order to prevent the development of inappropriate or untimely policies (Granville 2003).

There are various methods for identifying key contributors to uncertainty in a model. Before a simulation is carried out, the magnitude of the variation of each input can be compared. For linear models in particular, the magnitude of the estimated variation indicates potential to contribute to output uncertainty. Coefficients of variation (determined by dividing the variable variance by its mean value) can also be used to identify a priori potentially important inputs for linear models. Sensitivity analysis techniques are also appropriate, since the uncertainty about a highly influential variable is more likely to propagate through the model and affect model predictions. For example, after the simulation has been carried out, scatterplots of inputs versus the corresponding model outputs provide a visual sense of whether one influences the other. The input and output values can be regressed against each other in multivariate regression, and correlation coefficients[6] can be calculated, where coefficients >0.5 indicate substantial dependence (Cullen and Frey 1999). The specific methods used to evaluate uncertainty in HEIDI II are described in the methods section (Chapter 3).

Numerical methods for probabilistic analysis are useful for several reasons: they accommodate a wide variety of assumptions, can evaluate the effects of correlation and dependencies, and their accuracy increases as the sample size is increased. LHS (Latin

---

[6] The type of correlation coefficient may depend on the function under study, i.e. for nonlinear monotonic functions, use of rank correlation may be most appropriate.

Hypercube sampling) may perform better than Monte Carlo simulation for a given sample size (number of iterations). However, LHS may have limitations with respect to estimating higher moments such as variance, skewness, or higher percentiles, which are more sensitive to extreme values (Cullen and Frey 1999). In both sensitivity and uncertainty analysis, it is important to consider the possibility that variables may be correlated, and to account for this in the analysis.

The importance of including uncertainty analyses in HEIDI II cannot be overstated. HEIDI II is designed as a ranking tool – and it must be clear how sure the predictions are that any given substance is ranked higher than the next. Both the degree of separation between the rankings and the level of certainty about whether adjacent rankings are distinct will be important for policy decisions which are informed through use of this tool.

1.2.3.3 A note on variability

It is important to distinguish between uncertainty and variability. Uncertainty denotes a lack of knowledge – about the true value of a parameter, the correct way to structure a model, or the most appropriate scenario construction, and is typically characterized using probability distributions. Variability is an inherent, empirical distribution of values for a given parameter within a population sample, and is most often characterized using frequency distributions. Variability is irreducible, and may occur in various dimensions: across space, time, geographic area, age, gender, or other specific population subgroups (Hattis and Anderson 1999).

Bailar and Bailar note that heterogeneity (inherent variability) must be distinguished from uncertainty (highlighting the specific cases of differences between children and adults, sensitive subpopulations, and synergies with prior, concurrent, or later exposures to other agents) (Bailar and Bailar 1999). Hoffman and Hammonds (Hoffman and Hammonds 1994) also note the need to distinguish whether uncertainty in a model is due to lack of knowledge or variability, indicating that the presence of both in a single model may require two-dimensional Monte Carlo simulation to produce alternative distributions of output. Carrying out Monte Carlo analyses using distributions that describe both variability and uncertainty may complicate interpretation of the results (Cullen and Frey 1999).

1.2.3.4 Choosing Ranges and Distributions

Model evaluation should occur concurrently with model development, with iterations of analyses being performed as knowledge about the behaviour of the model increases. As a result, progressive “runs” may use various degrees of knowledge about the input variables. Initial runs may be designed to assess which variables are influential to the model output and which do not have to be specified with a high degree of knowledge. The range of variation selected to describe each input value in such a case may be based on informed guesses or intuition, and be revised at a later time (McKay 1988). The selection of appropriate parametric information must consider the purpose and type of information being conveyed by each model component. Morgan and Henrion identify several types of quantities that may exist within a model, including empirical quantities, defined constants, decision variables, value parameters, and model domain parameters (Morgan and Henrion 1990).

Where possible, selection of probability distributions should be informed – perhaps by a review of the literature, from empirical data, or through expert knowledge. Some common probability distributions are described in Appendix A.

In practice, selecting probability distributions may sometimes be a somewhat arbitrary process. However, the effect of selecting certain probability distributions can be explored either by repeating the simulations using alternate probability distributions, or by using the original simulations to approximate a response surface and studying it under different distributions (McKay 1988). If significant differences in model output are observed when alternative plausible input distributions are used, it may be beneficial to spend more time identifying the best representation for inputs.

1.2.4 Purpose and Objectives

- To test and validate HEIDI II
- To evaluate the model through application of sensitivity analysis, importance analysis, and uncertainty analysis
    - To identify appropriate ways of characterizing both uncertainty and variability within the model
    - To identify an appropriate form of the model which incorporates the maximum amount of information while maintaining parsimony

    - To identify variables which have a large influence on model predictions
    - To identify variables which contribute the most uncertainty to the predictions
    - To examine how uncertainty and variability affect our understanding of the rankings produced by HEIDI II
- To use HEIDI II to make predictions about important emissions for health impacts at Canadian refineries
- To use HEIDI II to explore how predictions change under various scenarios
- To use HEIDI II to explore the implications of uncertainty for predictions
- To explore methods of ranking stochastic data
- To discuss interpretation of predicted ranking under various scenarios
- To identify limitations of HEIDI II and possible areas for improvement

1.2.5 Rationale

A great deal of effort on the part of many stakeholders, and in particular, on the part of NERAM, was involved in the conceptualization and creation of HEIDI II. This tool was designed with the intent that it should be used (in conjunction with other tools and methods) by regulators, industry, NGOs, and other stakeholders for determining realistic and useful emissions reductions for the petroleum refining industry in Canada. The additional work completed here (a) increases the capabilities of HEIDI II and its usefulness to the stakeholders, (b) identifies the most important variables for achieving high rankings, (c) explores the effects of uncertainty on the model predictions, (d) using up-to-date information, provides clear, comprehensive summaries of HEIDI II's predictions for each of Canada's refineries alongside thoughtful discussion of the implications of these predictions, and (e) explores predictions that could emerge from alternate scenarios that might be considered useful by interested stakeholders.

1.3 Disclaimer

Much of the testing and validation of HEIDI II was done using predicted case incidence as an endpoint. This is in no way intended to suggest that the case incidence values predicted from HEIDI II are representative of real numbers of cases of illness caused by airborne emissions from petroleum refineries. The values predicted by HEIDI II are intended to be used for comparative purposes only. They have not been ground-truthed and are based on several assumptions inherent to the model, which are documented elsewhere in this thesis (see especially, Appendix C) and in the technical report accompanying the publicly available version of HEIDI II (McColl, Gower et al. 2004). In particular, generic meteorology and geography were used to describe vastly different geographic locations across Canada.

HEIDI II should be used as a screening-level tool, with predicted health impacts (predicted case incidence, or predicted DALYs) to be used for ranking emitted substances within a facility. Health impact values predicted at different facilities are not directly comparable.

1.4 Methods

The starting point for this project is considered to be a lightly tested deterministic version of HEIDI II coded in Excel (McColl and Gower 2004; McColl, Gower et al. 2004). The methods describe further testing and validation of the deterministic version, and development, testing, and validation of a probabilistic version of HEIDI II, coded in a more sophisticated computing environment, Matlab (Mathworks 2002). Methods for identifying sources of uncertainty in model predictions and important variables for predicting priority substances for reduction are described. Once an acceptable model was developed, it was used to make predictions and explore implications about priority emissions from refineries across Canada.

1.4.1 Development, Testing, and Validation

Development, testing, and validation must occur in an integrated way (Saltelli, Tarantola et al. 2004), where the purpose and scope of the model determines model design, model formulation sets up how the model is assembled in order to achieve the model's goals, and correct computation ensures that appropriate numbers and coding is used to produce error-free predictions that accurately reflect the formulation of the model (See Figure 4). As the figure implies, errors can be introduced in any of these three aspects of the model, at any stage of model development; it is crucial that they be evaluated continuously throughout the development and testing process.

The general approach followed to develop the HEIDI II probabilistic model included the following steps:

1. Catalogue and describe all model variables
2. Test and validate deterministic model
3. Assign probability distributions to each model variable where possible
4. Conduct sensitivity analysis to assess impact of different variable values
    a. For uncertain/variable inputs
    b. To assess various possible scenarios
5. Conduct uncertainty analysis to determine possible range /distributions of predictions

6. Test and validate probabilistic model; make recommendations about final form of HEIDI II [ongoing throughout development process]

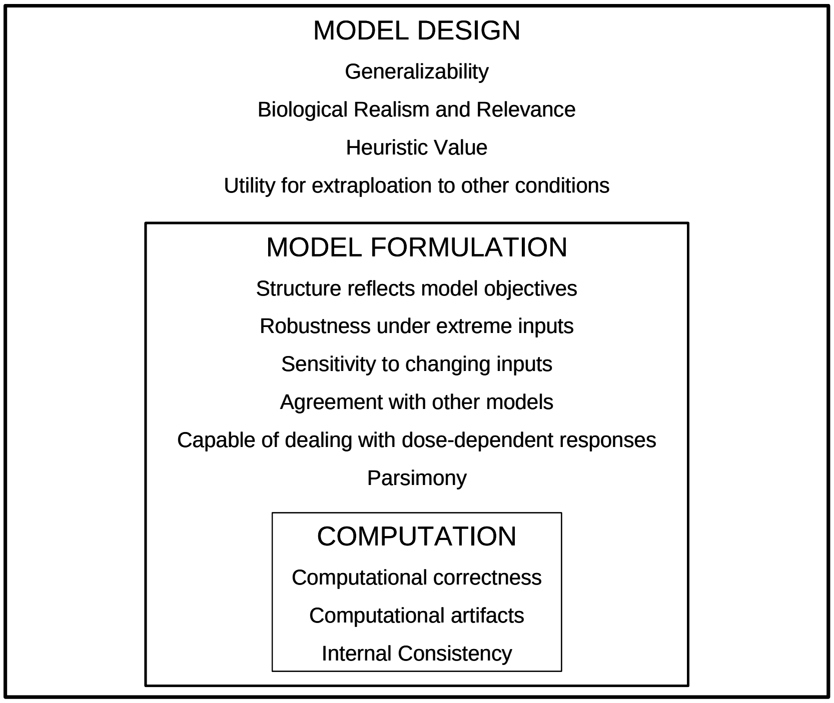


Figure 4: Aspects of the model which must be considered in an integrative and ongoing way during development, testing and validation. See Table 3 for specific testing methods

1.4.1.1 Model Inventory

An inventory of all model variables, including original data source, type of variable, and mathematical relationship(s) to other variables was compiled (See Appendix B). This allowed ordered testing of each variable to ensure appropriate representation in the model according to the model design.

1.4.1.2 Testing and Validation of the deterministic Excel version

The process described in Figure 5 was applied iteratively by the researcher as the model gained complexity. It was initially used to test the deterministic version of the model and later used for testing and validation during development of the probabilistic version. Following the approach depicted in Figure 5, and using the tabulation of model variables as a guide, each variable was examined within the module where its functionality resides. Module-by-module testing was completed first, and then HEIDI II was tested and validated as a whole.

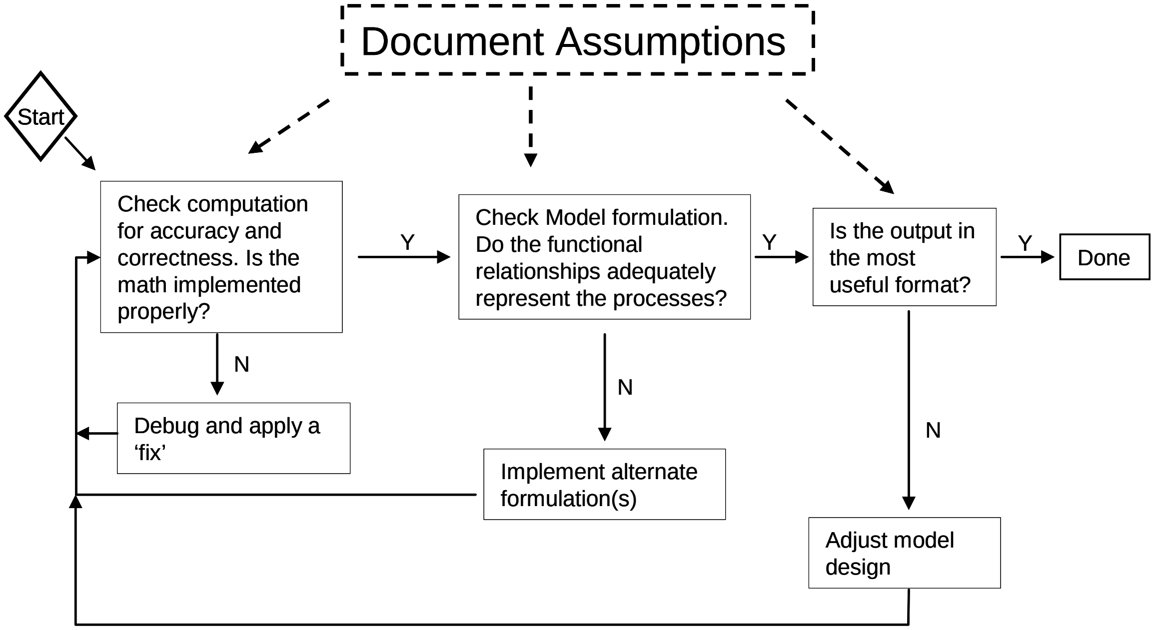


Figure 5: Basic Testing and Validation Approach for HEIDI II. This approach was used for each module individually, and then for the model as a whole.

The individual variables were classified as being subject to variation as a result of mainly (i) variability, (ii) uncertainty, or (iii) scenario choices. The uncertain and/or variable inputs were first tested while keeping the scenario variables at pre-selected default values. Once the functional relationships and variable values were confirmed as being reasonable for the model, the effects of applying the various scenarios available to the user (i.e., different refineries, stack heights, photodegradation times, emission year data etc.) were tested. The specific criteria and methods used to complete the testing and validation (for both the deterministic and probabilistic versions) are described in Table 3. The validation process also requires documentation of all assumptions made during model development and assembly, and any identified model limitations (See Appendix C).

Table 3: Criteria and methods used for testing and validation of HEIDI II throughout the development process for the probabilistic model

Validity Criterion	Definition	Methods used to test whether HEIDI II met this criterion
Computation		
Internal Consistency	How each model item independently relates to each other model variable and how they are related overall (i.e., populations in each zone add up to total population, total of fraction of PM observed in each zone adds up to one)	• Determine how each variable in HEIDI II relates to each other variable (tabulations, flow charts). If more than one method of calculating a variable is possible, values are similar from each calculation method. • Redesign HEIDI with (n-1) degrees of freedom to redefine variables in terms of each other
Absence of numerical (computational) artifacts	Examples: rounding-off errors which may affect non-monotonic functions (such as the ranking procedure), true 0 vs. notional 0, overflow and underflow effects, dealing with ties in the ranking, missing values handling	• Visual/graphical inspection of results at each stage along the model pathway to ensure realism of results • Documenting software handling of relevant issues such over-/underflow • Programming of HEIDI II in second environment (i.e., Matlab) to ensure predictions are the same
Computational Correctness	Model does not contain mathematical mis-specifications or oversights	• Visual inspection of results to assess realism • Disaggregation of HEIDI II into component modules to test inputs and outputs • Dimensional analysis – ensure that formulas predict correct units • Programming of HEIDI II in second environment (i.e., Matlab) to ensure predictions are the same
Model Formulation		
Model form is correct	Overall structure and equations, regardless of parameter values, accurately reflects model objectives	• Literature review to summarize current practice, knowledge, and thought re processes being characterized in HEIDI II, especially wrt thresholds and linear vs. nonlinear dose-response relationships • Document simplifying modeling assumptions • Annotation/documentation of reference sources
Robustness to changing input parameters	Model does not break down under differing input and exposure scenarios	• Apply emissions across a wide range of values to ensure that predicted case incidence reflects the dose-response form of the model selected. • Apply a wide range of values in place of each input variable • Visual inspection of results to assess realism under this range of emissions scenarios, also under each input/scenario selection option
Sensitivity to changing input parameters	Changes to key input parameters result in appropriate changes in model outcomes	• Sensitivity analysis – assess whether changes in inputs result in reasonable changes in outputs • Separately assess sensitivity at high and low doses

Parsimony	Model is not over-parameterized or unduly complex	• Sensitivity analyses should indicate which variables are most/ least important in output predictions. • This identifies which variables need to be characterized in terms of uncertainty/variability and which do not • If any of the scenarios available to the user do not actually alter predictions, they should be removed, and documentation provided to explain the change in model formulation.
Model Design		
Generalizability	The model is suitable for more than one application or use	• Determine whether HEIDI II could be adapted to (i) other industries (ii) include more substances (iii) other geographical areas, such as the U.S. context • What steps would be involved, complexity of achieving this, scenarios that could not be included (i.e., exposure other than inhalation?)
Biological realism and relevance	Underlying biological mechanisms are correctly specified	Assess limitations of dose-response methodology used, impact on predictions of HEIDI II. Compare to other methodologies, such as EPA's linear dose-response models; use of RfD rather than ED_{05} Compare predictions from a linear vs. threshold model for class 3 substances (CACs).
Agreement between different models characterizing the same process		Comparison to rankings that would be obtained using TRACI characterization factors Possible comparison to rankings obtained by HEIDI I for those chemicals that were assessed in the original prototype
Heuristic value	Model provides useable indicator variables that inform policy decisions	Discussion of CCME/NFPRER requirements, value of priority ranking strategies
Capacity to deal with dose-dependent biological responses		Discussion of approaches used for each different substance class (linear for carcinogens and CACs, Mantel-Bryant for air toxics)
Useful in extrapolation to other conditions		• Identify various scenarios for which HEIDI II can be used. Identify other scenarios which might be useful; assess difficulty of addressing with HEIDI • Assess utility of HEIDI II in low-dose situation. Is there an emissions level below which HEIDI II is unable to effectively prioritize (i.e., below-threshold predictions?) or a population level below which predictions are unrealistic?

In preparation for upgrading HEIDI II to probabilistic format, it was recoded in Matlab, a computational environment that allows greater flexibility in implementing and testing various model formulations. The program offers the additional advantage that evaluation time during Monte Carlo simulations was reduced compared to the Excel/Crystal Ball approach[7]. Once the deterministic model output from the two software programs (Excel and Matlab) was shown to match, the model development steps required to extend the Matlab model were undertaken.

1.4.2 Model Development: Probabilistic adaptation of HEIDI II.

Once HEIDI II was recoded in Matlab and predictions from the Excel and Matlab environments were in perfect agreement, probabilistic elements were introduced. Adapting HEIDI II into a probabilistic model essentially constituted a series of adjustments in model design. As development proceeded, at each update to the model (i.e., with new data, implementation of mathematical relationships or computations, or design elements), the process depicted in Figure 5 was re-initiated.

Distributions were identified to represent model variables where possible. For each variable, sources of uncertainty, the level of uncertainty, and the level of evidence were catalogued (see Appendix C). Specific (extra) sensitivity analyses deemed to be of interest for any individual variable were documented, and possible correlations with other model variables were identified. For each variable, justifications, notes, and comments about the parameterization of the variables, data sources, and limitations of the variable representation were also recorded. In cases where probability distributions could not be established, the implications of using point values were also assessed and recorded.

The default model for testing and analysis of the probabilistic model was selected to be a hypothetical worst-case scenario, using a stack height of 30 metres and a photodegradation time of 12 hours. This scenario uses the maximum annual emission observed across all Canadian refineries to represent each individual substance emitted, and therefore incorporates an emission for every substance included in the model (which is not the case for any individual Canadian refinery). It also uses high enough emissions

---

[7] Crystal Ball (Decisioneering 2000) is a forecasting and risk analysis software add-in for Microsoft Excel, and allowing probability distributions to be assigned to spreadsheet values. It was used in preliminary analyses but is not referred to further in this document as Matlab was used for all results presented.

that some predicted incidence of disease might be expected, but uses realistic emissions levels – as they are levels that have been recorded at real refineries. A political motivation for employing this as a default scenario was that it does not single out one real refinery for more in-depth analysis than the others. A stack height of 30 metres was chosen since it was thought to be most representative of the stack heights that exist at Canadian refineries (Hicks 2005), and 12 hours was selected as an annual average of the amount of daylight that might be expected during the day[8].

1.4.2.1 Focused settings for conducting Sensitivity Analysis

Although each variable in HEIDI II is likely subject to both uncertainty and variability, given the data available, it is not possible to sufficiently distinguish the two to enable assigning two separate probability distributions. However, it is usually apparent whether uncertainty or inherent variability dominates the reasons why a variable may take on a range of values. Distinguishing the variables by predominant "source" of variation informs the interpretation of the results of the sensitivity analysis (see Table 4).

1.4.2.2 Sensitivity Analysis (SA)

Although HEIDI II's final output is a rank order, full-model SAs were performed using *predicted incident cases* as the output of interest. Because rank order is a categorical rather than continuous output, using rank as the output for SA results in a loss of information (i.e., variation in input could change predicted case incidence for at least one substance but not alter rank order, or where only one substance in a class is associated with any predicted case incidence, rank order would not change no matter what variation occurred in inputs for that substance). Predicted health impact may be a more relevant indicator of how well the model performs. Although DALYs are intended to be the health impact measure upon which ranking/prioritization is based, in HEIDI II they are simplistically operationalized as point values (in terms of DALYS per person per year), and no relevant information about uncertainty in DALYs is available. Focusing on

---

[8] The amount of time for photodegradation might be more properly estimated based on annual average amounts of "sunlight"; in any case, the amount of either daylight or sunlight depends on the geographic location within Canada, and the assumption of 12 hours may not be appropriate for all locations. It does provide a useful base-case however, and sensitivity analysis addresses whether the amount of sunlight is an important predictor of the amount of each substance delivered to populations near refineries.

predicted case incidence rather than DALYs as an output is thus unlikely to result in a loss of information from the sensitivity analysis, and additionally, may be a more intuitive metric for the reader.

Table 4: The major contribution to variability (i.e., parametric uncertainty vs. inherent variability) for inputs used in HEIDI II directs the interpretation of the sensitivity analysis results

Dominant reason to perform SA	**Variables/formulations tested**
Assess impact of parametric uncertainty (the true value of a variable is not known, perhaps because of technological limitations in measurement, lack of data, human error, or systematic uncertainty) : (a) for variables that appear to be influential in the sensitivity analysis, the uncertainty of the parameter value is an important factor in limiting the predictive ability of the model. Improved datasets for these variables would enhance the model's predictive precision. (b) for variables that appear to be non-influential in the SA, the extent of the uncertainty manifested in the model predictions is likely small relative to that resulting from other variables, and better precision in characterizing the variable will not improve the model's predictive ability.	• k – substance-specific photodegradation rate constants • Atmospheric [OH][9] • C-R (concentration-response data) • Class 1: unit risk • Class 2: threshold Mantel-bryan slope • Class 3: RR • Specific analysis for especially uncertain values
Assess implications of inherent variability (where a variable may truly take on a range of values within a given population or dataset; improved measurement techniques will not reduce variability): (a) for variables that appear to be influential in the SA, the inherent variability is an important determining factor in predictions. Gaining a better sense of the true extent of the variability through improved monitoring or more frequent measurements may be useful. For contexts where data might be locally gathered and available, and less variable than the more broad data used in HEIDI II, substitution of this data into HEIDI II may result in more precise predictions. For variables that can be affected by policy decisions (i.e., background levels of airborne pollutants), HEIDI II may offer a method of assessing the extent of health improvements that could potentially be achieved. (b) for variables that appear to be non-influential in the SA, the different values the variables may take on do not affect the model predictions. Attempts to adjust the factor through policy or other intervention will likely not improve health of the affected population	• Annual emissions • Background concentrations
Compare predictions from different model formulations (model uncertainty) Assesses whether different formulations of the model affect the predictions; if not, then the most parsimonious formulation is desirable.	• Different values for Mantel-Bryan slope • Approaches for characterizing background data • Calculation of photodegradation
Assess implications of scenario uncertainty	• High vs. low dose • Stack height

---

[9] [OH] may also be inherently variable since it depends in part on ambient pollution levels and local meteorology and geographic conditions

Provides information about the range of predictions that might be expected under alternate sets of conditions which may occur at any given refinery.	- Amount of time for photodegradation - Population distribution around refinery

1.4.2.2.1 Local Sensitivity Measures

Various measures of sensitivity may be calculated when performing local sensitivity analysis (which is where the values assigned to only one variable are altered to determine the effect on model predictions). The measures used to explore the sensitivity of inputs in HEIDI are described below:

SR – Sensitivity Ratio

The sensitivity ratio (SR) measures percent change in output relative to percent change in input (U.S. Environmental Protection Agency 2001):

$$SR = \frac{\frac{(y_2 - y_1)}{y_1} * 100}{\frac{(x_2 - x_1)}{x_1} * 100}$$

This measure normalizes the amount of change in output (here, in predicted incident cases) by the amount of variation in the particular input variable. For HEIDI II, this measure was useful for assessing the effect of uncertainty in variables that functionally acted on all substances in the same way but had substance-specific probability distributions (i.e., concentration-response parameters for a particular class of substances, where the same type of function was applied to calculate incidence for all class 2 substances, but the probability distribution of the toxicity data which determined where the function was anchored was different for each substance).

Percent change in output

The percent change in output alone can be assessed for two input values, x1 and x2:

$$\% \text{ change} = (y_2 - y_1)/y_1$$

The x1 and x2 values selected to test the sensitivity of the model can either be a fixed percentage of themselves (i.e., what is the effect of changing an input by 5%?), or be determined by the standard deviations of the inputs. Some inputs are inherently likely to take on a wider range of values than others, so when the standard deviation is used to determine y1 and y2, the percent change in output accounts for the impact of anticipated “realistic” variability in an input on predicted incidence. This is a simpler metric that was useful in HEIDI II for comparing the relative importance of inputs whose distributions are not substance-specific (such as [OH]), since the x1 and x2 values would remain unchanged for each substance-specific evaluation.

Absolute change in output value

The absolute change in predicted incidence provides information about whether a large or small relative change in predicted incidence that was observed in the SA might be meaningful. In some cases, large percent changes in predicted incidence were related to absolute changes on the order of 10^{-12} or smaller. Given the limitations of HEIDI II, values this small cannot be reasonably interpreted as representing real variation, and do not represent a meaningful difference in predicted incidence in a regulatory or policy context in any case.

Local SA for substances subject to uncertainty or variability

For examining inputs that are subject to uncertainty or variability, the local sensitivity measures were calculated based on the change in predicted case incidence for each substance associated with a change of 1 standard deviation (both increases and decreases) in input. For each calculation, only one variable of interest was altered at a time; the others were held constant. The variables of interest were:

- emissions
- rate constant for photodegradation (k)
- atmospheric concentration of hydroxyl radical
- background (ambient) concentration of each substance
- concentration-response (C-R) parameter for each substance.

For some substances, the SR could not be calculated. This occurred when either the input value or the predicted value was zero (resulting in a value of infinity being calculated for either the numerator or denominator of the SR), or when the input was not a single number. For example, the C-R value of BTEX was a complex combination of the C-R parameters for benzene, toluene, xylene, and ethylbenzene, and the concentration-response values for class 3 substances were complicated amalgamations of relative risk values for children, adults and seniors. To evaluate the sensitivity of these inputs, the other local measures of sensitivity plus results from the global sensitivity analyses were considered.

Extra sensitivity analyses were performed for C-R values for several individual substances including Ni, PAH, and V as a result of particularly high uncertainty surrounding their toxicity values.

Local SA for various scenarios possible within HEIDI II

Local measures of sensitivity were also applied to estimate the implications of selection various scenarios for the HEIDI II model:

Inputs that define model scenarios and have user toggles: stack height and photodegradation time

For user-selected inputs such as stack height and photodegradation time, the range of model predictions was explored across the range of allowed inputs. The interaction of stack height and photodegradation was assessed using response surfaces for total predicted case incidence at various distances from the refinery. The absolute and percent change in predicted case incidence for each alternate scenario was compared to the default scenario.

Inputs that define model scenarios without user toggles: population and background

The effect on predicted case incidence of altering the population distribution around the refinery was investigated. For the hypothetical refinery scenario, a standard population of 1 000 000 was manipulated to create the following population density/dispersion scenarios

a) homogeneous
b) heterogeneous outward – where population density increases moving from zone to zone away from the refinery (using 1x, 2x, 3x, 4x, 5x population density for each subsequent "circular slice" moving away from refinery)

c) heterogeneous inward – where population decreases with distance from the refinery (similar to the refinery being situated at the centre of an urban area),
d) all population in the north
e) all population in the south
f) all population in the east
g) all population in the west

Sensitivity analysis was used to compare two different background scenarios. The first, which was used in the deterministic version of HEIDI II, employed site-specific values for ambient concentrations of each substance modeled. Many of the values were based on incomplete data or data from monitors that were not directly adjacent to the refineries. An alternate, "low/medium/high" background scenario was proposed, where the divisions between each category were determined based on the population of each community and the imperfect location-specific background data that was used in the original HEIDI II model. The method and values used to choose the low/medium/high scenarios are detailed in Appendices C, G, and H.

Response Surfaces

Response surfaces may be created to investigate the possibility of interaction between model inputs. These are "maps" of model predictions in three dimensions: output is on the vertical axis (z-axis), and each of two inputs are varied along x and y axes. These provide good visual representations of whether two variables may interact to affect the model output, and provide focus for further (numerical) investigations, if needed.

Possible interactions with class 2 "estimated threshold"

For class 2 substances which were assumed to be threshold-acting, response surfaces were plotted to investigate the possibility of interaction between the concentration-response parameter (estimated threshold) selected for each of the class 2 substances with (i) background concentration of each of the substances (ii) mantel-bryan slope factor used to anchor the concentration-response curve.

1.4.2.2.2 Global Sensitivity Analyses

In global sensitivity analysis, the effect on model predictions of simultaneous variation of all variables is explored. Monte Carlo simulations were run where the values of all probabilistically-defined inputs were simultaneously allowed to vary according to their probability distributions. According to Cullen and Frey (Cullen and Frey 1999), a good way of identifying influential variables in a Monte Carlo Simulation is to create a scatterplot of input values vs. the associated outputs. Scatterplots of input vs. predicted case incidence were created for each substance to determine the influence of the input variables of (i) OH atmospheric concentration, (ii) k values (which determine rate constant of reaction with OH), (iii) background concentration, and (iv) toxicity values, on the output of predicted case incidence.

Spearman rank correlation coefficients were calculated for each input/substance combination. Calculating the correlation coefficients between inputs and output (using predicted case incidence as the output of interest) helps to identify significant contributors to variance in the output (Cullen and Frey 1999). The rank correlation coefficient is useful in cases where scale may be very different, as in HEIDI II where k is on the order of 10^{-12}, while ED05 values can be on the order of 10^{5}.

The number of iterations used for the simulation was initially varied to ensure that an adequate number of runs were being used to assess trends and correlation. Final analyses were run with 100,000 iterations which was sufficient to show trends where they existed without overburdening the computational time and resources required.

1.4.2.2.3 SA in general

The sensitivity analysis results were used to identify which variables are and are not influential for predicting case incidence. SA results were used throughout the model development and validation process to determine which variables most needed to be characterized in terms of uncertainty or variability (or both) for the model output to accurately reflect the current level of knowledge about the variables and processes included in the model. The information obtained from the sensitivity analyses was also used to formulate important components of the model (i.e., how best to represent background concentrations).

Finally, the sensitivity analyses (especially identification of influential variables) were also important to help interpret model results for policy applications.

1.4.3 Model Predictions (Uncertainty Analysis Results)

Frequency distributions for predicted case incidence from exposure to each emission at the hypothetical worst-case refinery were created using Monte Carlo simulations with 100 000 iterations. For class 1 and class 2 substances, the proportion of the frequency distribution curve below the *de minimis* risk level of 10^{-6} was identified, and substances for which the entire frequency distribution was below the *de minimis* risk level were documented. The distributions were truncated at the 99th percentile to improve graphical representations of the distributions, but the full distribution was used for the numerical analysis. For class 3 substances the whole distribution was above the *de minimis* risk level, so this type of analysis was not relevant. Instead, the 5th, mean, and 95th percentile values for predicted case incidence were extracted, along with the mean risk level.

The same approach was followed for each of the 20 real refineries in Canada. A list of class 1 and class 2 substances for which a proportion of the predicted case incidence frequency distribution was above the *de minimis* level was retained to enable identification of common substances of concern. The 5th percentile, mean, and 95th percentile values for predicted case incidence and the mean risk level were calculated for class 3 substances at each refinery.

1.4.4 Ranks at the Hypothetical Refinery

The distribution of ranks predicted for each substance during the simulation was determined on a within-class basis. The number of times each substance was assigned each possible rank during the simulation was determined and extracted for each class. For class 2 substances, 25 ranks were possible, but only the top ten ranks are presented, to improve clarity.

These frequency distributions indicated that there was overlap in which substances were identified as being highest priority. As a result, various methods for ranking the substances both within each class and across classes were compared. The methods used were

a) rank from the deterministic model
b) rank based on the mean value predicted in the Monte Carlo Simulation,
c) test of second-degree stochastic dominance (described in chapter 5), and
d) rank based on proportion of cumulative probability distribution exceeding 10^{-6} for substance-specific predicted case incidence.

Each of these values was determined separately using predicted case incidence, predicted simple DALYs and predicted complex DALYs (except method (d)).

The top three ranked substances were identified within each class, and also from the across-class rankings. This enabled determination of whether the priorities were consistent across ranking methods. This (i) allowed assessment of the utility of different ranking methodologies and (ii) provided evidence about whether the model was capable of identifying high priority substances.

Correlation coefficients comparing the ranks predicted for each substance using each of the within-class ranking approaches were calculated to check how similar the results were across ranking methods.

1.4.5 Further Analysis

1.4.5.1 Impact Equivalents

As an alternate way to compare and communicate the relative impact of the different substances within each class, impact equivalents were calculated for class 1 and class 2 substances. Predicted case incidence, simple DALY, and complex DALYs were calculated in terms of benzene equivalents for class 1 substances and mercury equivalents for class 2 substances.

1.4.5.2 Exposure from multiple refineries

Because there are four refineries in close proximity in Sarnia, predictions from individual refineries in the area may not be relevant for the population. An ad hoc analysis was conducted to determine whether HEIDI II could be useful in this situation where the population is exposed to emissions from more than one refinery. To check that the populations within the 25 km zone captured by HEIDI II's analysis for each individual refinery were roughly the same set of people, the number of adults, children, senior, and total population surrounding each refinery was compared across refineries.

Analysis indicated that roughly the same population is captured when looking within 25 km of each refinery (i.e., the refineries are close enough together that the same people are living within 25 km of any of the four facilities). When the populations were compared by quadrant, the variation was much higher (up to 2), indicating that the location of highest population density relative to the location of each refinery was not consistent.

A theoretical refinery was imagined to be located at the geographic location which minimized the distance from each actual refinery, and the theoretical emissions were represented by the sum of all the emissions emitted from each of the four refineries. The "average" population distribution was calculated by averaging the actual population of children, adults, and seniors living in each quadrant around the real refineries.

The predicted case incidence at this theoretical Sarnia refinery was compared to that predicted at individual refineries in the Sarnia area and to the predictions for a hypothetical worst-case refinery, to assess whether the priorities identified in each case were similar and to investigate any obvious differences between the results for predicted case incidence.

1.4.5.3 Comparison of HEIDI II to another model

An effort was made to compare results from HEIDI II to those predicted by another available model. TRACI is a stand-alone, Windows-based tool that was developed by the U.S. EPA. It uses a run-time version of Microsoft Access to characterize the potential impacts of a variety of environmental stressors, including human health cancer effects, human health noncancer effects, and human health criteria-related effects (Bare, Norris et al. 2003). TRACI is one of few available impact analysis tools that explicitly distinguishes human health cancer and noncancer effects and also allows for assessment of airborne emissions only, as HEIDI II does. Currently, TRACI is offline for updating, but the characterization factors used in TRACI were available and enabled a comparison between the results predicted by the two models.

TRACI

The characterization factors developed for TRACI were obtained from Jane Bare, one of the model's authors (Bare 2004). TRACI includes a wide range of impacts, including the following relevant human health (HH) impact categories: HH Cancer Air (kg benzene eq /kg), HH Noncancer Air (kg toluene eq /kg), and HH Criteria Air-Point Source (kg PM2.5 eq / kg).

The characterization factors for the relevant impact/substance combinations were extracted from TRACI, applied to the hypothetical worst-case emissions scenario, and then ranked within impact categories and across impact categories. The priority order was compared to the rankings produced by the deterministic version of HEIDI II, since TRACI is itself deterministic and the rankings produced by HEIDI II as a probabilistic model were often similar to those produced by the deterministic version.

1.4.5.4 Application of HEIDI II to another industry

In order to test the generalizability of HEIDI II, an attempt was made to apply the model to emissions from another industry. The Nanticoke power generation facility was selected since it was in a similar geographic area as that assumed by the meteorology of HEIDI II, and adjacent to a refinery that was included in HEIDI II, which allowed re-use of population data. Coal-fired power generation was selected because as in the case of petroleum refineries, the predominant route of exposure for most emissions is by inhalation.

Emissions data was obtained from the NPRI database, and for the substances not already included in HEIDI II, data on background, photodegradation potential, concentration-response, and health impact was gathered from similar sources as those used when data was initially compiled for HEIDI II. HEIDI II was first reprogrammed for the Nanticoke power generation facility as a deterministic model in Excel, and then as a probabilistic model in Matlab.

The difficulties in adapting the model were recorded, and the results of HEIDI II's predictions for the facility presented.

2 Part 2: Results

2.1 Model Validation and Analysis

Computational validation techniques involve mathematical and dimensional "double-checking", model formulation techniques are best done through adept use of techniques such as sensitivity analysis and model design questions are often best addressed through thought and discussion. General comments, results, and issues which arose during the validation process are addressed in Table 5. The bulk of testing and validation of the HEIDI II model was performed using techniques of sensitivity analysis (SA), and is addressed in the remainder of the chapter. Issues that require thoughtful consideration rather than mathematical analysis are addressed in either the discussion section of this chapter or this document's final discussion.

2.1.1 Basic Validation

Following on from Table 3, which was presented in the Methods chapter, the results and comments which resulted from some of these efforts are presented below and are addressed in the comments in Table 5.

2.1.2 Sensitivity Analysis

In HEIDI II, SA was used to help provide recommendations about the most parsimonious and information-rich model form, identify scenarios potentially associated with greatest predicted health impacts, and provide an initial sense of the range of predicted health impacts from refinery airborne emissions.

In order to conduct a complete SA, an inventory of the model variables and associated uncertainty and variability was compiled. Distributions for the model variables were proposed and justified where possible, and possible correlations identified. This inventory served as the basis for designing both local and global sensitivity analyses (See Appendix C). Distributions could not be assigned to some input variables due to lack of information; for example, all of the dispersion modeling was performed externally to

Table 5: Results and comments arising from basic validation efforts

Validity Criterion	Comments
Computation	
Internal Consistency	Consistency in predictions was found when variables were calculated via alternate possible methods and compared. There was very little need to redesign with (n-1) degrees of freedom as most of the functions were linear.
Absence of numerical (computational) artifacts	Inspection of results ensured realistic predictions, predictions from two software programs (excel and matlab) match. In excel the number precision is 15 digits; all values predicted fell in between the largest and smallest allowable values which are on the order of 10^{308} and 10^{-308} for both excel and matlab. (The Mathworks 2002; Microsoft Office online Excel 2003)
Computational Correctness	- Dimensional analysis predicted appropriate units for the excel version - Perfect agreement of Excel and Matlab predictions was achieved for the deterministic models
Model Formulation	
Model form is correct	See discussion and Appendix C regarding simplifying model assumptions
Robustness to changing input parameters	- Functional relationships were tested using values ranging from 0.0001*central value – 1000*central value for each variable to confirm functional relationships. - Probabilistic model did not break down under conditions of varying inputs.
Sensitivity to changing input parameters	- Local sensitivity analysis were carried out for all variables except meteorological variables - All SA was done using hypothetical refinery central values. Low dose SA used (hypothetical refinery emissions)/100
Parsimony	- Sensitivity ratios were calculated, local and global sensitivity analyses were carried out - Some aspects of the model were identified for potential removal to improve parsimony (see discussion and recommendations)
Model Design	
Generalizability	- An attempt was made to adapt HEIDI II to a coal-fired power plant (Nanticoke). Which addresses (i) and (ii) - See also discussion
Biological realism and relevance	See discussion
Agreement between different models characterizing the same process	- Predictions were compared to priorities using TRACI characterization factors - Comparisons to the prototype were invalid since the theoretical population and emissions scenarios are not comparable
Heuristic value	See discussion – especially with respect to cost-benefit of reductions in priority substances
Capacity to deal with dose-dependent biological responses	See discussion
Useful in extrapolation to other conditions	- A theoretical “Sarnia refinery” was tested to see how well HEIDI II could predict impacts from multiple refineries in one geographic area/affecting one population - Low dose sensitivity analysis indicated that predicted incidence tends to zero for most class 2 substances at lower doses

HEIDI II and was operationalized in the model through a series of "adjustment factors" such as the generic multipliers applied to annual emissions of each substance to predict concentration in each of 20 locations surrounding any given refinery. These restrictions are also documented in Appendix C.

Sensitivity analyses in HEIDI II were phased. Initially, local sensitivity analysis (where one input is varied and all others are held constant) was performed for each input variable and substance. As described in the methods section, within-module local SAs were performed first, followed by variable and substance-specific local sensitivity analysis for the model as a whole. Scenarios and functional relationships were also tested by module and model using local SA. The module-by-module local SA results served mainly as validity checks and will not be presented here. Global sensitivity analysis (where all inputs are allowed to vary simultaneously) was used to confirm conclusions made based on local SAs and to investigate the anticipated range of outputs from HEIDI II.

2.1.3 Local Sensitivity Analysis Results

Sensitivity was calculated based on change in predicted case incidence for the hypothetical worst-case refinery scenario. For many substances, predicted case incidence was zero across all tested input values. For others, while predicted case incidence was zero at the base case, adjusting inputs resulted in a positive predicted case incidence for some input values tested. The direction and magnitude of change in predicted output depended on whether the input variables were increased or decreased from their central values.

2.1.3.1 Uncertain Inputs

2.1.3.1.1 k and OH

k (atmospheric OH rate constant) and OH (atmospheric concentration) are mathematically related to predicted output in exactly the same way: they are multiplied by each other to generate the first-order rate constant used in the function used to describe photodegradation. However, while the distributions defined for k were substance-dependent, the value used to describe the distribution for OH was not. As shown in Table 6, the importance of the uncertainty in k and OH was greater for class 1 than class 2 substances (class 3 substances were assumed not to photodegrade). Any reduction in delivered concentration would directly affect predicted incidence for class 1 substances (since a linear, non-threshold dose-response was applied for class 1 substances), while for class 2 substances variation in k would only affect predicted incidence to the extent that the delivered concentration breached the substance-specific C-R threshold. In general, the impact of uncertainty in k appears to outweigh the importance of the uncertainty in OH on predicted incidence in absolute terms. Uncertainty in either k or OH alone does not alter the absolute predicted incident cases by one in a million. The impact of uncertainty in OH on predicted incidence is greatest for substances which photodegrade fastest.

The greatest impact on predicted incidence appears to result from uncertainty in the k value for PAH: varying k across the range defined by ±1 stdev results in ~50% change in incident cases from one extreme to the other.

Table 6: Sensitivity of predicted incidence to k and OH using several sensitivity measures. Local sensitivity analyses were conducted using +/- 1 stdev from the variables' central values. * represents substances for which predicted incidence was zero at baseline, or both before and after the SA, preventing calculation of some sensitivity measures. 'N/A' indicates that the measure was not relevant, i.e., metals do not photodegrade, therefore k and OH do not affect the model predictions for these substances.

Substance	**k**						**OH**					
	Sensitivity Ratio		**% change output**		**Absolute change**		**Sensitivity Ratio**		**% change output**		**Absolute change**	
Increase or decrease in stdev	+	-	+	-	+	-	+	-	+	-	+	-
Class 1												
1,3-Butadiene	-0.03	-0.50	-6.8	34	4.2E-03	-2.1E-02	-0.14	-0.24	-3.0	5.5	1.9E-03	-3.4E-03
Benzene	-0.02	-0.02	-5.0	1.6	9.7E-03	-3.1E-03	-0.02	-0.02	-0.5	0.5	9.5E-04	-9.6E-04
Ethylene (as oxide)	-0.08	-0.13	-22	10	1.7E-02	-7.4E-03	-0.11	-0.12	-2.6	2.7	1.9E-03	-2.0E-03
Nickel (and its compounds)	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
PAH (as benzo(a)pyrene)	-0.05	-0.53	-12	38	1.7E-01	-5.2E-01	-0.20	-0.31	-4.4	6.9	6.0E-02	-9.3E-02
Formaldehyde	-0.10	-0.17	-23	15	1.5E-02	-9.4E-03	-0.14	-0.15	-3.1	3.4	1.9E-03	-2.1E-03
Acetaldehyde	-0.12	-0.26	-25	17	1.6E-03	-1.1E-03	-0.20	-0.22	-4.4	5.0	2.8E-04	-3.1E-04
Class 2												
1,2,4-Trimethylbenzene	*	*	*	*	*	*	*	*	*	*	*	*
Ammonia (Total)	0.00	0.00	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00
BTEX[10]			-9.8	4.4	3.0E-08	-1.3E-08	0.0	0.0	-1.3	1.4	3.8E-09	-4.1E-09
B	-0.04	-0.06										
T	-0.05	-0.06										
E	-0.05	-0.07										

---

[10] Because the input variables for BTEX are a combination of the values of B,T,E,X, the sensitivity ratio can be calculated to assess percent change in predicted incidence relative to percent change in emissions of each component of the mixture.

X	-0.05	-0.07										
Cyclohexane	*	*	*	*	*	*	*	*	*	*	*	*
Dicyclopentadiene	*	*	*	*	*	*	*	*	*	*	*	*
Diethanolamine (and its salts)	*	*	*	*	*	*	*	*	*	*	*	*
Hydrogen sulphide	-0.24	-0.44	-54	31	1.7E-09	-9.8E-10	-0.36	-0.39	-8.2	8.8	2.5E-10	-2.8E-10
Isoprene	*	*	*	*	*	*	*	*	*	*	*	*
Mercury (and its compounds)	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Methanol	*	*	*	*	*	*	*	*	*	*	*	*
Methyl ethyl ketone	*	*	*	*	*	*	*	*	*	*	*	*
Methyl isobutyl ketone	*	*	*	*	*	*	*	*	*	*	*	*
Methyl tert-butyl ether	*	*	*	*	*	*	*	*	*	*	*	*
Naphthalene	-0.01	-2.09	-1.7	140	5.1E-14	-4.0E-12	0.0	0.0	0.0	0.0	0.0	0.0
n-Hexane	-0.27	-1.54	-58	110	4.0E-12	-7.3E-12	0.0	-0.01	0.0	0.26	0.0	-1.8E-14
Phenol	-0.09	-0.10	-18	7.0	1.5E-09	-5. 9E-10	-0.14	-0.03	-3.2	0.65	2.7E-10	-5.5E-11
Propylene	*	*	*	*	*	*	*	*	*	*	*	*
Styrene	*	*	*	*	*	*	*	*	*	*	*	*
Sulphuric acid	-0.02	-0.02	-4.5	1.4	4.3E-05	-1.3E-05	-0.02	-0.02	-0.43	0.43	4.1E-06	-4.2E-06
Vanadium and its compounds	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Zinc (and its compounds)	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A

2.1.3.1.2 Toxicity data

Table 7 shows that adjusting the C-R (concentration-response parameter) by 1 standard deviation has a dramatic impact on predicted incidence, especially for class 2 substances where percent changes of up to 10^{15} were observed and absolute numbers of predicted cases increased by as much as 4600 (in the case of PAH). The values observed for class 1 and class 3 substances for SR reflect the linear no-threshold functions used to characterize dose-response. For class 2 substances, the large increases in predicted incidence that occur for a reduction in threshold suggest that overestimation of threshold values could be an important source of error. A change of 1 standard deviation in relative risk (RR) estimates for class 3 substances appears to result in important changes in predictions for mortality and morbidity, particularly for sulfur dioxide, which is associated with the largest emissions of the three CACs. Considering that the effects attributable to each of the three CACs would be additive under a linear no-threshold assumption, this is cause for concern.

Table 7: The sensitivity of predicted incidence to uncertainty in the C-R values used (unit risk for class 1 substances, TC05/NOAEL/LOAEL for class 2 substances, and RR for class 3 substances). * indicates values for which zero incidence was predicted

Substance	C-R value					
	Sensitivity Ratio		% change output		Absolute change	
Increase or decrease in stdev	+	-	+	-	+	-
1,3-Butadiene	1.0	1.0	3.4E5	-100	-210	0.06
Benzene	1.0	1.0	3.4E5	-100	-640	0.19
Ethylene (as oxide)	1.0	1.0	3.4E5	-100	-250	0.08
Nickel (and its compounds)	1.0	1.0	3.4E5	-100	-1.7E05	52
PAH (as benzo(a)pyrene)	1.0	1.0	3.4E5	-100	-7.5E04	22
Formaldehyde	1.0	1.0	3.4E5	-100	210	0.06
Acetaldehyde	1.0	1.0	3.4E5	-100	210	0.01
1,2,4-Trimethylbenzene	*	*	*	*	0.0	-4.3E02
Ammonia (Total)	-1.0E-01	-4.7E+07	-1.0	4.5E07	1.8E-14	-8.0E-07
BTEX[11]			-1.0	1.2E10	3.0E-07	-3.5E03
B	-4.2E-3	-1.2E10				
T	-1.0E-1	-9.2E8				
E	-4.2E-3	-1.2E10				
X	-4.2E-3	-1.0E7				
Cyclohexane	*	*	*	*	0.0	-2.5E-01

---

[11] Because the input variables for BTEX are a combination of the values of B,T,E,X, the sensitivity ratio can be calculated to assess percent change in predicted incidence relative to percent change in ED05 for each component of the mixture

Dicyclopentadiene	*	*	*	*	0.0	-3.0E01
Diethanolamine (and its salts)	*	*	*	*	0.0	-3.8E+00
Hydrogen sulphide	-4.2E-03	-7.4E12	-1.0	7.4E12	3.1E-09	-2.3E04
Isoprene	*	*	*	*	0.0	-1.3E-04
Mercury (and its compounds)	-4.2E-03	-1.8E11	-1.0	1.8E11	4.1E-09	-7.3E02
Methanol	*	*	*	*	0.0	-3.0
Methyl ethyl ketone	*	*	*	*	0.0	-5.4E-01
Methyl isobutyl ketone	*	*	*	*	0.0	-4.3E-02
Methyl tert-butyl ether	*	*	*	*	0.0	-6.3E-02
Naphthalene	-4.2E-03	-7.5E13	-1.0	7.5E13	2.9E-12	-2.2E02
n-Hexane	-4.2E-03	-5.7E13	-1.0	5.7E13	6.9E-12	-3.9E02
Phenol	-4.2E-03	-8.4E10	-1.0	8.4E10	8.5E-09	-7.1E02
Propylene	*	*	*	*	0.0	-5.5E01
Styrene	*	*	*	*	0.0	-1.2E01
Sulphuric acid	-4.2E-03	-9.0E08	-1.0	1.3E09	9.6E-04	-8.6E05
Vanadium and its compounds	-3.7E-03	-1.0E07	-1.0	1.0E07	1.0E-01	-1.1E06
Zinc (and its compounds)	-1.0E-01	-6.0E06	-1.0	5.8E06	4.4E-09	-2.5E-02
SOx chronic mortality	*	*	28	-28	91	-91
SOx chronic bronchitis	*	*	36	-36	200	-200
SOx asthma hosp	*	*	43	-43	3	-13
SOx asthma ER	*	*	43	-43	22	-22
NOx chronic mortality	*	*	28	-28	9.00	-9.0
NOx chronic bronchitis	*	*	36	-36	19	-19
NOx asthma hosp	*	*	43	-43	1.20	-1.2
NOx asthma ER	*	*	43	-43	2.10	-2.1
primary chronic mortality	*	*	28	-28	7.90	-7.9
primary chronic bronchitis	*	*	36	-36	17	-17
primary asthma hosp	*	*	43	-43	1.10	-1.1
primary asthma ER	*	*	43	-43	1.90	-1.9

Together with Table 6, these results suggest that to improve predictions of the health impacts resulting from exposure to these refinery emissions, it would be most effective to plan research that would reduce uncertainty in the toxicity values used rather than the uncertainty in estimates for k and OH.

2.1.3.2 Variable inputs

2.1.3.2.1 Annual Emissions

Fluctuations in annual emissions that were observed between 2001-2003 were sufficient to alter the predicted incidence by 100 % for some substances including PAH, ammonia, naphthalene, sulphuric acid, and zinc. As Table 8 shows, the results suggest that the potential change in predicted incidence might exceed the *de minimis* risk level for nickel, PAH, formaldehyde, and most of the class 3 substances, but would be extremely small in absolute terms for class 2 substances.

These results suggest that accurate and up-to-date knowledge about the emissions at a particular refinery is required for HEIDI II to provide useful predictions, and that actions taken to reduce many emissions from petroleum refineries, particularly of class 1 and class 3 substances, would result in large relative decreases in predicted health impact.

Table 8: Sensitivity of predicted incidence to fluctuations in annual emissions. Substances for which predicted incidence was zero in all cases are omitted.

Substance	**Annual emissions value**					
	Sensitivity Ratio		**% change output**		**Absolute change**	
Increase or decrease in stdev	+	-	+	-	+	-
1,3-Butadiene	1.00	-1.00	28	-28	-0.02	0.02
Benzene	1.00	-1.00	61	-61	-0.12	0.12
Ethylene (as oxide)	1.00	-1.00	55	-55	-0.04	0.04
Nickel (and its compounds)	1.00	-1.00	6.6	-6.6	-3.42	3.42
PAH (as benzo(a)pyrene)	1.00	negative emissions	173	-31	-38	1.00
Ammonia (Total)	65	negative emissions	7800	negative emissions	-1.4E-12	1.8E-14
BTEX[12]			51	-51	-1.6E-07	1.5E-07
B	0.84	0.83				
T	1.8	1.7				
E	1.9	1.9				
X	0.08	1.5				
Hydrogen sulphide	5.3	4.0	40	-31	-1.3E-09	9.6E-10
Mercury (and its compounds)	1.7	0.27	7.0	-1.1	-2.9E-10	4.5E-11
Naphthalene	3.6	2.0	180	-98	-5.2E-12	2.8E-12
n-Hexane	0.78	2.8	16	-58	-1.1E-12	4.0E-12
Phenol	0.89	1.2	7.7	-11	-6.5E-10	8.9E-10
Sulphuric acid	5.9	2.0	260	-88	-2.5E-03	8.5E-04
Vanadium and its compounds	3.2	2.8	22	-19	-2.3E-02	2.0E-02
Zinc (and its compounds)	2.5	1.1	200	-85	-8.9E-09	3.7E-09
SOx chronic mortality	1.00	-1.00	9.2	-9.2	30	-30
SOx chronic bronchitis	1.00	-1.00	9.2	-9.2	50	-50
SOx asthma hosp	1.00	-1.00	9.2	-9.2	2.80	-2.80

---

[12] Because the input variables for BTEX are a combination of the values of B,T,E,X, the percent change in predicted incidence from the mixture relative to changes in each of the individual substance-specific inputs was calculated.

SOx asthma ER	1.00	-1.00	9.2	-9.2	4.70	-4.70
NOx chronic mortality	1.00	-1.00	2.4	-2.4	0.77	-0.77
NOx chronic bronchitis	1.00	-1.00	2.4	-2.4	1.30	-1.30
NOx asthma hosp	1.00	-1.00	2.4	-2.4	0.07	-0.07
NOx asthma ER	1.00	-1.00	2.4	-2.4	0.120	-0.120
primary chronic mortality	1.00	-1.00	40.9	-40.9	12	-12
primary chronic bronchitis	1.00	-1.00	40.9	-40.9	19	-19
primary asthma hosp	1.00	-1.00	40.9	-40.9	1.10	-1.10
primary asthma ER	1.00	-1.00	40.9	-40.9	1.80	-1.80

Ambient levels of each of the substances included in HEIDI II fluctuate over time and from location to location. Table 9 suggests that the largest relative changes in predicted incidence observed throughout the local SAs were precipitated by adjusting the background concentration for some substances. The associated absolute change in predicted incidence is expected to be very small however. Potential increases in background concentrations are much more important for predicting large relative increases in incidence than equivalent decreases are for predicting relative decreases in incidence – although this may often be an artifact since background concentrations cannot extend below zero.

Table 9: Sensitivity of predicted incidence to fluctuations in ambient concentrations. Substances for which predicted incidence was zero in all cases are omitted. '--' indicates results could not be calculated

Substance	Background concentration					
	SR		% change output		Absolute change	
Increase or decrease in stdev	+	-	+	-	+	-
1,2,4-Trimethylbenzene	--	--	--	--	-6.2E-10	0.0
Ammonia (Total)	background = 0		0.0	0.0	0.0	0.0
BTEX[13] B T E X	35 26 31 31	1.3 1.2 1.3 1.2	9800	-100	-3.0E-05	3.0E-07
Hydrogen sulphide	0.02	0.02	4.0	-1.5	-1.2E-10	4.7E-11
Mercury (and its compounds)	26.68	1.44	5800	-100	-2.4E-07	4.1E-09
Naphthalene	500.64	1.45	1100	-100	-3.1E-09	2.9E-12
n-Hexane	557.73	1.18	2300	-100	-1.6E-08	6.9E-12

---

[13] Because the input variables for BTEX are a combination of the values of B,T,E,X, the percent change in predicted incidence from the mixture relative to changes in each of the individual substance-specific inputs was calculated.

Phenol	17.54	1.57	3000	-100	-2.6E-07	8.4E-09
Propylene	--	--	--	--	-1.6E-12	0.0E+00
Sulphuric acid	background = 0		0.0	0.0	-3.7E-04	0.0E+00
Vanadium and its compounds	0.42	0.22	-15	-1.6	1.6E-02	-1.60E-02
Zinc (and its compounds)	37.77	1.22	-97	-4.3E-05	4.2E-09	-4.20E-09

The SR could not be calculated for many substances throughout the local SAs – often because the predicted case incidence values were zero in the base case. In order to gain a sense of the extent of increase in predicted case incidence that could occur with variations in each of the input variables, the absolute change in predicted case incidence must be considered.

2.1.3.3 Class-by-class

Since substance class determines the function used for dose-response in HEIDI II, it is helpful to compare the importance of each input variables to predicted incidence within classes. Figure 6 and Figure 7 confirm that variability in emissions and uncertainty in the unit risk values are the greatest contributors to variation in predicted incidence for class 1 substances, based on individual inputs that would be classified as variable or uncertain.

2.1.3.3.1 Class 1

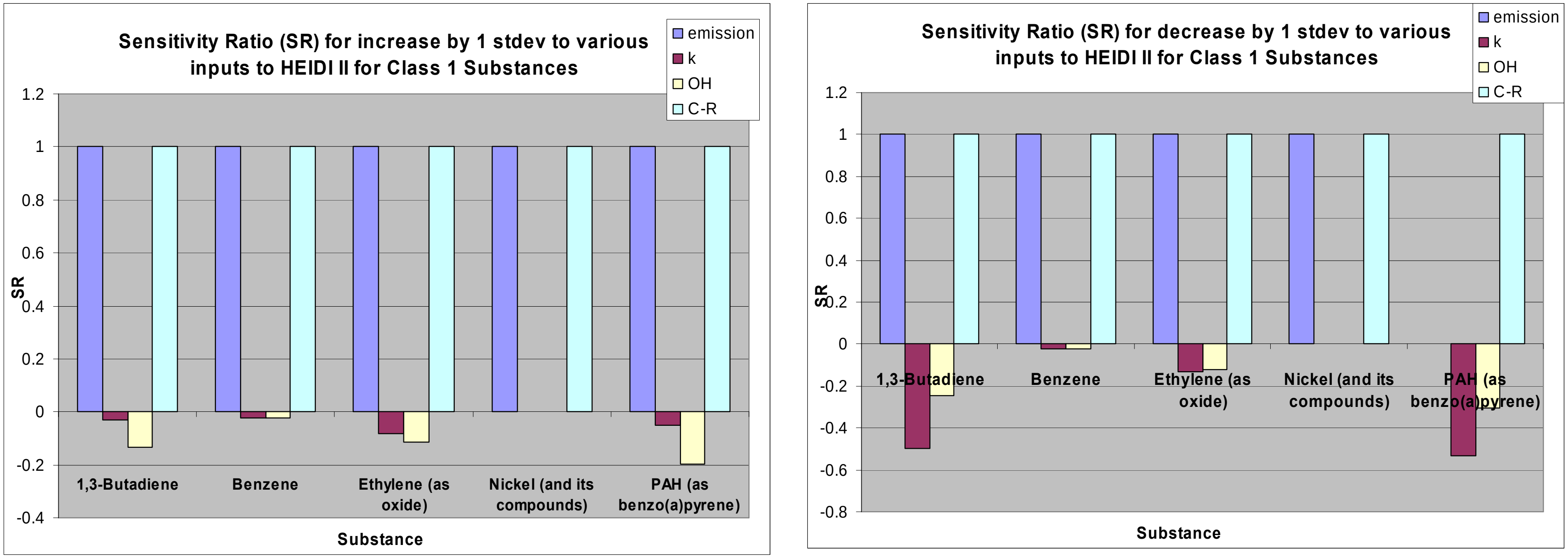


Figure 6: Sensitivity ratios confirm that linear relationships exist between the emissions level and predicted incidence, and between unit risk and predicted incidence. SR evaluates percent change in output relative to percent change in input: for these two variables the percent change is directly related through the slope value so SR = 1. The negative SR values for OH and k indicate an inverse relationship between each of the variables and predicted incidence. (A decrease in photodegradation rate through either smaller k or less ambient OH would result in some increase in predicted case incidence from exposure to 1,3-butadiene, Ethylene oxide, PAH, acetaldehyde, and formaldehyde.) The figures above suggest that decreases in k or OH relative to central value have more of an effect on predicted incidence than increases. Lower value of either k or OH is associated with higher exposure and therefore higher predicted incidence. Therefore, overestimation of either k or OH might be more important in underpredicting incidence (compared to an underestimation of k or OH which would have a smaller effect on overpredicting incidence). Background was excluded from the figures since it is assumed not to affect predicted excess incidence for class 1.

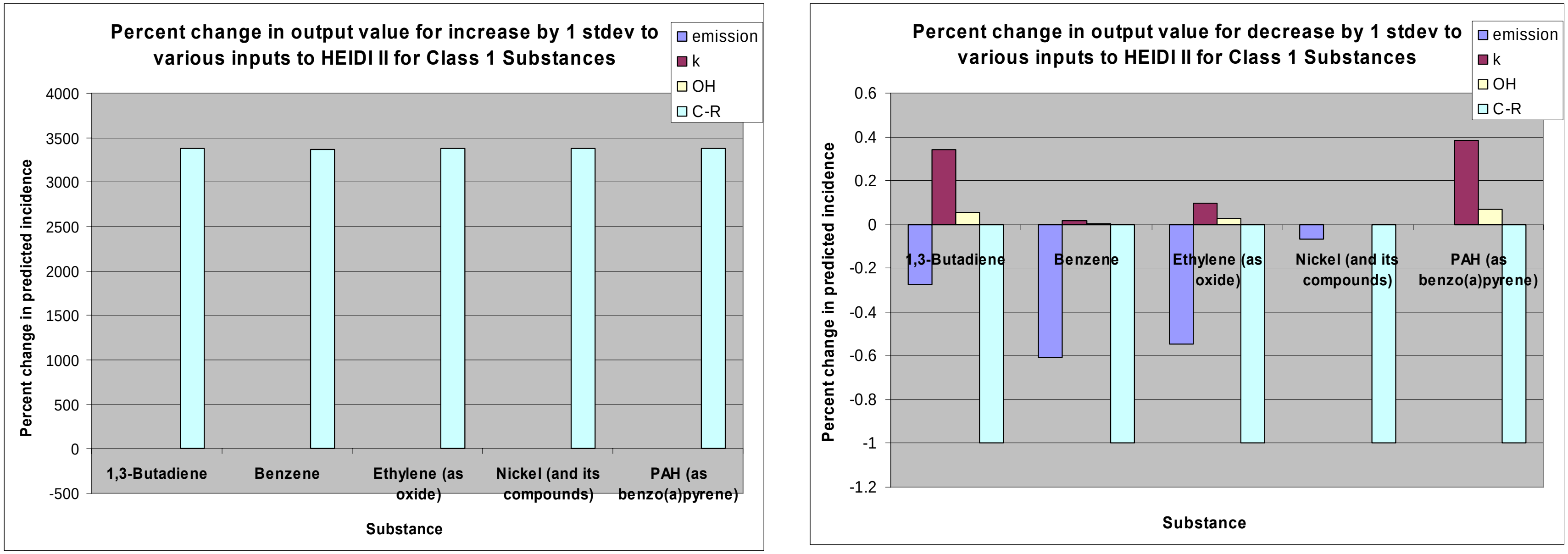


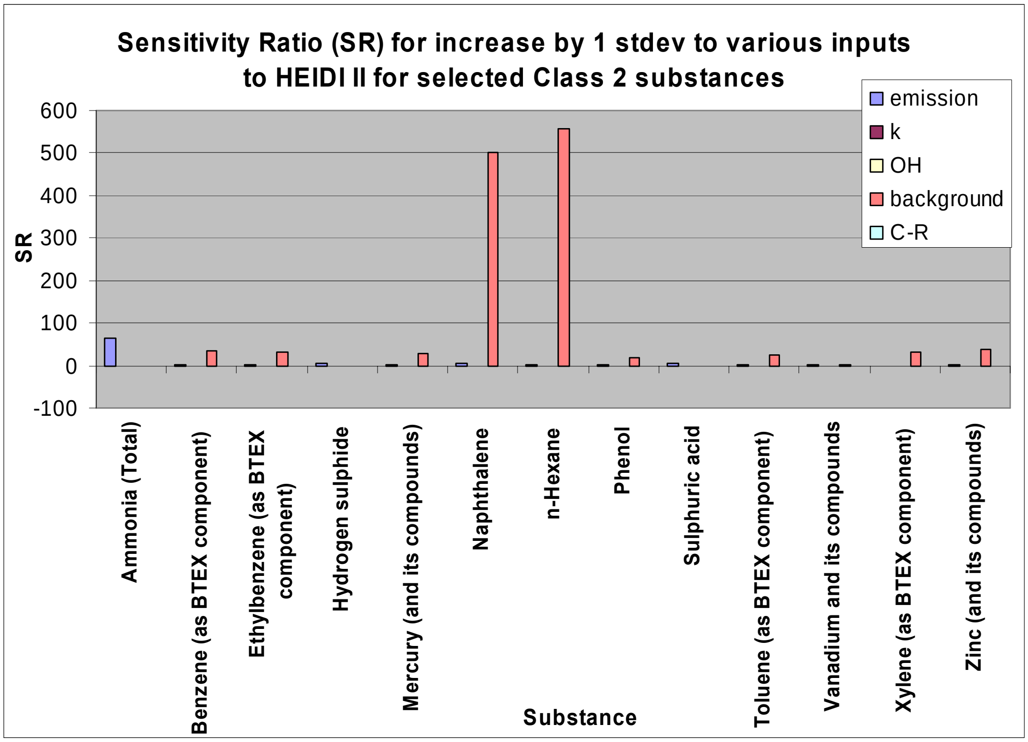
Figure 7: Percent change in predicted case incidence with a one standard deviation change in input. The effect of increasing the unit risk value overwhelms the effect of increasing any other input variable for class 1 substances. For decreases from the central estimate, the maximum possible percent change is 100% since negative values for predicted incidence cannot occur. The relative differences in the effect of emissions of predicted incidence stem from the baseline level of predicted incidence (i.e., nickel and PAH were associated with larger initial predicted incidence, so the increase that occurred by altering the emissions input was smaller relative to the increase which was observed for substances whose baseline predicted incidence was very low. In general, C-R seems to be the most influential variable, followed by emissions, k, and [OH]. In absolute terms, the largest changes in predicted incidence are observed for nickel – as a result of the relatively large unit risk value associated with its toxicity. Altering the value by 1 stdev imposes a drastic change in toxicity on the substance.

2.1.3.3.2 Class 2

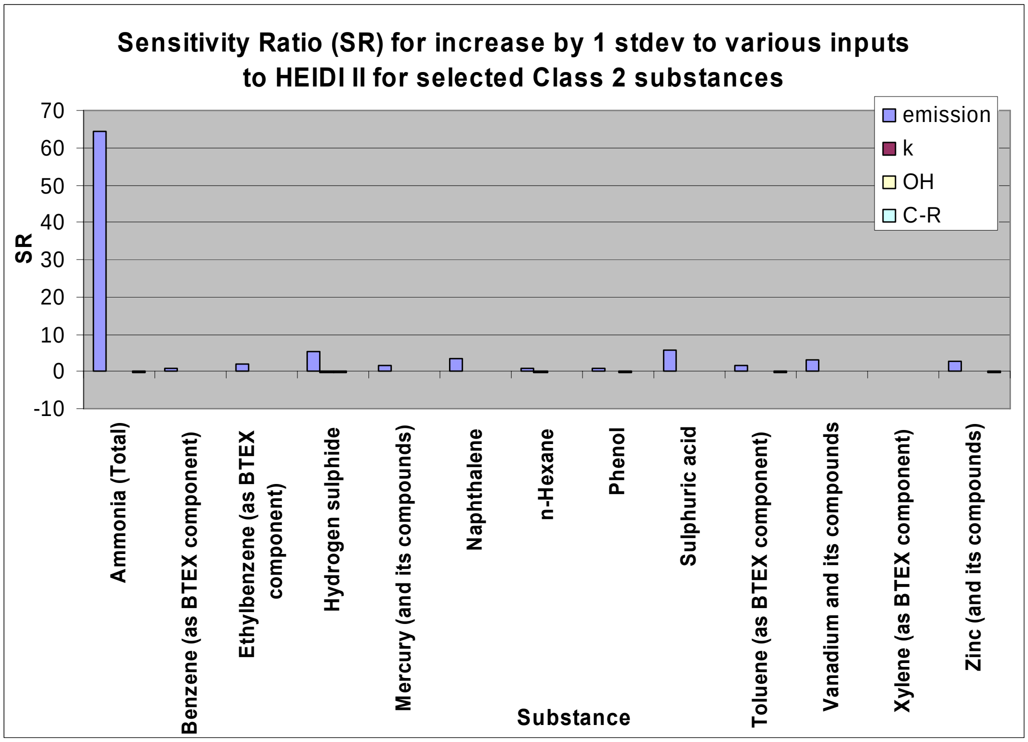
Because of extremely large differences in absolute predicted incidence and even percent change in predicted incidence for class 2 substances, the SR appears to be the best indicator for comparing the effects of varying the different inputs that affect predicted incidence for these systemic toxins. Figure 8 (A) suggests that variation in background levels of some substances (in particular, naphthalene and n-hexane) may have a large relative impact on predicted incidence. Once background is removed from the figure, it is possible to see that emissions also play a large role in influencing predicted incidence, as shown in Figure 8 (B). Figure 8 (C) shows the relative effects of increasing the remaining inputs: OH, k, and C-R (which is an ED05 for these class 2 substances). An increase in the ED05 does not have a large effect on predicted incidence for any substance, suggesting that underestimation of ED05 is not usually an important source of error.

The patterns of importance by input variable are different when a decrease from the central value occurs: C-R becomes an important predictor of incidence, where a small decrease in ED05 can result in a large increase in predicted incidence (the inverse relationship results in negative values of SR) See Figure 9.

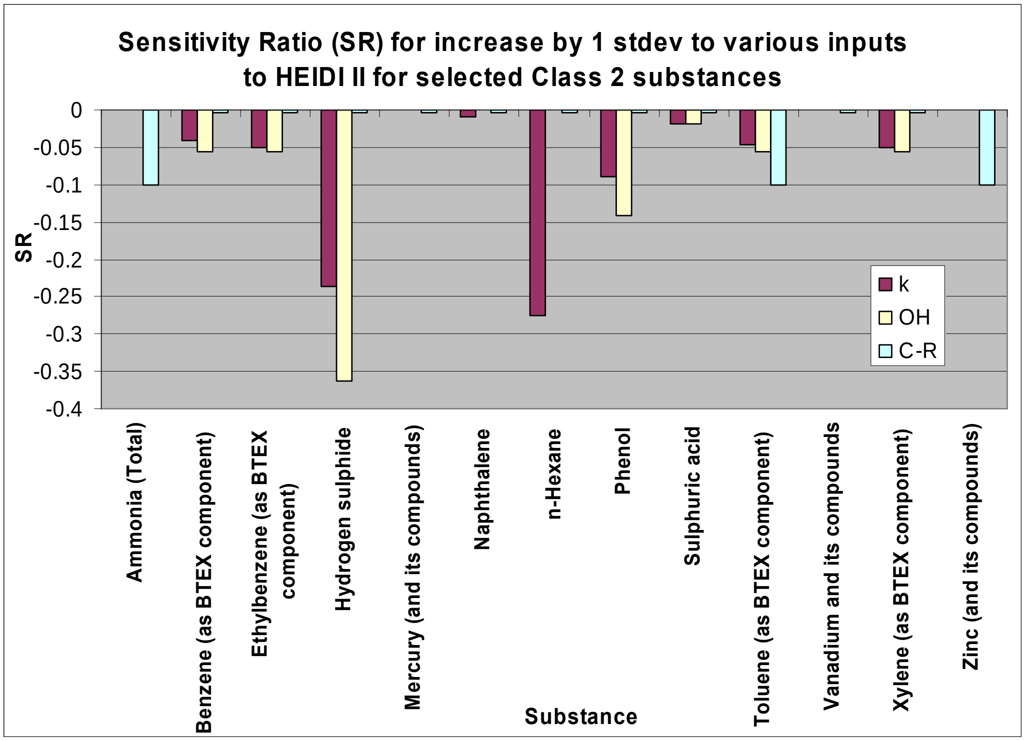
For all variations in input, predicted incidence as a result of exposure to naphthalene and n-hexane seems to be most influenced by changes in inputs, especially background, emission, and C-R. This may be because the baseline predicted incidence is very low (on the order of 10^{-12}) such that any change appears to be large when compared to changes in predicted incidence for other substances.



8(A) Background becomes an important predictor of incidence for several substances when its input value is increased from the base case by 1 stdev.

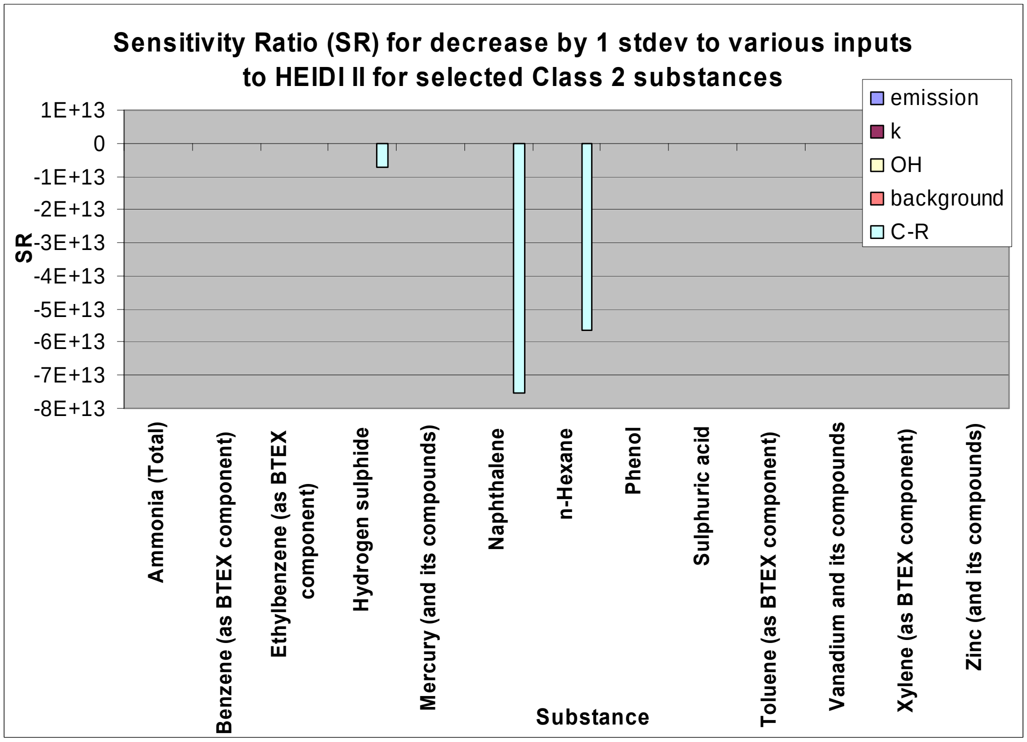


8(B) After background, emissions is the most important predictor of case incidence for class 2 substances

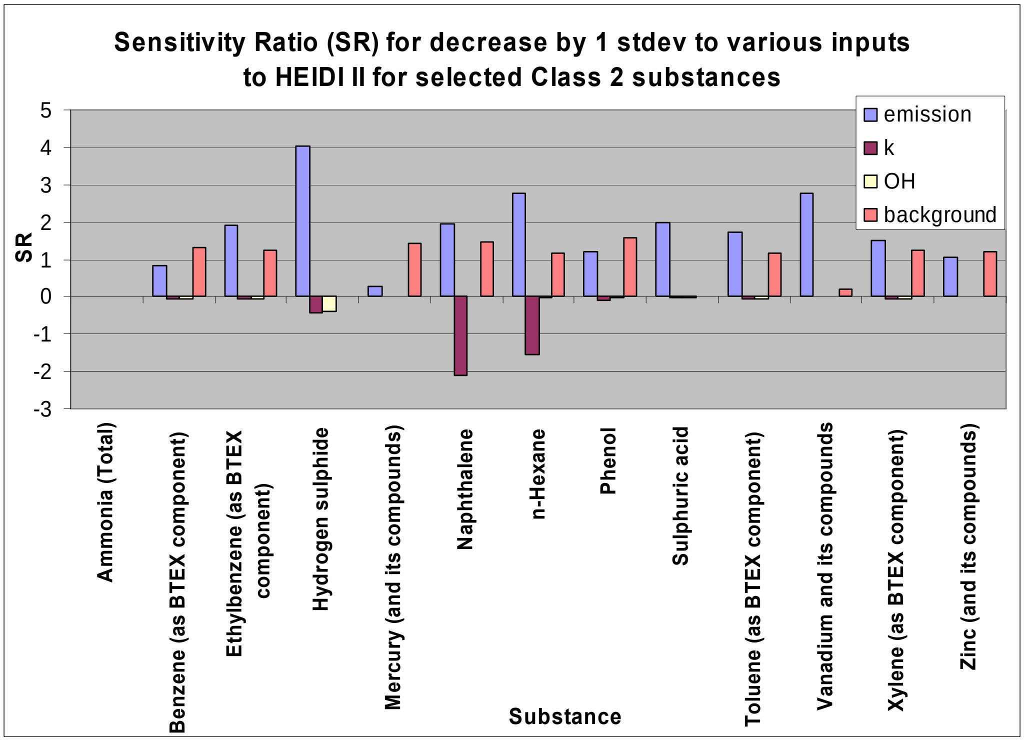


8(C) With background and emissions removed from the figure, k and OH seem to have the most influence on incidence when their values are increased from baseline

Figure 8: Sensitivity ratio for case incidence with one standard deviation increase in input values for selected class 2 substances.



9 (A) Concentration response (ED05) has the greatest influence on predicted incidence when values are decreased from baseline

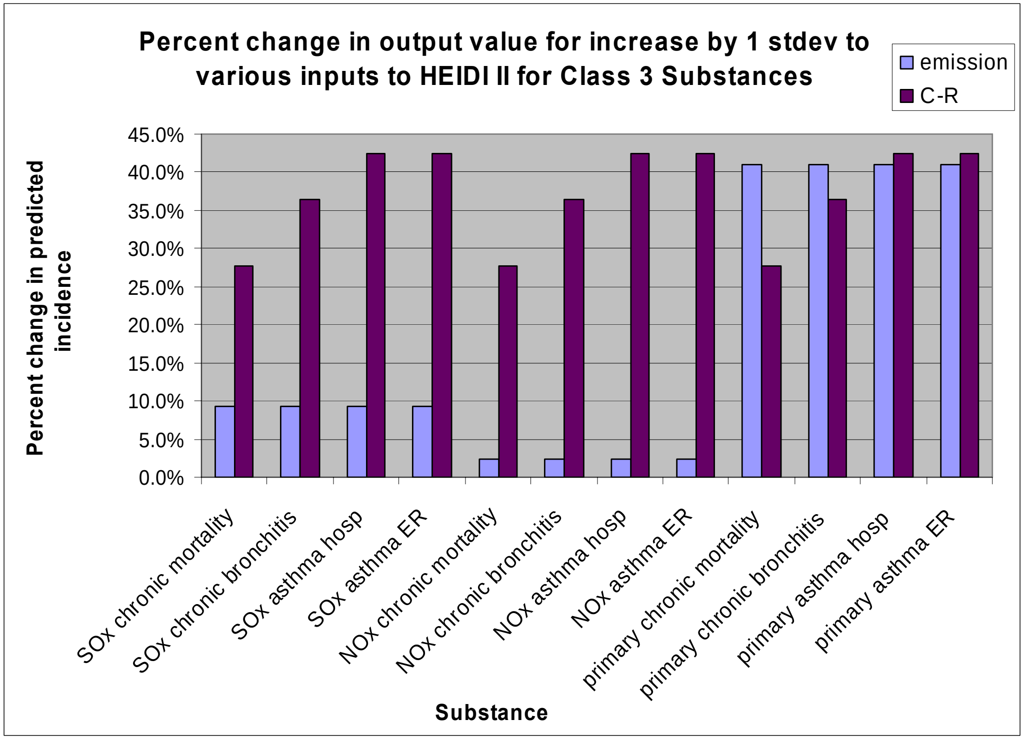


9 (B) With C-R removed from the figure, emissions seem to have the largest influence on predicted incidence has the greatest influence on predicted incidence when values are decreased from baseline.

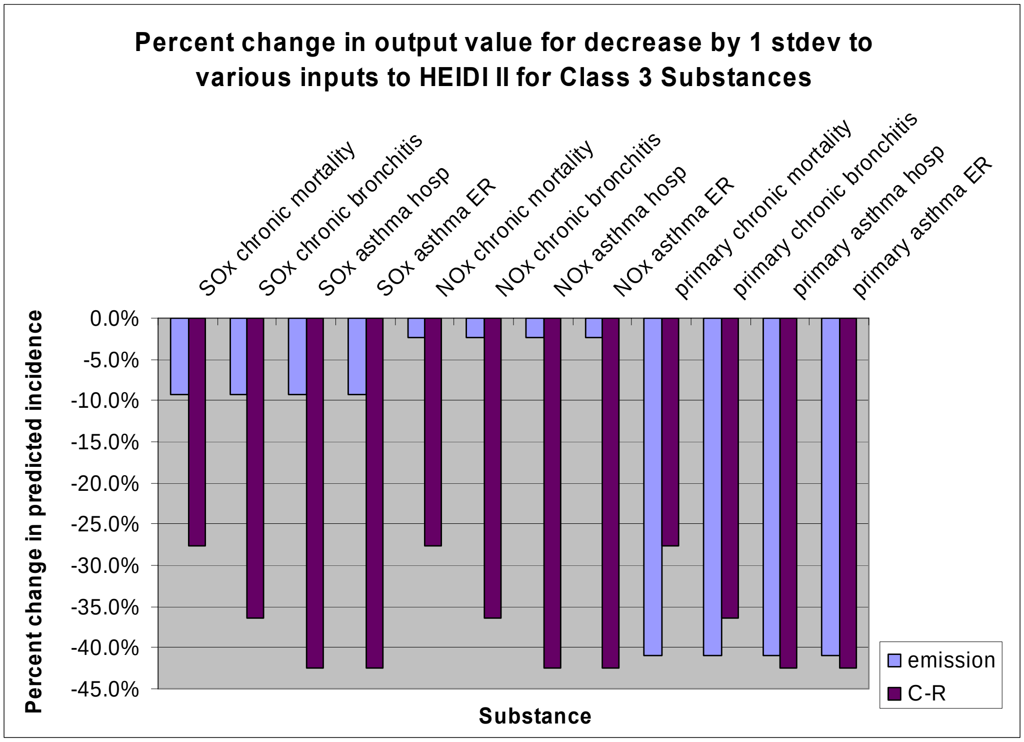
Figure 9: Sensitivity Ratio for case incidence with one standard deviation decrease in input vlaues

2.1.3.3.3 Class 3

The class 3 substances are assumed to act according to a linear non-threshold dose-response function, so background is not considered to affect predicted incidence. As well, the class 3 substances do not photodegrade, so k and OH do not affect predicted incidence. Figure 10 shows that the emission level and the C-R value relative risk values have a regular and predictable effect on predicted incidence for class 3 substances, with emissions affecting all outcomes from a particular "type" of $PM_{2.5}$ to the same degree, regardless of "outcome type", and the C-R value affecting each "outcome type" to the same degree, regardless of $PM_{2.5}$ "type".



(A)



(B)

Figure 10: Predicted case incidence for Class 3 substances depends only on emissions and C-R data. Because the Class 3 C-R inputs depended on the population breakdown, a simple SR could not be calculated. Thus, the percent change in predicted case incidence rather than the SR is graphed. Because the degradation of Class 3 substances was calculated outside HEIDI II and the dose response relationship used was linear non-threshold, the predicted case incidence would not be expected to depend on k, OH, or background. The regular patterns above reflect the consistent input for emissions for each Class 3 substance, the consistent input for C-R for each Class 3 outcome type, and the linear dose-response function.

While the percent change in predicted case incidence and the SR are useful for identifying the extent of relative change incurred by variation in input variables, they do not inform about levels of predicted case incidence. For some substances, the predicted case incidence fluctuates by a large relative amount but remains below the *de minimis* level. Because HEIDI II compares across substances and uses substance-specific data for each of the input variables, it is helpful to examine the absolute changes in predicted case incidence. The tables presented above indicate that while some input variables may have a large influence on the relative change in predicted case incidence, the sensitivity of predicted case incidence to variation in the inputs is more important for Class 1 and class 3 substances, in terms of actual predicted number of cases.

For increases in input variables affecting class 2 substances, the most influential variable for predicted case incidence is either background or ED05 value, depending on the direction of variation. However, even the greatest changes in predicted case incidence do not typically reach one case.

2.1.3.3.4 Toxicity values for V, Ni, PAH

Several substances may be subject to greater than average uncertainty in their toxicity values. As a result, it is prudent to check the model using alternate possibilities for the toxicity values. Although not all the endpoints are identical, these values are selected in an effort to place limits on the upper and lower bounds of toxicity that might be expected. Shaded areas in the tables below represent values currently in use in HEIDI II.

Vanadium

The ED05 values used in HEIDI II was based on a LOAEL devised by the WHO and published in 2000. Very few agencies have published reference values for either vanadium or vanadium pentoxide, citing a lack of adequate qualitative data. This includes Health Canada, EPA (IRIS), and CalOEHHA (RAIS), and the ASTDR, hindering development of an appropriate suite of values to test in HEIDI II. The recently released IARC monograph on vanadium pentoxide (IARC (International Agency for Research on Cancer) 2006) confirms that while there is sufficient evidence for carcinogenicity in animals, there is not enough evidence to confirm carcinogenic effects in humans (IARC (International Agency for Research on Cancer) 2006). Vanadium's classification as Group 2B – possibly carcinogenic to humans, remains unchanged for the moment. There is currently little ability to distinguish various forms of V or V_2O_5 in terms of either their toxicity or predominance in the environment. Table 10 summarizes the available data[14]. The distribution (mean, 5th percentile, 95th percentile) used to describe V in the probabilistic model was (20, 9.8E-2, 70.6).

---

[14] Agencies such as the OSHA, ACGIH, NIOSH also provide PEL values for Vanadium fume and dust and pentoxide. Using these PELs to back-calculate C-R values which might be useful in HEIDI II results in values which fall within the range described by the data presented here.

Table 10: Predicted case incidence from Vanadium exposure using alternative inputs for C-R data (shading indicates values that were actually used for all analyses of HEIDI II)

Source	Value and type	Notes	Suggested C-R value	Predicted case incidence (all other model parameters at default)
WHO, 2000	20μg/m^3 as LOAEL	Suggest 1 μg/m^3 as a reference level, safety factor of 20 is based on no susceptible subpops identified and minimal nature of adverse effects	20μg/m^3	0.10
IIEQ (Illinois Institute for Environmental Equality)	clinical signs of subtle chronic intoxication (green tongue, cough, vascularization of the cornea, conjunctivitis, colic, respiratory tract irritation, mucus, and rhinorrhea) at concentrations of about 100 μg/m^3 or less	vanadium pentoxide	≤ 100	4.11E-04 (using 100 μg/m^3)
IIEQ (Illinois Institute for Environmental Equality)	subclinical chronic intoxication resulting in metabolic disorders occurred at about 1-20 μg/m^3	vanadium pentoxide	1-20	440 (using 1μg/m^3)

Nickel:

The unit risk value used in HEIDI II was based on oxidic, sulphidic and soluble nickel compounds (combined). The actual composition of the nickel compounds to which populations around refineries are exposed is not known and may fluctuate with the composition of other substances which are emitted simultaneously. Possible alternate values for unit risk are:

Table 11: Predicted case incidence from Nickel exposure using alternative inputs for Ni C-R data

Source	Value and type	Notes	Predicted case incidence (all other model parameters at default)
Based on Health Canada TC05	1.25E-3 per μg/m^3 (Unit Risk)	oxidic, sulphidic and soluble nickel compounds combined	52
EPA	2.4E-3 per μg/m^3 (Unit Risk)	Refinery dust	99
EPA	4.8E-4 per μg/m^3 (Unit Risk)	Nickle subsulfide	20

The distribution (mean, 5th percentile, 95th percentile) used to describe Ni in the probabilistic model was (1.25E-3, 1.3E-6, 3.6E-3).

PAH

There are also several available values for PAH unit risk. PAH is a mixture of individual chemicals which fall under the classification of polycyclic aromatic hydrocarbons – each with its own toxicity value. The values presented here all follow the convention of expressing PAH toxicity in BaP equivalents, as this was the method selected for describing the mixture's toxicity in HEIDI II.

Table 12: Predicted case incidence for PAH using alternative inputs for C-R data. All methods are based on some estimation based on the amount of BaP in the PAH mixture (i.e., BaP equivalents).

Source	Value and type	Predicted case incidence (all other model parameters at default)
MOE	$2.3*10^{-2}$ per μg/m^3 (Unit Risk)	1.4
WHO	8–10×10^{-2} per μg/m^3 (Unit Risk)	5.9 (using $10*10^{-2}$)
RIVM (1986)	$1*10^{-2}$ per μg/m^3 (Unit Risk)	0.59

The distribution (mean, 5th percentile, 95th percentile) used to describe PAH in the probabilistic model was (2.3E-2, 2.5E-5, 6.8E-2).

Inspection of these alternate values indicate that for each substance identified, these "reasonable alternate C-R values" do not necessarily fall within the 95th percentile range defined by the distributions that will be applied to the C-R data for the probabilistic values. For vanadium, the upper bound C-R value of 100 proposed by the IIEQ is above the 95th percentile of V's probability distribution as used in HEIDI II. Higher thresholds would reduce the predicted incident cases for Vanadium, so the impact of not including this upper-bound estimate of toxicity for V could be overprediction of incidence and an underestimate of the variation in predicted incidence. For PAH, the upper bound value of $10*10^{-2}$ per μg/m^3 proposed by WHO exceeds the 95th percentile value defined for PAH unit risk in HEIDI II, which could result in underprediction of cases.

Using the individual "reasonable alternate C-R values" suggested above in local SA at the worst-case hypothetical refinery results in predicted case incidence values from $4*10^{-4}$ up to ~400 for the range of values used to test Vanadium, from 20-99 cases for values tested for Nickel, and from <1 - ~6 cases for PAH. These potential variations confirm how little is known about the specific toxicity of many substances, and also that the impact on humans, especially in the case of Ni and PAH, where the potential health outcome is cancer, could be considerable. Additionally, the values tabulated here represent results of limited experimentation and do not represent the true range of uncertainty about the toxicity of these substances

2.1.3.3.5 Potential interaction of background and C-R for class 2 substances

The C-R values used for class 2 substances were "derived threshold estimates" [15] values used to anchor the Mantel-Bryan C-R formulation. Local sensitivity analyses indicated that predicted case incidence was dependent on background exposure for selected substances. The total exposure of a population surrounding a refinery may depend highly on the background levels, especially if emissions of specific substances are low relative to background concentrations. If the background levels approach the model's "derived threshold estimates" for class 2 substances, additional exposure contributed by a refinery emission could cause additional predicted case incidence of disease. However, if the background levels are far below the toxicity threshold, emissions contributed by the refinery are unlikely to push exposure levels over the threshold, and so disease is unlikely to be predicted.

There could be an interaction between substance-specific background levels and the toxicity values selected to represent their "derived threshold estimates". To better understand this phenomenon, response surfaces were created depicting the interaction between background and the "derived threshold estimate" values. These response surfaces investigate the range of values from 1-99th percentile of the distributions used in HEIDI II for background and threshold. The response surfaces indicated that even at combined extreme values for background and threshold (all other inputs held at central values), the *de minimis* risk level was exceeded for only five substances (See Table 13).

---

[15] Although they are being used to anchor the Mantel-Bryan distribution, they are variously based on TC05, LOAEL, and NOAEL values, some of which are extrapolated from animal experiments. It is probably not appropriate to label them as "thresholds" when they are only approximations in any case. Additionally, the terminology "threshold" suggests a definite cutoff point, whereas the Mantel-Bryan function allows for a continuous, sublinear function to represent dose-response for class 2 substances.

Table 13: Approximate number of predicted incident cases per million people at the hypothetical refinery for extreme values of background and C-R

Substance	**Cases predicted per million people at 1st percentile for C-R[16] and 99th percentile for background**
1,2,4-trimethylbenzene	~2
BTEX	~680 000
naphthalene	~1
n-hexane	~5
Vanadium	~100 000

The two cases of particular concern appear to be Vanadium and BTEX. For V, the relevant outcome is relatively mild (nasal and upper airway irritation). High values of predicted case incidence for BTEX occur only at extreme values for background and toxicity, but given the relevant outcome of CNS toxicity, may be of concern. For all substances, most of the predicted incidence was at or close to zero as shown in Figure 11 and Figure 13.

---

[16] Because C-R is an ED05 value, it predicts higher incidence for lower values. Thus, the first percentile of the PDF for the ED05 is selected rather than the 99th percentile.

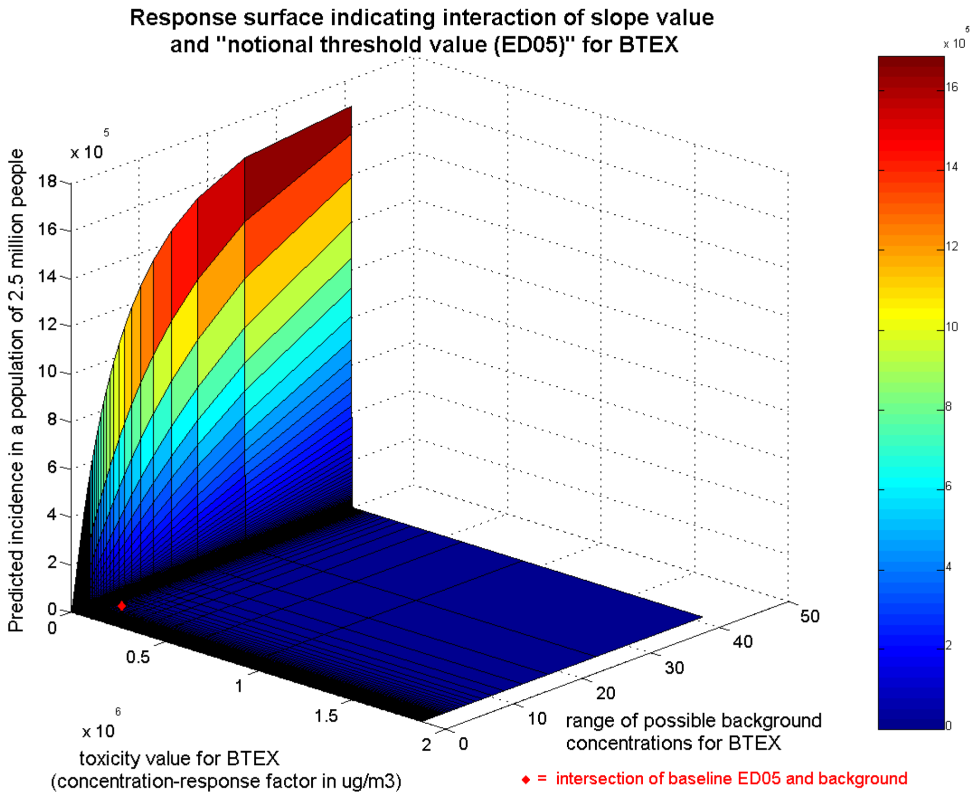


Figure 11: BTEX – predicted incidence across the range of values allowed for C-R and background. Relevant equivalent human health outcome is moderate CNS neurotoxicity

Figure 11 shows the predicted incidence associated with BTEX across the 99th percentile of values in the distributions for ED05 and background, and indicates that the majority of predicted incidence is zero. However, it is difficult to tell anything about the highest percentiles on this figure. A closer look at the first 20th percentile for C-R and the top 20th percentile for background (i.e., “zooming in” on the area of highest predicted incidence) provides a better sense of how fast predicted incidence of CNS neurotoxicity due to BTEX exposure increases at these values. (See Figure 12).

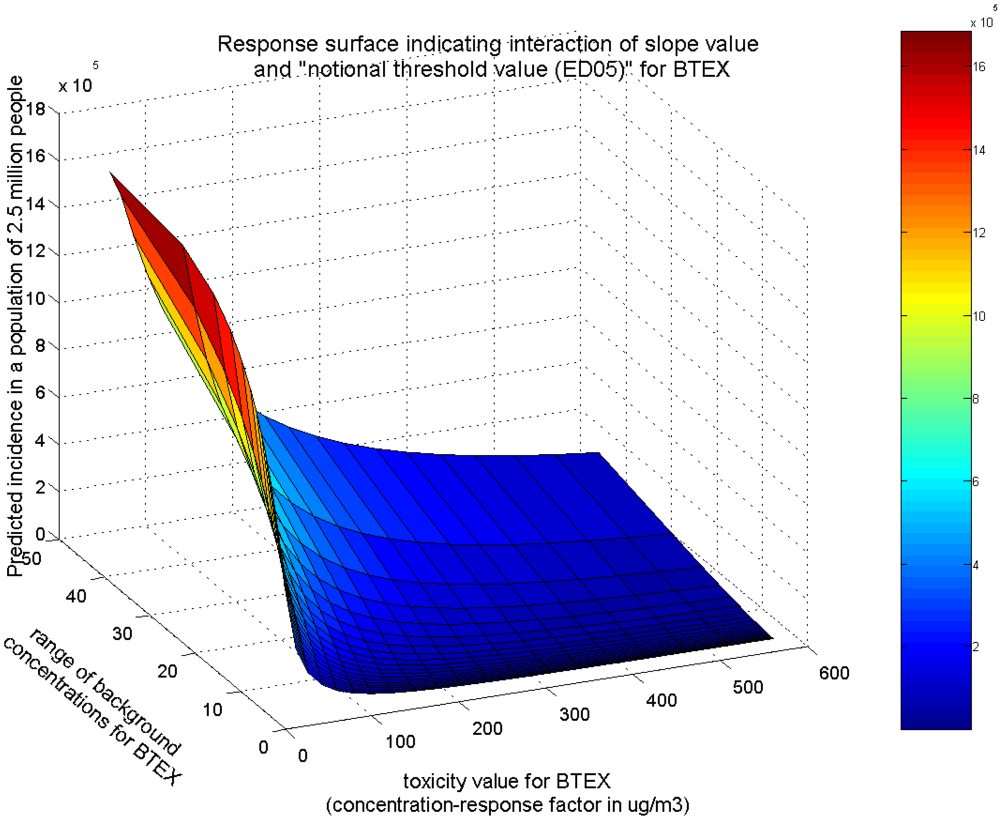


Figure 12: BTEX – predicted incidence across the 20th percentile of values for C-R and background leading to highest predicted incidence. Relevant equivalent human health outcome is moderate CNS neurotoxicity

A similar response surface is produced for Vanadium: most of the response surface is at zero with high predicted incidence for low toxicity value inputs as shown in Figure 13. A closer look at the first 20th percentile for C-R and the top 20th percentile for background (i.e., “zooming in” on the area of highest predicted incidence) provides a better sense of how fast predicted incidence of upper airway irritation due to Vanadium exposure increases at these values. See Figure 14.

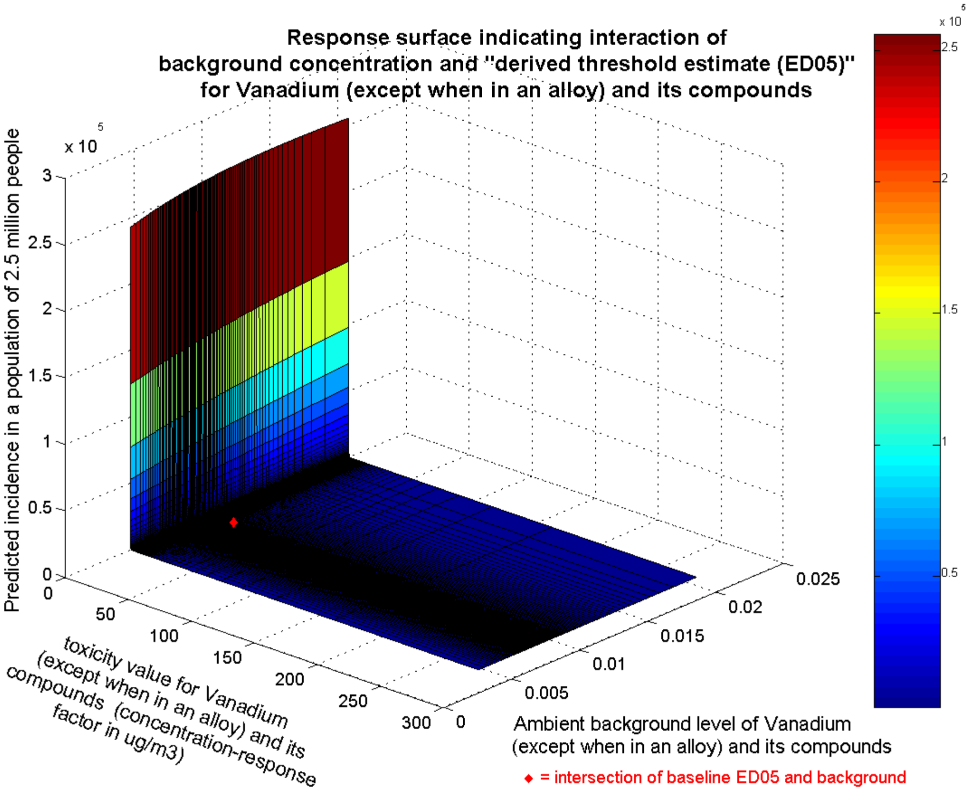


Figure 13: Vanadium. Predicted incidence across the range of values allowed for C-R and background. Relevant equivalent human health outcome is nasal and upper airway irritation.

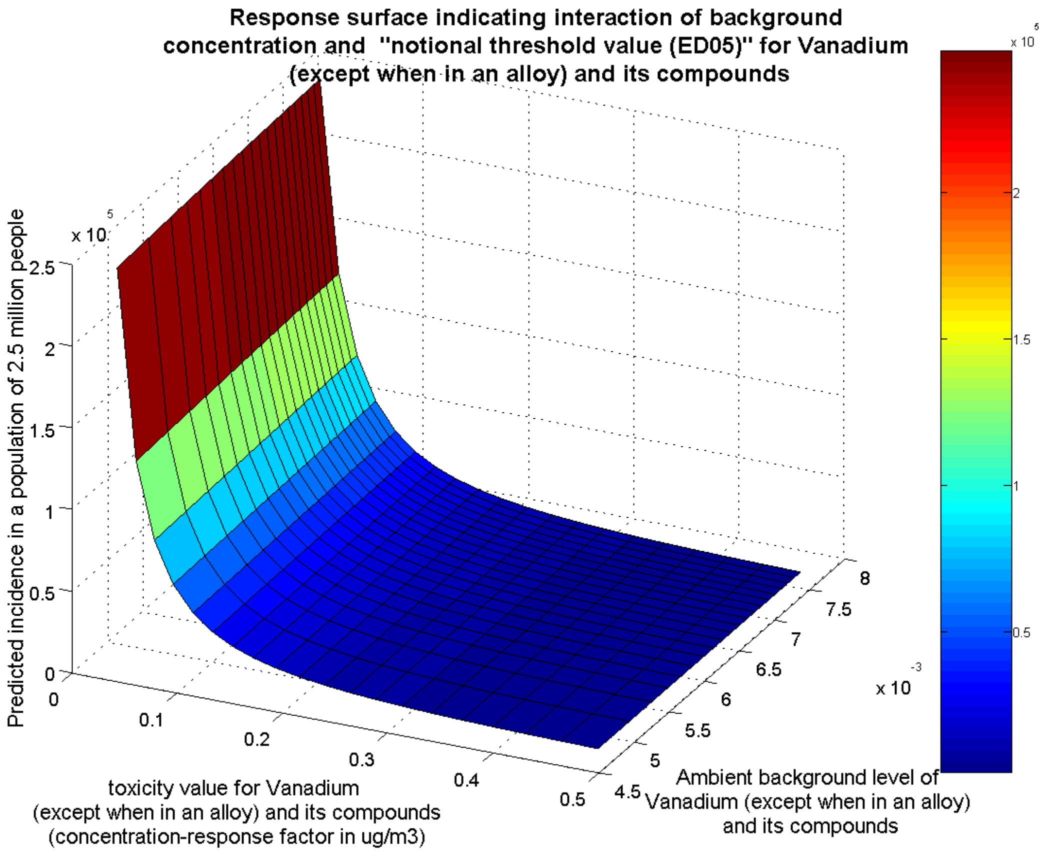


Figure 14: V – predicted incidence across the 20th percentile of values for C-R and background leading to highest predicted incidence. Relevant equivalent human health outcome is upper airway irritation.

2.1.3.3.6 Potential interaction of Mantel-Bryan slope and C-R values

The C-R values used for class 2 substances were "derived threshold estimate", or ED05 values used to anchor the Mantel-Bryan C-R formulation. The Mantel-Bryan formulation for dose-response also relies on a slope value (for the probits per dose increase). In HEIDI II, the central value used was 1.5, which was found to provide good dose-response across the range of possible air concentration values, and to provide results that align well with the *de minimis* risk level calculated with the conventional threshold formula (See Appendix C for more details). The values used for these two substances could interact when predicting incidence. A sample graphic is provided for Vanadium in Figure 15. It includes the 1-99th percentile of toxicity data for Vanadium and shows that at most toxicity values the value of the slope selected has little impact on predicted incidence, and that at the slope value used in the model (1.5), there might be a slight increase in predicted incidence from baseline only for the lowest 2 percentiles of possible threshold values.

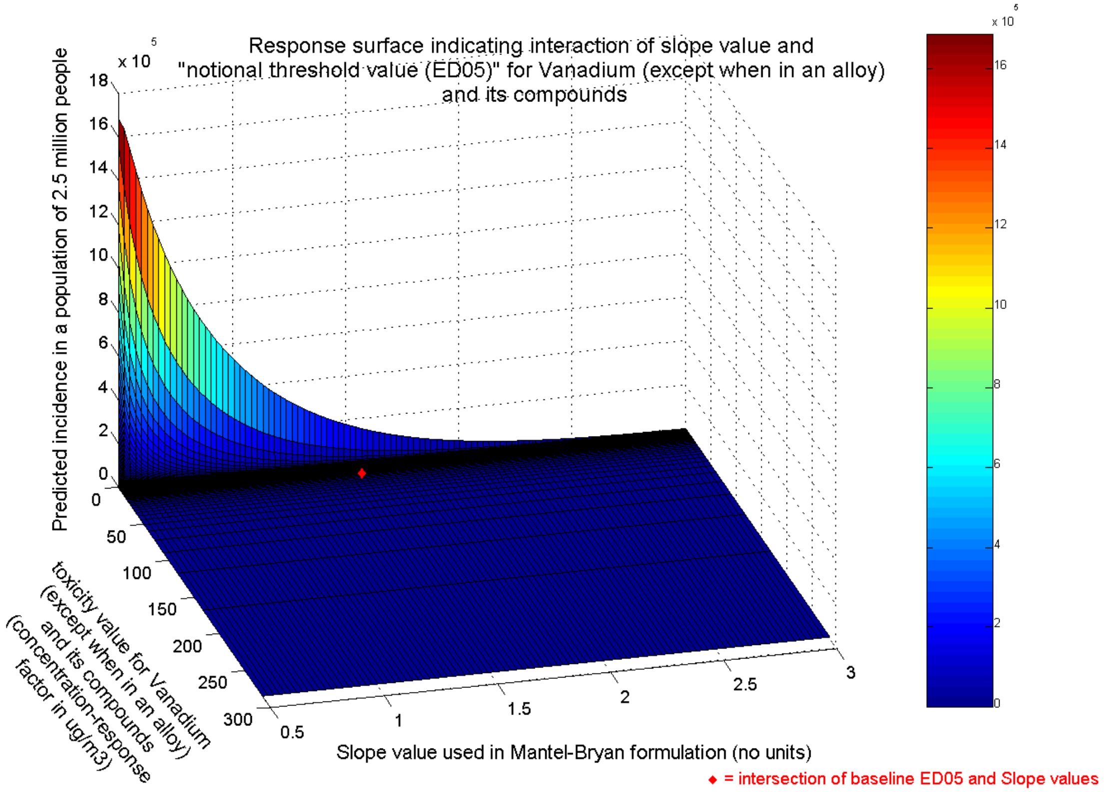


Figure 15: Vanadium. Predicted incidence across the range of values allowed for C-R and Slope. Relevant equivalent human health outcome is nasal and upper airway irritation

2.1.3.4 Alternate Model Formulations

There are various ways to “assemble” a model and select data to represent the model variables. It is appropriate to test alternative formulations of the model – to find the most parsimonious representation that adequately represents the data.

(i) Background scenarios

The original incarnation of HEIDI II used site-specific data for background concentrations. However, much of the data was incomplete or from monitors that were not ideally sited to collect background levels (i.e., not directly in the community, or located downwind from the refinery). Thus, a general division of background levels into “high”, “medium”, and “low” was proposed, with refineries assigned to each level based on population surrounding the refinery and whatever site-specific background data was available. The values used to represent the background concentrations were derived from combining the site-specific data for refineries assigned to each of three categories (high/medium/low - See Appendix C).

Sensitivity analysis indicated that for most substances, the change in predicted case incidence (or DALYs) was small with the new background scenario. The largest changes in predicted incidence were observed for styrene and isoprene, followed by zinc, 1,2,4-trimethylbenzene, and MEK. It is worth noting that these were differences in absolute values on the order of 10^{-14} and smaller (in some cases, changes are at the level of 10^{-28}). With this change in predicted population health impact, the rank order of each of these substances remained low, and often did not change. Thus the simpler high/medium/low background scenarios were retained for the probabilistic version of HEIDI II.

(ii) Mantel-Bryan Slope

A component of the C-R function for class 2 substances is the slope selected for the Mantel-Bryan formulation. 1.5 was used as the default, but possible values ranging from 1-5 were evaluated. When the Mantel-Bryan slope is decreased to 1 from 1.5, the percent increase in predicted population health impact is large, especially for those substances with the highest ED05 values. However, it is worth noting that the original predicted impacts for those substances were so small that increasing them even several million-fold does not affect their rank order (i.e. ranked at a tie in last place)! Where the slope was increased, the changes in predicted population health incidence tended towards zero.

(iii) Application of photodegradation in HEIDI II

A shortcoming of HEIDI II is its approach to photodegradation of class 1 and class 2 substances: the photodegradation equation, which was intended mainly to reflect the average amount of sunlight daily, is uniformly applied to concentrations delivered to each quadrant. However, substances take more time to reach the more distant locations, and so may undergo more photodegradation as they travel. At the closest locations, exposures are likely being underpredicted by HEIDI II, since the emissions may have very limited time to photodegrade before exposure occurs, while at the more distant locations, exposures are potentially overpredicted by HEIDI II.

Table 14: Percent change in predicted incidence at 25 km from the refinery for two photodegradation times: 8 hours and 16 hours. Only substances that had predicted incidence>0 for the 25 km zone are included

Substance	Stack Height (m)		
	30	*15*	*5*
1,3-Butadiene	51.1%	51.1%	51.1%
Benzene	5.1%	5.1%	5.1%
Ethylene (as 5% Ethylene Oxide)	27.3%	27.3%	27.3%
Nickel (and its comps)	0.0%	0.0%	0.0%
PAHs (BaP surrogate class)	51.5%	51.5%	51.5%
Formaldehyde	29.1%	29.1%	29.1%
Acetaldehyde	39.7%	39.7%	39.7%
Mercury	0.0%	0.0%	0.0%
Phenol	26.5%	17.6%	26.5%
Sulphuric Acid	5.6%	5.4%	5.6%
Vanadium	0.0%	0.0%	0.0%
Zinc (and its compounds)	0.0%	0.0%	0.0%

Table 15: Percent change in predicted incidence at 1 km from the refinery for two photodegradation times: 8 hours and 16 hours. Only substances that had predicted incidence>0 at 1 km for at least one of the stack height scenarios are included. (Val = 0 indicates that the percent change could not be calculated since one of the predicted incidence values was zero.)

Substance	Stack Height (m)		
	30	*15*	*5*
1,3-Butadiene	51.1%	51.1%	51.1%
Benzene	5.1%	5.1%	5.1%
Ethylene (as 5% Ethylene Oxide)	27.3%	27.3%	27.3%
Nickel (and its comps)	0.0%	0.0%	0.0%
PAHs (BaP surrogate class)	51.5%	51.5%	51.5%
Formaldehyde	29.1%	29.1%	29.1%
Acetaldehyde	39.7%	39.7%	39.7%
1,2,4-Trimethylbenzene	Val=0	100.0%	85.1%
Ammonia	0.0%	0.0%	0.0%
Dicyclopentadiene	Val=0	100.0%	96.6%
Diethanolamine (and its salts)	Val=0	Val=0	97.0%
Hydrogen Sulphide	0.0%	0.0%	0.0%
Mercury	0.0%	0.0%	0.0%
Naphthalene	47.3%	48.1%	59.6%
n-Hexane	50.0%	53.1%	75.0%
Phenol	19.8%	20.1%	21.3%
Sulphuric Acid	4.2%	3.8%	3.0%
Vanadium	0.0%	0.0%	0.0%
Zinc (and its compounds)	0.0%	0.0%	0.0%

To test the effect of this error, two photodegradation times were selected, and the difference in predicted incidence at a location far from the refinery and a location close to the refinery were assessed. Table 14 and Table 15 show the percent change in predicted incidence at two distances from the refineries with different photodegradation times. The potential for error is consistent across stack heights for class 1 substances, but differs across stack heights for class 2 substances. For the 5 metre stack height the potential error is greatest at closer locations and for the 30 metre stack height, it is marginally greater at distant locations. The results suggest that the relative error in predicted incidence could be large. Also – because it is different for each substance, it could potentially alter the rank order that HEIDI II produced to identify priority substances. Unfortunately the complexity required to incorporate photodegradation difference by time traveled away from the refinery is prohibitive.

A second shortcoming of the method by which photodegradation was applied is that the breakdown products of the photodegradation process are not accounted for. Accounting for this would require a complex alternate model formulation and raises the problem of "double-counting" when estimating toxicity.

2.1.3.5 Scenario Uncertainty

"User-selected inputs"

These include stack height input, which can be 5, 15, or 30 metres, and time allowed for photodegradation, which can theoretically vary between 0-24 hours. The following figures explore the range of possible outputs associated with different input values for these variables. The first few figures explore the effect of stack height and photodegradation on delivered concentration (Module 1 alone), since this helps to understand how changes in stack height or photodegradation affect exposure and therefore predicted incidence.

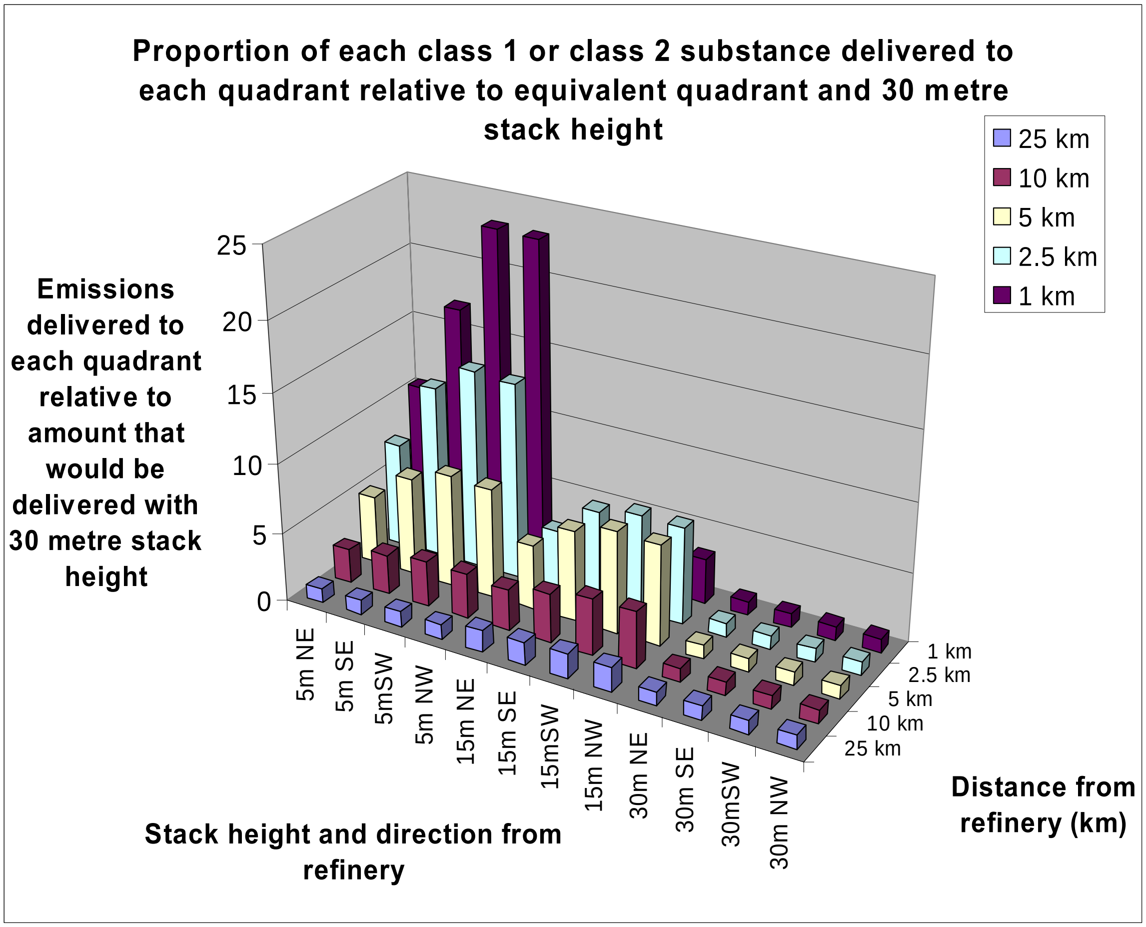


Figure 16: HEIDI II predicts that low stack heights deliver a much higher concentration to nearby locations, while intermediate stack heights deliver larger concentrations to intermediate distances. The stack height has a similar impact on class 3 substances (not shown) although the actual delivered concentrations would differ due to formation of secondary PM as distance increases from the refinery.

Figure 16 shows that the highest concentrations of each substance are delivered to the nearby locations, and with the lowest stack heights. Although this figure does not display it well, absolute concentrations of each substance also decrease with increasing distance from the refinery. The stack height affects every emission in the same way. Figure 17 shows how the effect of photodegradation is substance-specific, depending on the rate constant for the reaction of each emission with ambient OH. Figure 17 provides an assessment of the proportion of each substance remaining after a variety of allowed times (t) for photodegradation, and given the substance-specific degradation rate constant, k:

$$\text{Proportion} = \frac{Conc(0,k)}{Conc(t,k)}$$

The extent to which photodegradation time affects delivered concentration will depend on the specific emission of interest, and will be less important for substances that degrade slowly.

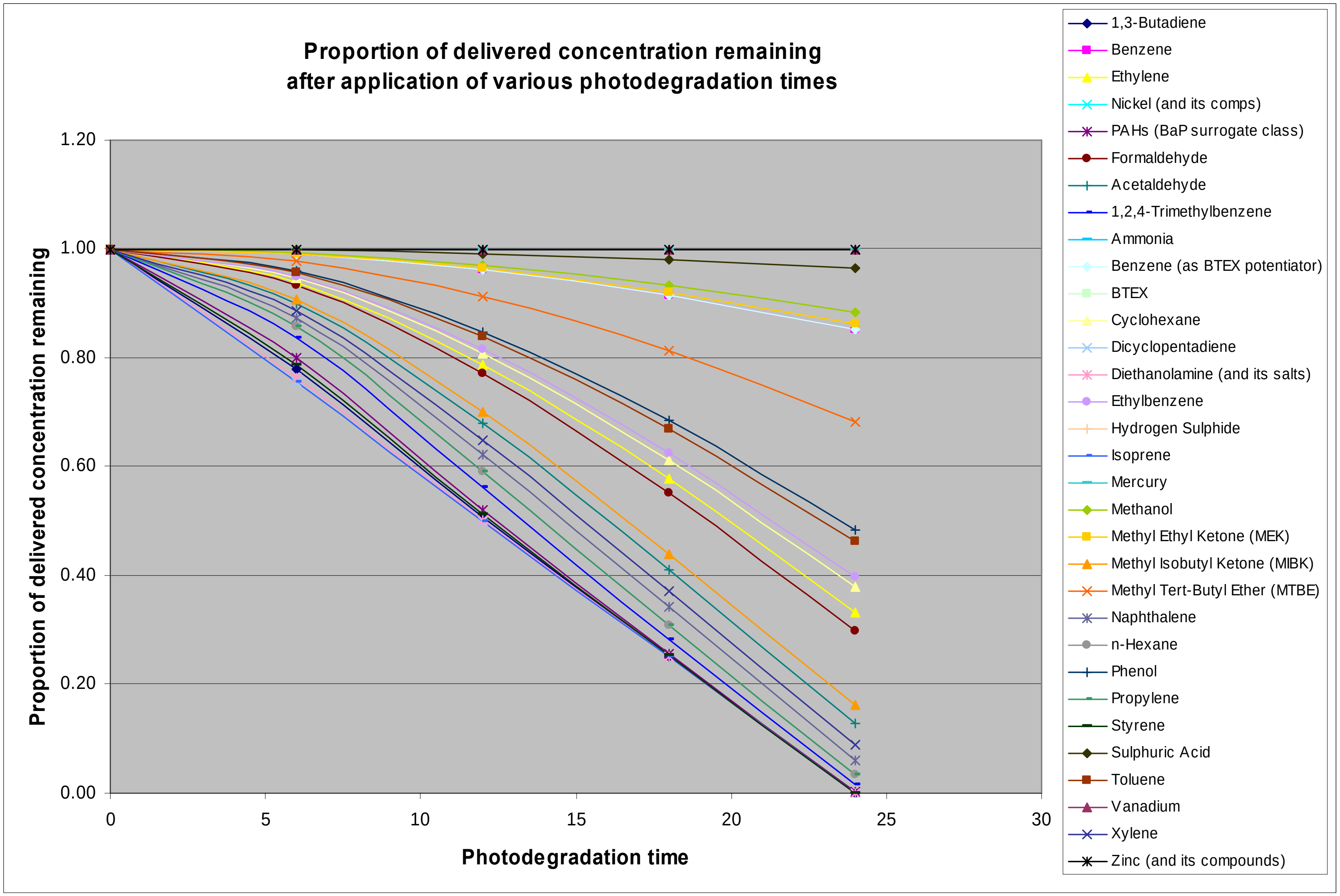


Figure 17: The proportion of each substance remaining at any given location around the refinery depends on the degradation rate constant of the substance and the time available for photodegradation. Some substances, such as the metals, do not photodegrade at all. Class 3 substances are not considered to undergo photodegradation reactions.

Ethylene, which has an intermediate photodegradation rate constant, is used as an example substance to explore the interaction between photodegradation time and stack height (See Figure 18. and Figure 19). These figures indicate that the overall relationship between stack height, photodegradation time, and delivered concentration around the refinery is complex. The summary value of predicted case incidence that emerges from the various combinations for these inputs values is thus likely to be complex as well. In general, a larger value of k (faster degradation) results in a steeper curved slope along the photodegradation time axis, and in all cases, more photodegradation time results in less exposure). Figure 18 explores the interaction for zones closest to the refinery: at this location, the combination of low stack height and little time for photodegradation results in the highest delivered concentrations – about 2.5 times higher than what would be observed with a 30 metre stack height and 0 hours of photodegradation. Figure 19 indicates that at all distances, the impact of different photodegradation times on delivered concentration with a 30 metre stack is minor. Since 30 metres is the most realistic representation of stack height for most Canadian refineries (Hicks 2005), the amount of time available for photodegradation may not be relevant for determining exposure to most substances. Examining predictions results across a range of rate constants suggests that these results are generalizable to all class 1 and class 2 air toxics (class 3 substances do not undergo photodegradation).

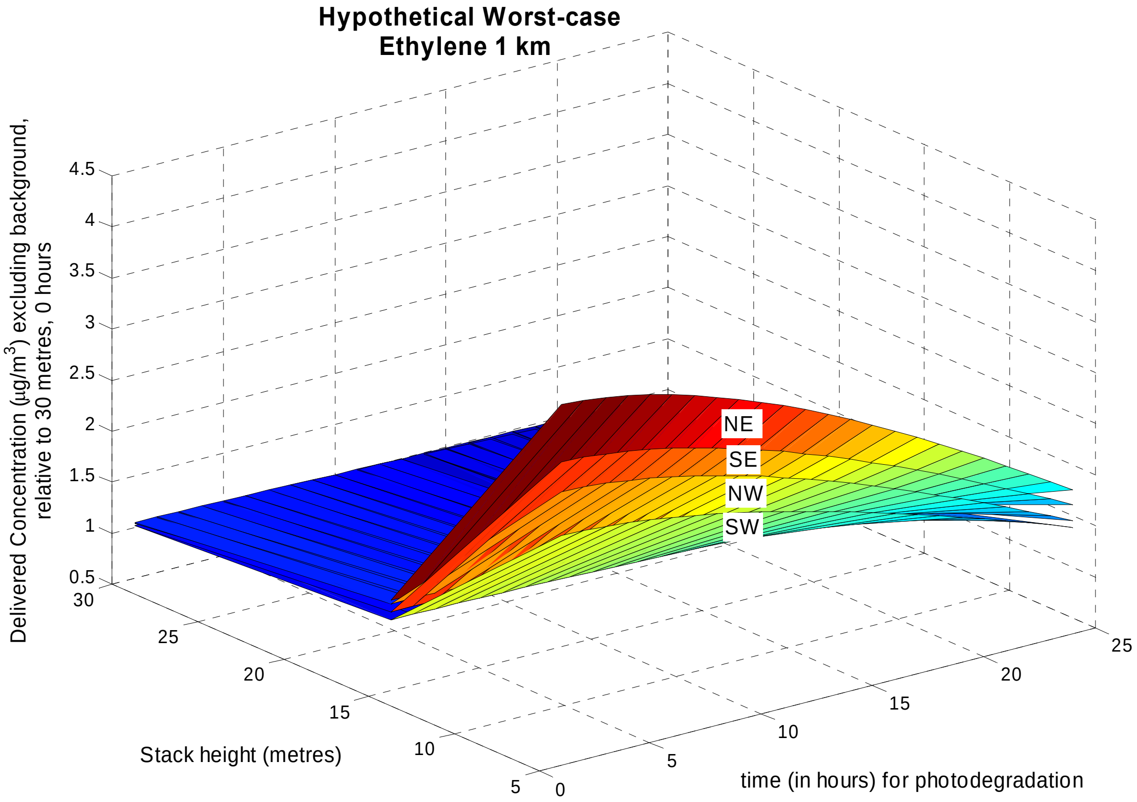


Figure 18: Ethylene (as oxide) (in the 1 km NE quadrant) is used as an example. In this quadrant, at high stack heights, the time available for photodegradation does not affect the delivered concentration. However, at low stack heights, the delivered concentration depends more strongly on photodegradation time.

Figure 19[17] looks at a specific quadrant at various distances from the refinery. It shows that the 30 metre stack is associated with the lowest exposure at any photodegradation time and distance from the refinery, but that the relative contributions to exposure for stack heights of 5 m or 15 m depend on a combination of photodegradation time and distance from the refinery. The highest exposure occurs for the shortest photodegradation times combined with the shortest stack height.

---

[17] The model can only be run for three specific stack heights: 5m, 15m, or 30m. The discontinuity that appears in these figures is an artifact of the limited number of data points for stack height.

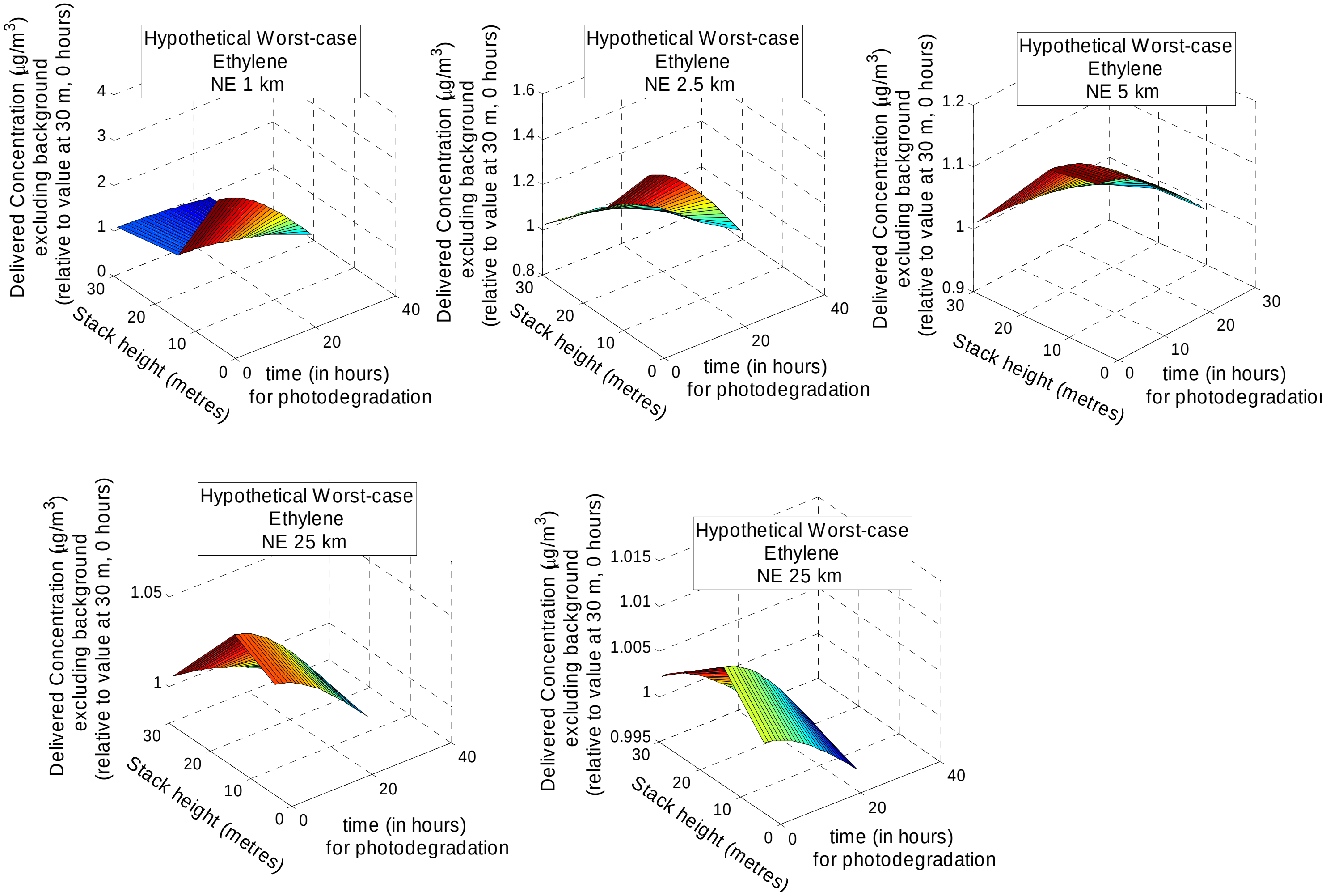


Figure 19: The interaction between stack height and photodegradation time. Here, the set of interactions across all NE quadrants with increasing distance from the refinery demonstrates how the delivered concentration is greatest for the 5 metre stack close to the refinery, but at farther distances, the 15 metre stack begins to contribute more to the delivered concentration. The NE quadrant was chosen for this analysis because it is directly downwind of emissions.

Table 16 shows the predicted case incidence values for ethylene, under various stack height/photodegradation time scenarios (and using a homogeneous population of one million people). The greatest predicted case incidence occurs with the least amount of sunlight and with the 15 metre stack height. The only scenario that predicts lower incidence than the default scenario is the 16 hours, 30 metres scenario. This indicates that the default scenario used for most analyses may not be the most conservative scenario. However, it is probably the most realistic.

Table 16: Predicted case incidence of leukemia from ethylene (class 1 substance) exposure at the worst-case refinery. Note that reporting values to three decimal places may not be appropriate as it provides a false sense of precision and accuracy associated with these values. Also note that for no scenario is there likely to be even one predicted case in a population of one million.

Predicted case incidence (leukemia) from Ethylene at worst-case refinery					Percent change in predicted case incidence relative to default (30 metres, 12 hours)		
Stack height	Hours of sunlight				Hours of sunlight		
	8	12	16		8	12	16
5	0.10	0.09	0.07		180%	150%	100%
15	0.10	0.09	0.08		180%	150%	110%
30	0.04	0.04	0.03		14%	0%	-17%

Table 17: Predicted case incidence from exposure to sulphuric acid and phenol, class 2 substances. The extent to which incidence is altered with changes in stack height and photodegradation inputs depends on the individual substance. This is a function of the interaction of the nominal "threshold" and the total changes in exposure around the refinery resulting from various stack height/ photodegradation time scenarios. Although there is a large percent increase in predicted case incidence for many of the scenarios relative to default, the absolute value for predicted case incidence remains low (predicted case incidences are in a population of one million). Sulphuric acid has one of the lowest photodegradation constants, while phenol has a relatively high photodegradation constant.

Predicted case incidence (benign nasal and upper airway tumors from Sulphuric Acid at worst-case refinery					Percent change in predicted case incidence relative to default (30 metres, 12 hours)		
Stack height	Hours of sunlight				Hours of sunlight		
	8	12	16		8	12	16
5	4.2E-08	4.1E-08	4.0E-08		16000000%	16000000%	16000000%
15	3.0E-11	3.0E-11	2.9E-11		11000%	11000%	11000%
30	2.7E-13	2.7E-13	2.7E-13		0%	0%	0%
Predicted case incidence (mild CNS neurotoxicity) from Phenol at worst-case refinery					Percent change in predicted case incidence relative to default (30 metres, 12 hours)		
	Hours of sunlight				Hours of sunlight		
Stack height	8	12	16		8	12	16
5	9.7E-10	9.2E-10	7.4E-10		170%	160%	110%
15	9.6E-10	9.1E-10	7.6E-10		170%	160%	110%
30	4.1E-10	3.6E-10	2.9E-10		15%	0%	-19%

Table 16 and Table 17 show that the stack height is much more important for determining impacts of refinery emission than the amount of photodegradation time/sunlight available.

Class 3 substances do not undergo photodegradation but rather transformation by chemical reactions. These were predicted as a part of the external dispersion modeling. Because the dose-response function for class 3 substances is linear non-threshold, a sense of the change in predicted case incidence with stack height can be inferred by considering the general effect of stack height on delivered concentrations (see Figure 16) in combination with the distribution of population around the refinery.

The populations (numbers and geographical distribution of people) associated with each refinery were selected based on Canadian census data (Statistics Canada 2002). However, populations may fluctuate and the distribution around any specific refinery may have important implications for total predicted case incidence. The influence of the following population scenarios on total predicted case incidence around a refinery (with all other variables held at the default) was assessed:

- homogeneous
- heterogeneous outward – population density increases linearly moving from zone to zone away from the refinery
- heterogeneous inward – population decreases with distance from the refinery (similar to the refinery being situated at the centre of an urban area)
- All population in the north
- All population in the south
- All population in the east
- All population in the west

The general trends in predicted case incidence were the same for class 1 and class 2 substances, (although the absolute predicted case incidence values were different for each substance). Figure 20 uses nickel as an example to describe the pattern:

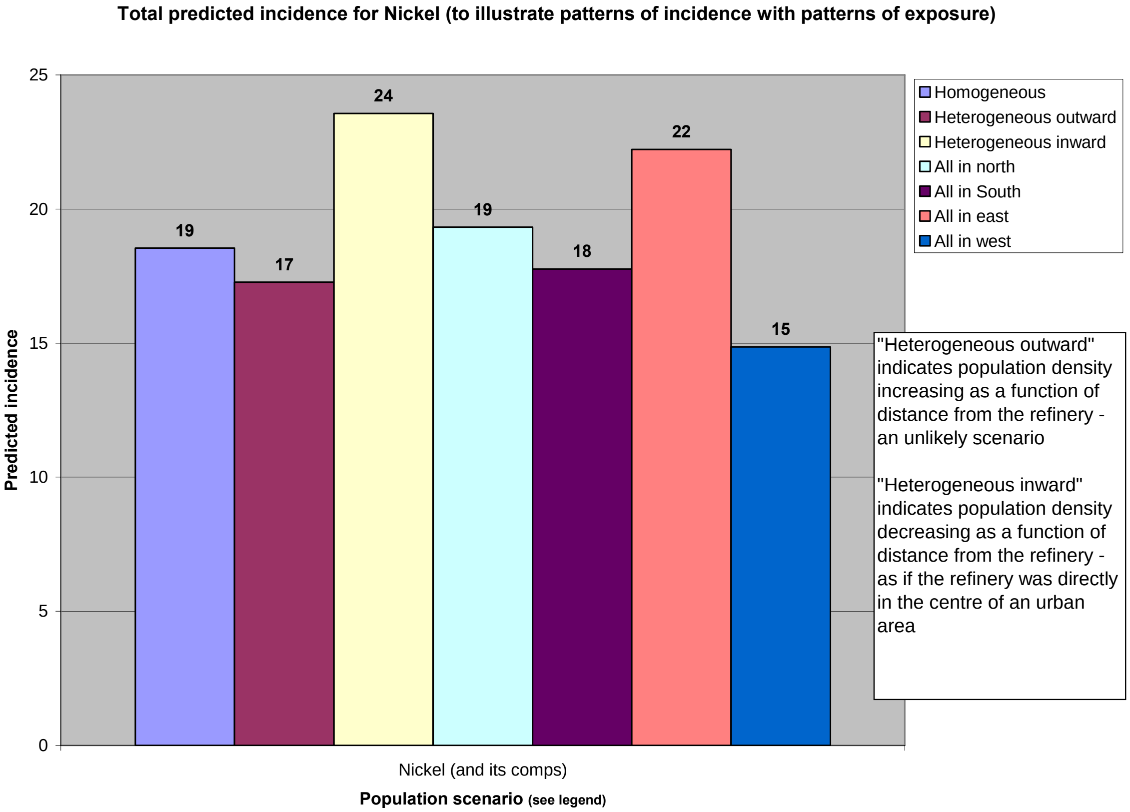
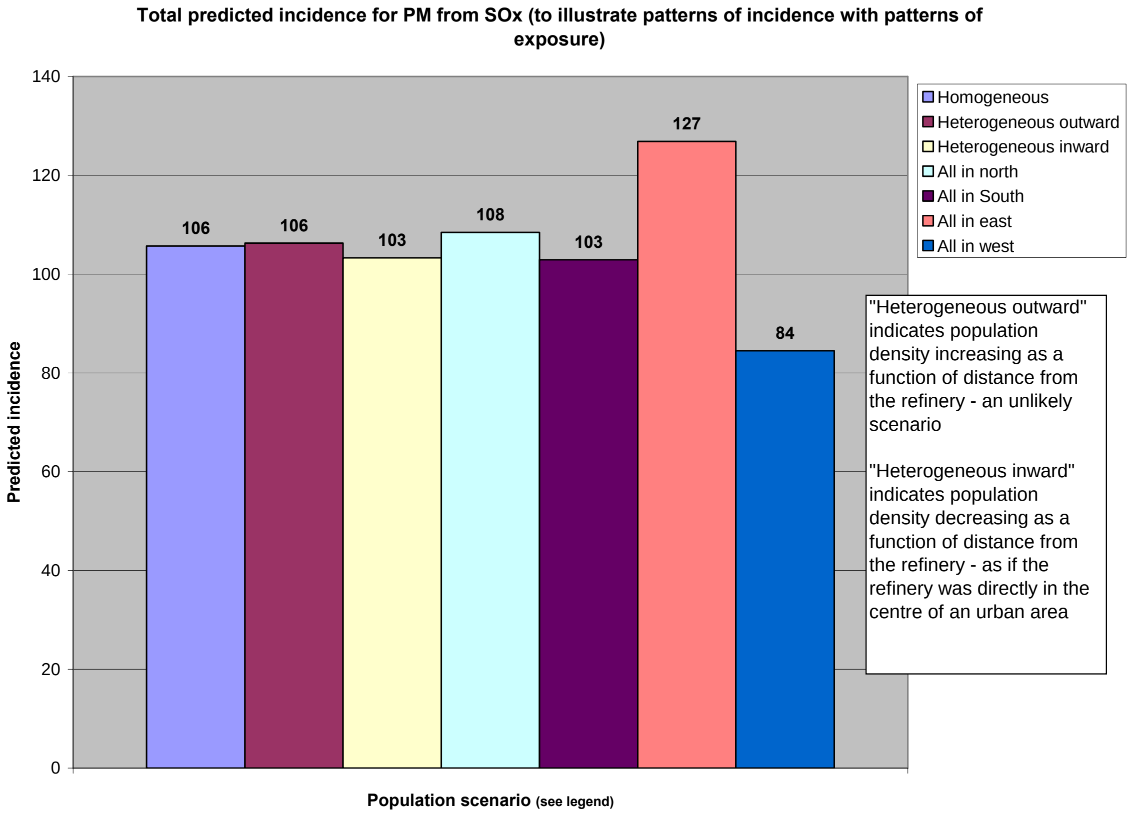


Figure 20: Nickel, like all class 1 and class 2 substances, decreases in concentration with distance from the refinery. For class 1 and two substances, having the refinery at the centre of a heavily populated area would result in highest predicted case incidence.

The greatest predicted case incidence is observed for “heterogeneous inward” – this makes sense since delivered concentrations are higher closest to the refinery. Heterogeneous outward places most of the population farther from the refinery where concentrations should be lower – this is reflected in the lower relative predicted case incidence. Prevailing winds were set as being from the SW to the NE – the patterns of predicted case incidence reflect this with higher predicted case incidence observed in the north and east scenarios where delivered concentration is likely to be higher.

Looking at the percent change in incidence that would be predicted compared to the homogeneous population distribution around the refinery, the following points are noted: (i) predicted case incidence is higher in areas where delivered concentration should be higher, and (ii) the “heterogeneous inward” scenario results in the largest magnitude of altered predicted case incidence compared to the base case.

The pattern for the secondary PM (NO_x and SO_x) is somewhat different, with relatively similar predicted case incidence for homogeneous, heterogeneous inward, heterogeneous outward, or all in north or south scenarios. The only population scenarios that elicit notably different predicted case incidences than the homogeneous scenario are the all in east or all in west scenarios. This is likely a function of how degradation/transformation was calculated for class 3 substances. For primary and secondary PM, the calculation of transformation and degradation accounted for the reduced amount of primary PM and increased amounts of SO_x and NO_x at each successive distance from the refinery. The strong increase in SO_x concentrations with distance from the refinery essentially overwhelms the reductions in predicted case incidence that might be expected for a heterogeneous inward scenario (due to fewer people living farther from the refinery) as compared with the "homogeneous" scenario.



"Heterogeneous outward" indicates population density increasing as a function of distance from the refinery - an unlikely scenario

"Heterogeneous inward" indicates population density decreasing as a function of distance from the refinery - as if the refinery was directly in the centre of an urban area

Figure 21: Concentration of SOx increases with distance from the refinery, in contrast to all class 1 and 2 substances. In this case, only the "All in East" and "All in West" scenarios produce different predicted case incidence than the "homogeneous population" scenario. Siting of refinery that is protective for SOx exposure is therefore not the same as siting which would be protective for class 1 and class 2 substance exposures.

The local sensitivity analyses were followed by global analyses, where all uncertain or variable inputs were allowed to vary simultaneously according to predetermined probability distributions.

2.1.4 Global Sensitivity Analysis Results

2.1.4.1 Parametric uncertainty and Variability

In a global sensitivity analysis, the effects of allowing all input variables to vary at the same time is investigated, typically using a technique such as Monte Carlo simulation.

The scatterplots of inputs/outputs created after initial Monte Carlo simulations indicated that there were always one or two extreme values predicted for both inputs and outputs. Truncating the distributions of values predicted at the 99th percentile eliminated the most extreme (and unlikely values) and provides a better sense of the scatter in values. Table 18 was created using 50 000 iterations. With this number of iterations, the correlation coefficients were stable.

Cullen and Frey suggest that correlation values of > |0.5| between model inputs and outputs indicate substantial correlation, while values > |0.2| may be of interest. For input/output combinations in HEIDI II, only correlation between predicted incidence and toxicity values exceeds either of these cutoff points for any substance. Correlations between predicted case incidence and background often exceeded |0.1|.

Table 18 confirms that the toxicity parameters are the most influential variables (of those that are either variable or uncertain or both) for predicted case incidence for class 1 and two substances. Background concentration becomes mildly important for some substances (BTEX, cyclohexane, n-hexane, propylene, and styrene). The background levels used do not appear to be significantly higher (relative to amount emitted) for these substances as compared to other substances, and the toxicity values do not appear to be particularly low. However, the GSD used to characterize the distributions for the background for these particular substances was relatively high. The higher degree of skew in the lognormal distributions used to represent ambient concentrations may have resulted in the total delivered concentration exceeding the threshold for these substances more often.

Table 18 indicates that there are varying levels of correlation between the ED05 values and the predicted impact for class 2 substances. In general, substances with lower thresholds exhibit greater correlation with predicted incidence. This likely reflects the greater proportion of times that the delivered concentration value exceeds the threshold during a simulation with multiple iterations - and therefore exerts an effect on predicted incidence values. In contrast, each time a delivered concentration value below the threshold is predicted for a given substance, regardless of the C-R value, zero case incidence would be predicted, leading to a low correlation.

For a select few substances (BTEX, cyclohexane, n-hexane, propylene and styrene), background becomes important. This suggests that the delivered concentration from refinery emissions rarely reaches the threshold concentration without the addition of background levels. Background is likely to have the greatest influence in cases where its presence routinely causes the threshold to be exceeded. With the exception of BTEX, the (absolute) predicted impacts for these substances are negligible. However, in the case of BTEX, this indicates that the combined presence of benzene, toluene, ethylbenzene, and xylene in the ambient environment and from individual industries poses a threat to health.

Table 18: Spearman (rank) correlation coefficients for inputs values and predicted incidence calculated with distributions truncated at 99th percentile and using 50000 iterations. Correlation coefficients > |0.1| are highlighted. This data highlights the overwhelming importance of the C-R data in predicting incidence for most class 1 and class 2 substances. "N/A" indicates not applicable to predicting incidence.

Substance	***Atmospheric [OH]***	***Rate Constant***	***Background***	***C-R Value*** *Class 1: unit risk Class2: ED05*	***Mantel-Bryan Slope (Class 2)***
Class 1					
1,3-Butadiene	-2.6E-02	-1.1E-02	N/A	1.0	N/A
Benzene	2.6E-03	-2.1E-03	N/A	1.0	N/A
Ethylene Oxide (as ethylene metabolite)	-9.8E-03	-2.2E-02	N/A	1.0	N/A
Nickel (and its compounds)	-6.7E-04	N/A	N/A	1.0	N/A
PAHs	-2.7E-02	-2.4E-02	N/A	1.0	N/A
Formaldehyde	-3.3E-03	-1.5E-02	N/A	1.0	N/A
Class 2					
1,2,4-Trimethylbenzene	-7.0E-03	8.3E-04	7.2E-02	-7.0E-01	-0.59

Ammonia (Total)	-1.9E-03	2.8E-03	N/A	-7.1E-01	-0.65
BTEX	1.0 E-03		0.25[18]		-0.40
B		1.6 E-03	0.30	-0.27[19]	
T		1.3 E-03	0.22	-3.7E-02	
E		4.9 E-03	4.5 E-02	-1.6E-02	
X		1.5 E-04	1.7 E-02	-9.4E-02	
Cyclohexane	-1.8E-03	-3.8E-03	0.11	-0.45	-0.59
Dicyclopentadiene	-2.8E-03	-7.2E-03	N/A	-0.88	-0.41
Diethanolamine (and its salts)	-3.0E-03	-4.4E-03	N/A	-0.87	-0.44
Hydrogen sulphide	-8.6E-03	5.0E-03	4.2E-03	-0.93	-0.30
Isoprene	2.0E-03	-2.0E-03	7.9E-02	-0.37	-0.49
Mercury	-2.4E-03	N/A	4.0E-02	-0.92	0.01
Methanol	-6.0E-03	-4.3E-03	N/A	-0.59	-0.61
Methyl ethyl ketone	-5.0E-03	-3.5E-03	2.9E-02	-0.47	-0.62
Methyl isobutyl ketone	-3.8E-03	-1.2E-04	7.1E-03	-0.45	-0.60
Methyl tert-butyl ether	-4.6E-03	4.0E-03	N/A	-0.55	-0.64
Naphthalene	-8.0E-03	-2.4E-03	3.5E-02	-0.77	-0.55
n-Hexane	9.0E-04	5.6E-03	0.12	-0.74	-0.56
Phenol (and its salts)	2.2E-04	-2.5E-04	N/A	-0.83	-0.48
Propylene	-6.4E-03	-3.2E-03	0.15	-0.59	-0.62
Styrene	3.8E-03	8.1E-04	0.13	-0.60	-0.61
Sulphuric acid	-5.3E-03	1.1E-04	N/A	-0.95	-0.23
Vanadium (except when in an alloy) and its compounds	-3.2E-03	N/A	1.4E-02	-0.86	-0.46
Zinc (and its compounds)	3.1E-03	N/A	6.4E-02	-0.58	-0.73

Table 19 shows the correlation for class 3 substances, calculated after truncating distributions at 99th percentile.

Table 19: Correlation between age-group and outcome-specific specific annual average mortality coefficient values with predicted case incidence. The predicted case incidence is highly correlated

---

[18] The first correlation coefficient listed is for a weighted background concentration for the BTEX mixture. Each of the following coefficients is for the background concentrations of the individual components of the mixture.

[19] The toxicity value used for BTEX was a weighted combination of the toxicity values for B, T, E, X which depended on the relative amounts delivered to each zone around the refinery and thus changed with the geographic space around the refinery. The correlation coefficients shown here are for the toxicity assigned to each of the components, suggesting that the toxicity of benzene contributes most to the overall toxicity of the mixture. The correlation of the individual components appears to be low relative to other substances. This may be because BTEX is the only substance for which the toxicity depended on the zone, which also determined delivered concentration and population.

with the epidemiological coefficients in HEIDI II. This is expected, since there are few other variables that predict class 3 incidence which are described probabilistically, and the dose-response relationship is assumed linear. N/A is used in the table where risk coefficients do not apply (i.e., children are not considered to be at risk of mortality from air pollution; this assumption is routinely made since the epidemiological studies on which the coefficients are based did not include children).

Substance	Input (toxicity RR)	Population	Sample Rank Correlation	Spearman Rank Correlation
PM from NOx	*mortality*	child	N/A	N/A
		adult	0.96	0.96
		senior	0.96	0.95
	chronic bronchitis	child	N/A	N/A
		adult	0.98	0.98
		senior	0.97	0.97
	Asthma hospitalization	child	0.96	0.97
		adult	0.98	0.98
		senior	N/A	N/A
	Asthma ER visit	child	0.96	0.97
		adult	0.98	0.98
		senior	N/A	N/A
PM from SOx	*mortality*	child	N/A	N/A
		adult	0.96	0.96
		senior	0.96	0.95
	chronic bronchitis	child	N/A	N/A
		adult	0.98	0.98
		senior	0.97	0.97
	Asthma hospitalization	child	0.96	0.97
		adult	0.98	0.98
		senior	N/A	N/A
	Asthma ER visit	child	0.96	0.97
		adult	0.98	0.98
		senior	N/A	N/A
Primary PM	*mortality*	child	N/A	N/A
		adult	0.98	0.97
		senior	0.97	0.97
	chronic bronchitis	child	N/A	N/A
		adult	0.98	0.98
		senior	0.98	0.98
	Asthma hospitalization	child	0.97	0.98
		adult	0.99	0.99
		senior	N/A	N/A
	Asthma ER visit	child	0.97	0.98
		adult	0.99	0.99
		senior	N/A	N/A

Table 19 indicates high correlation between the relative risk values used for each population/outcome combination with predicted case incidence. This is expected due to the highly linear nature of the functions used to predict health impact from CACs.

The datapoints selected during a simulation can be plotted as scatterplots to complement the correlation coefficients data, as shown in these examples: Figure 22, Figure 23, and Figure 24.

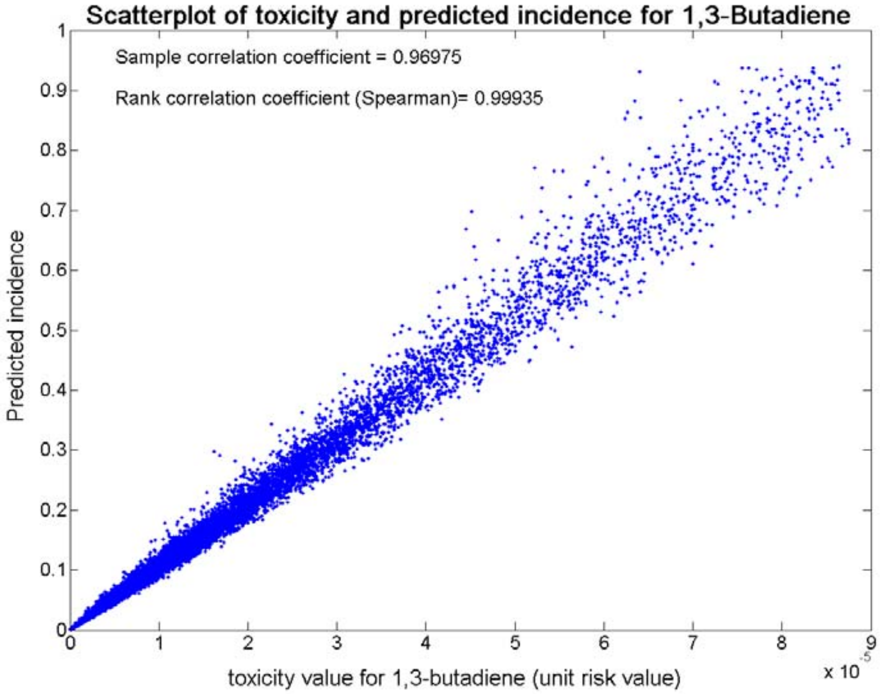


Figure 22: Sample scatterplot showing a strong linear relationship between C-R value and the predicted case incidence for 1,3-butadiene. This relationship was present for all class 1 substances.

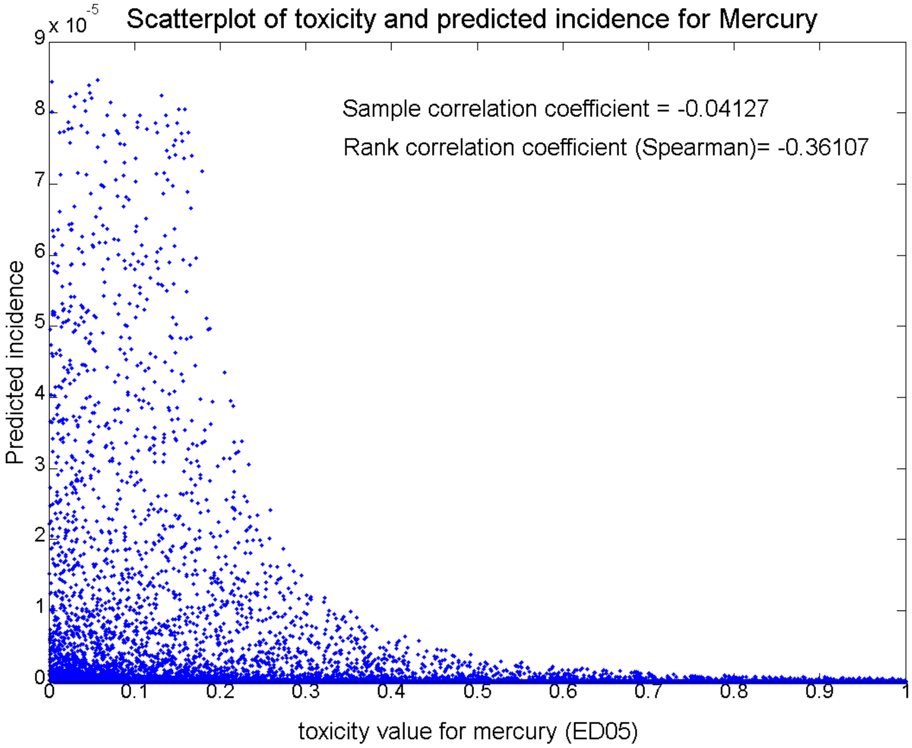


Figure 23: Sample scatterplot (for Mercury) showing the relationship typical of that observed between ED05 and predicted case incidence for class 2 substances where lower thresholds are more likely to result in higher predicated incidence, and incidence is predicted using a sublinear function .

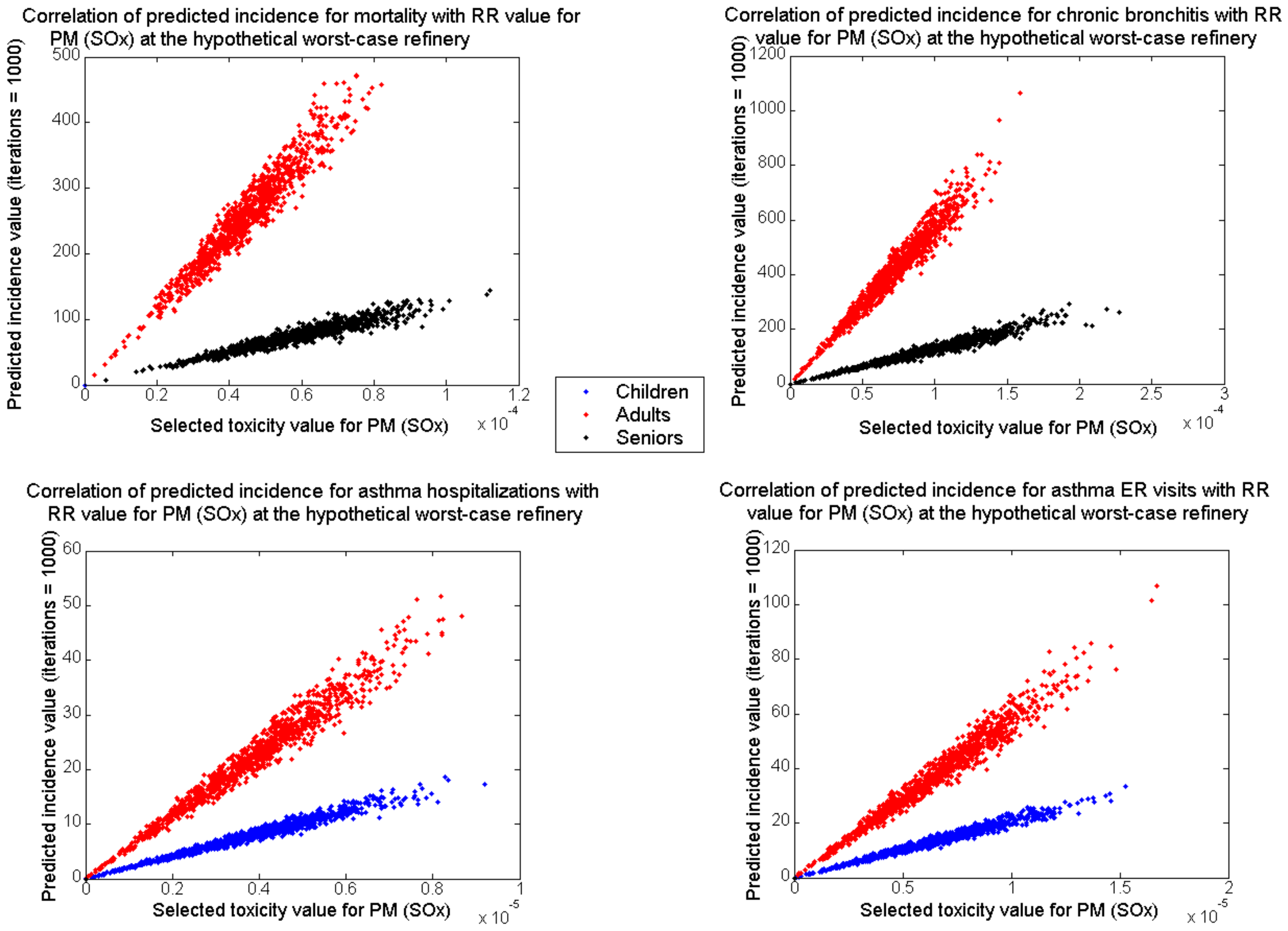


Figure 24: There is a clear linear relationship between C-R value and predicted case incidence for all class 3 substances, as illustrated in this figure. Predicted incidence is only modeled for outcomes that apply to each population (i.e., children are not considered to be at risk of mortality)

Other variables:

Predicted case incidence for class 3 substances are not mathematically related to [OH], k, or background concentrations, and class 1 substances are not mathematically related to background. Scatterplots generated for these combinations confirmed this (for purposes of validation) and are not presented here.

2.1.5 General conclusions about variables that are and are not important

Of the scenario variables under the user's control, the stack height appears to be most influential in determining delivered concentration, and the degree to which each stack height delivers a small or large concentration to a particular area around the refinery depends on the distance from the refinery. The stack height variable could potentially interact with the population variable, where a refinery with a 30 metre stack would be associated with a greater health impact if the population was mainly located at 25 km downwind than if the same number of people were clustered within 5-10 km of the refinery. Based on predictions using a 5 metre stack height, fugitive emissions are likely to be important for people living with 5-10 km of the refinery, but do not appear to affect the health of people living farther away.

The evidence presented above indicates that despite large uncertainty and variability in many input variables, predicted case incidence depends mainly on the concentration-response data selected for each substance. The uncertainty in background may play the most important role in predicting incidence for some class 2 substances, but the absolute difference in predicted case incidence in a population of 2.5 million is still less than one even if the background is being underpredicted at the 95th percentile of its uncertainty distribution. Additionally, the influence of even a minor overprediction of C-R values overwhelms the effect of background on predicted case incidence for any substance. There is an interaction effect between background levels and ED05 value for class 2 substances, where if the background is high and the threshold is low in a particular iteration of the model, the predicted case incidence is high. However, predicted case incidence values of note only appear to occur at extreme combinations for both, which would typically be unlikely to occur together in practice. The potential variability and uncertainty in k and OH is not important for predicting incident cases, thus these variables could be represented as point estimates in the model without any significant loss of information.

It appears that at certain combinations of variables at their 95th percentile levels, high levels of predicted case incidence can occur in the model for BTEX, Vanadium, HS, and Zn. The potential for predicted case incidence when all variables are simultaneously varying throughout the simulation will be investigated in the next chapter which provides the results of the Monte Carlo simulation. For now it is sufficient to note these substances for further investigation. For most class 2 substances, the predicted case incidence values are very low; well below a *de minimis* risk level of 10^{-6} even when values for at least two inputs are selected from the tails of their distributions – the most influential region.

2.1.5.1 Alternate model formulations?

Sensitivity analysis should assess not just the effect of varying individual input variable, but also the predictions of plausible alternate model formulations. This was partially addressed by changing the slope in the Mantel-Bryan formulation of the C-R for class 2 substances. There was a clear dependence of predicted case incidence on this value, suggesting that if this characterization of the dose-response relationship is inappropriate, the model predictions for predicted case incidence are also invalid. However, the HEIDI II model was developed as a screening tool. Under the assumption that all class 2 substances are subject to equivalent dose response relationships (just anchored at substance-specific ED05 values), use of a likely dose response relationship is probably sufficient to enable comparison of substances. The interaction between Mantel-Bryan slope and ED05 value was investigated and the results indicated that high values of predicted case incidence occurred only for slope values of 1 or less and that for slopes of 1.5 and greater, predicted case incidence was effectively zero across the range of potential ED05 values.

By analyzing three separate classes of substances with three distinct C-R characterizations, the model contains a type of internal sensitivity analysis. The general characteristics of model behaviour for each of the three classes can be compared to understand how different types of C-R characterizations affect output.

Table 20: Comparing how three different types of dose-response relationships (selected to represent different "types" of substances) affected the model output and behaviour

	Class 1	**Class 2**	**Class 3**
C-R characterization	Linear nonthreshold, depends on toxicological data (unit risk values)	Mantel-Bryan dose-probit formulation, depends on toxicological data, anchored at TC05 values	Linear nonthreshold, depends on epidemiological evidence (relative risk values)
Type of health outcome	Cancer	Systemic; range from mild (i.e., nasal irritation) to severe (i.e., CNS nuerotoxicity)	Mortality and respiratory morbidity
Magnitude range of emissions	~0-52 tonnes/year	~0-300 tonnes/year	~0-23000 tonnes/year
Magnitude range of predicted case incidence	~0.006 - 52	$< 10^{-14}$ – 0.1	2-539
Effect of background on predictions	None	Marginal for certain substances	None
Complexity of model	medium	complex	simple

2.1.6 Discussion

Truncating the output distributions in the global sensitivity analysis had the effect of eliminating the most extreme predictions from the distributions. A lognormal distribution was assumed for many of the variables' probability distributions. For the C-R data especially, the lognormal distributions were quite skewed. The result is that where high values of predicted case incidence are predicted (relative to the central estimates), the degree to which predicted case incidence becomes more extreme increases rapidly at the tail end of the distribution.

The predicted case incidence results presented in this chapter all resulted from inputs for a hypothetical worst-case scenario, where high emissions were being modeled for all substances – an unlikely scenario for any individual refinery. Most substances would be emitted at lower levels at any given refinery. In this way, the hypothetical refinery provides a conservative scenario, allowing assessment of impact at the highest likely emissions scenario. However, substance-specific results were independent, and the worst-case refinery was developed using the maximum emissions observed for each substance from across the refineries, so each substance-specific predicted incidence distribution could apply to at least one refinery in Canada. It might be useful to extend the validation to a "catastrophic" refinery scenario, where emissions are modeled as being significantly higher than what has been observed in practice.

The impact of stack height and photodegradation time on predicted case incidence is clear. The default scenario of 30 metres and 12 hours of degradation time is associated with the second-lowest predicted case incidence of all the possible stack height/photodegradation scenarios. The subsequent sensitivity analyses were all conducted at the default scenario. However, if the stack height (or "average stack height", which could be conceptualized as the combination of all onsite emissions from multiple stacks of various heights plus fugitive emissions) was lower than 30 metres, the predicted case incidence across all distributions would increase. For substances such as BTEX, HS, V, and Zn which were already identified as potentially having relatively higher predicted incidence at the tails of the probability distribution, this could be important at a particular refinery if the stack is actually lower than 30 metres.

The impact of stack height is important with respect to the physical distribution of the population around any given refinery. If the stack height in the model is changed, the location of maximum delivered concentration is also changed. The SAs provided above were done using the distribution of population close to the Imperial Sarnia refinery, which has the greatest number of people living within 25 km of any Canadian refinery. However, this distribution is not representative of all refineries. Policies for siting refineries can optimize (minimize) the impact of emissions on nearby densely populated areas through careful consideration of meterology, relative locations of the refinery and the population, and stack height. Improved mitigation should also be a component of risk management for refinery emissions.

The sensitivity analyses described above overlooked many factors which could influence the predictions of HEIDI II. SA was unable to assess the effect of uncertainty in the dispersion modeling results, the effect of variable meteorological conditions, or the cumulative health impact from simultaneous exposure to all refinery emissions.

HEIDI II assumed that airborne concentrations are representative of each individual's exposure, which is not realistic, since most Canadians spend most of their time indoors (Leech and Laporte 1996), which reduces their exposure to ambient airborne pollutants. As well, Canadians living near a refinery are unlikely to spend all of their time in the same location relative to the refinery, but will move further and closer in various directions as they travel to work and school, conduct errands, or meet social obligations. There is no adequate way to test the impact of neglecting “individual-level exposure” in HEIDI II.

2.1.6.1 So what should HEIDI II look like as a probabilistic model?

It appears that little information is likely gained in HEIDI II by retaining probability distributions (rather than point estimates) for variables such as k, [OH], and often, background levels for chemicals. The EPA points out that when deciding whether to use point values or probability density functions (PDFs) to characterize these types of variables, the risk communication process might be facilitated by focusing in on key variables and this is facilitated by quantifying only those variables using PDFs. However, they also point out that issues of perception and trust are important, and concerns exist that elimination of multiple small sources of variability would reduce the variability in the final output predictions (Office of Emergency and Remedial Response 2001). A key goal of NERAM’s original approach to HEIDI was to retain the maximum amount of transparency in the model. The run time of the model was not significantly increased by retaining the PDFs for these variables, and so there was no practical reason to use point estimates. Therefore, although the sensitivity analyses indicated that the variation in variables k, [OH], and sometimes background have little impact on the predicted case incidence, the PDFs for these variables were retained and allowed to fluctuate during the simulations.

To assess probable impacts, HEIDI should be run at the default, i.e. 30 metres and 12 hours. 30 metres is likely representative of most refineries and 12 hours is the best compromise across seasons in Canada. However, to assess worst-case possibilities, the model could be run with a 15 metre stack height and no photodegradation.

2.2 Model/Analytical Findings

2.2.1 Introduction

The sensitivity analyses conducted in the previous section provided some indication of specific substances which might be associated with predicted case incidence levels of concern, and the uncertain or variable inputs that would be related to the high predictions. In the following probabilistic analysis, Monte Carlo simulations were run with a high number of iterations to predict distributions of incidence for all substances. Each of the uncertain/variable inputs was allowed to vary simultaneously according to its selected probability distribution (See Appendix C). Distributions of predicted case incidence (or DALY years, if using DALY weights) allow comparison of the possible range of potential health impacts due to emissions from Canadian refineries, given both uncertainty and variability in the input data. The upper tails of the distributions could be thought of as describing a conservative scenario (given the amount of uncertainty in some inputs). This might include a sensitive population (since uncertainty in C-R values appears to be particularly influential), or where unusually high levels of background concentrations exist, or both. The distributions of predicted case incidence are first presented for the hypothetical worst-case refinery default scenario. Some predictions of annual incidence based on real emissions from Canadian refineries are also provided. These should be interpreted with caution and used mainly to compare substances with each other, as HEIDI II was developed as a screening tool and was not intended to be used to predict absolute incidence from exposure near specific refineries.

The original design for HEIDI II was to compare predicted health impacts based on a measure such as DALYs, which accounts for years and quality of life lost due to disease or disability, allowing comparison of endpoints with varying severity. However, most of the testing and validation of the model was carried out using predicted incidence[20]. The current operationalization of DALY weights in HEIDI II is fairly unsophisticated: they are expressed in terms of "DALYs per person" averaged over a population assumed to be equivalent to the Canadian population. The health impacts predicted by the model can be expressed in three ways: (i) predicted incidence, (ii)

---

[20] For reasons described in Chapter 3 - Methods ("Sensitivity Analysis" section).

predicted DALYs using a set of "simple DALY" weights which differentiate health conditions only into three levels of severity, and (iii) predicted DALYs using a set of "complex DALY" weights which assigns a distinct weight to each disease state. The different methods of predicting health impact allow comparison of model rankings generated using DALYs vs. those using predicted case incidence.

HEIDI II is ultimately intended to be a prioritization tool; the most relevant output of HEIDI II is a rank order intended to identify the substances having the highest impact on populations living close to refineries in Canada. Various approaches to ranking probabilistic outputs are explored in an attempt to determine which approaches work best and whether there is any consistency across refineries in predictions about which substances should be highest priority for reduction.

Unless otherwise specified, all simulations were run using the default stack height and photodegradation time parameters (30 metres and 12 hours).

2.2.2 Predicted case incidence at the hypothetical worst-case refinery

2.2.2.1 Classes 1 and 2

Frequency distributions for predicted case incidence were created using Monte Carlo simulations with 100 000 iterations, and the proportion of the cumulative frequency distribution curve below a lifetime (70 years) *de minimis* risk level of 10^{-6} was identified. For the purpose of creating legible plots, values above the 99th percentile were discarded during plotting.

Figure 25 provides an example cumulative probability distribution for predicted case incidence of lung cancer from exposure to Nickel at the hypothetical worst-case refinery. For nickel in this worst-case scenario, about 40% of the predicted case incidence values that emerged from the Monte Carlo simulation were above the *de minimis* risk level of 10^{-6}, suggesting a high probability that this scenario is associated with more cancer than is typically deemed acceptable by many regulatory agencies. The upper tail of the distribution suggests that there is a small chance that as many as 100 cases of lung cancer could be predicted per year within 25 km of the hypothetical worst-case refinery by emitted nickel.

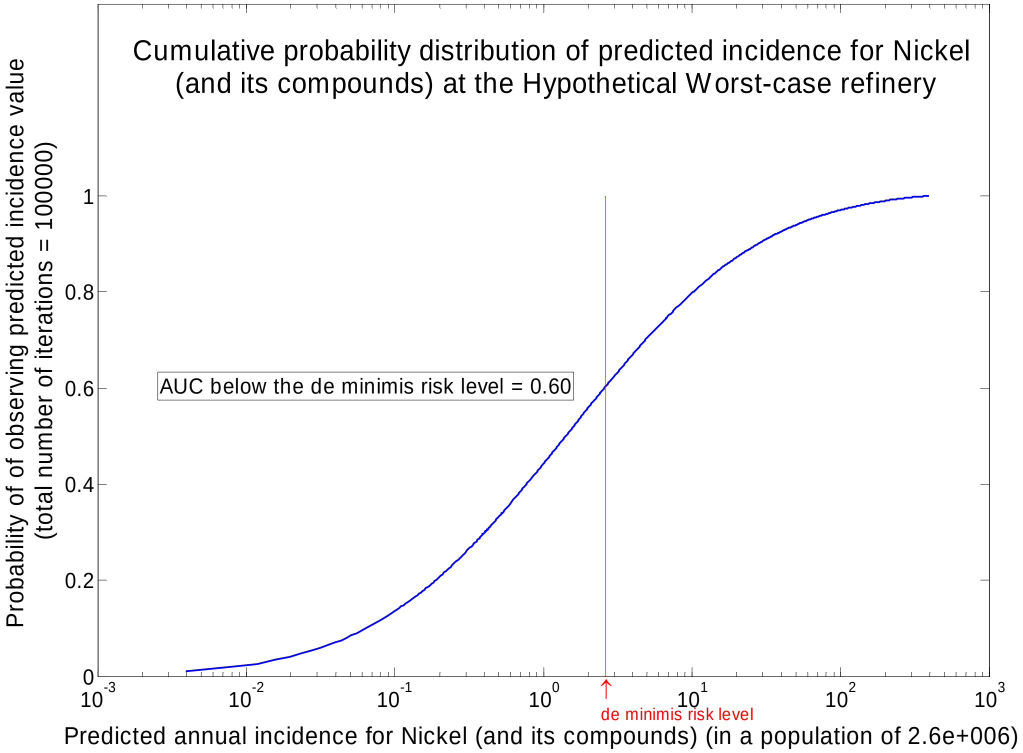


Figure 25: Cumulative probability distribution for predicted case incidence of lung cancer from Nickel (and compounds) at the hypothetical worst-case refinery. AUC = area under the curve, where total area equals 1.

Table 21 summarizes the percentage of the cumulative probability distribution exceeding the *de minimis* risk levels for each emitted substance in the default hypothetical worst-case scenario. The relevant human outcomes for those with the highest values are disparate, including lung cancer, CNS neurotoxicity, and nose irritation. It is difficult to compare chemicals on the basis of such diverse types of health outcomes; this table highlights the disadvantages of not including quality of life measures in determining health impact from exposure to diverse chemicals. Incidence above 10^{-6} was sometimes predicted during the simulations for substances related to serious health impacts such as cancer and CNS neurotoxicity (i.e., Ni, PAH, BTEX). This indicates that analysis at individual refineries is important to determine whether high potential level of risk exists with “real” emissions/population distribution combinations.

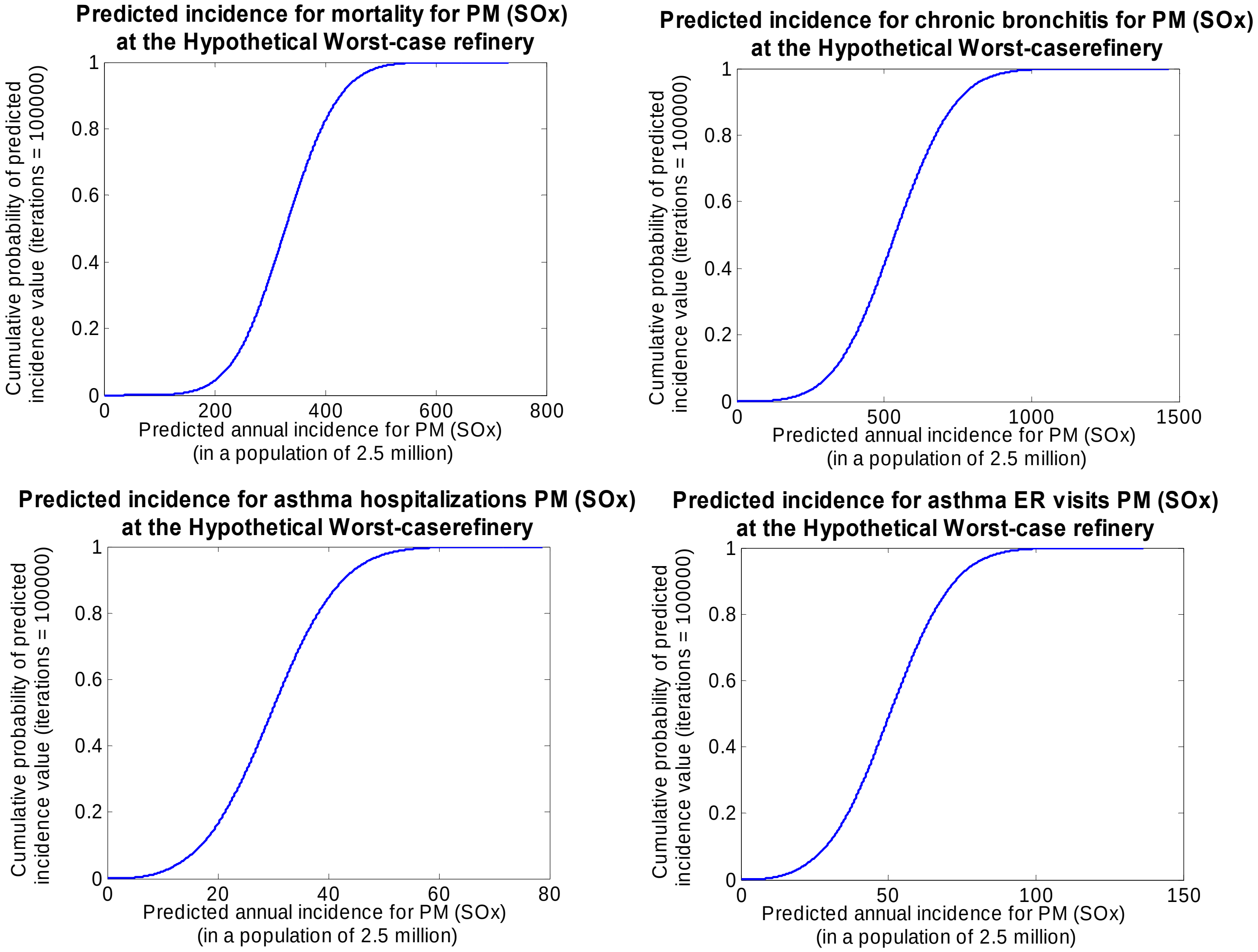
Table 21 also provides a sense of which substances were not predicted to be associated with any risk above the *de minimis* level at the hypothetical worst-case refinery. Many substances were associated with zero predicted case incidence in all simulations, including ammonia, isoprene, mercury, methanol, MEK, MIBK, MTBE, and phenol. This suggests that refinery emissions of these substances are not likely to be a health concern at any refinery in Canada. Depending on the substance, this is likely related to either very low emissions (i.e., mercury) or very low toxicity (i.e., MIBK) or a combination of both.

Table 21: Proportion of predicted case incidence above the 10^{-6} *de minimis* level for all class 1 and class 2 substances for the hypothetical worst-case refinery. This tabulation in conjunction with the relevant human outcomes provides a sense of why DALYs (or some sort of weighting scheme) is useful for prioritization of risk. Values greater than 0 are highlighted

Substance	**Proportion of predicted case incidence above 10^{-6}**	**Relevant outcome (for reference)**
Class 1		
1,3-Butadiene	0.00	Leukemia
Benzene	0.00	Leukemia
Ethylene (as 5% ethylene oxide)	0.00	Leukemia
Nickel	0.40	Lung Cancer
PAH (using Benzo[a] pyrene)	0.38	Lung Cancer
Formaldehyde	0.00	Nasal and lung cancer
Class 2		
1,2,4-trimethylbenzene	0.01	Moderate anemia
Ammonia	0.00	Skin and nose irritation
BTEX	0.20	CNS neurotoxicity
Cyclohexane	0.00	Reduced bodyweight
Dicyclopentadiene	0.00	Chronic renal disease
Diethanolamine	0.00	Throat irritation
Hydrogen sulphide	0.03	Nose irritation
Isoprene	0.00	Benign lung tumours
Mercury	0.00	Severe CNS neurotoxicity
Methanol	0.00	Physical teratogenesis
MEK	0.00	Developmental retardation
MIBK	0.00	Developmental retardation
MTBE	0.00	PNS neurotoxicity
Naphthalene	0.00	Benign lung tumors
n-hexane	0.00	PNS neurotoxicity
Phenol	0.00	Mild CNS neurotoxicity
Propylene	0.00	Benign nasal & upper airway tumours
Styrene	0.00	Mild developmental retardation
Sulphuric Acid	0.32	Benign nasal and upper airway tumors
Vanadium	0.46	Nasal and upper airway irritation
Zinc	0.00	Moderate anemia

2.2.2.2 Class 3 substances

Recall that the predictions of incidence for class 3 substances are different by virtue of (i) how they were generated (no accounting for photodegradation and the interdependence of concentrations of secondary PM on primary PM concentrations), and (ii) the type of C-R data used to predict incidence. For class 3 substances, epidemiological relative risk values for four separate outcomes per substances was used, whereas toxicity of class 1 and class 2 substances was based on unit risk or ED05 values which were estimated for the most critical endpoint, and often based on toxicological experiments on animals. The general characteristics of the predictions are also distinct. In particular, 100% of the cumulative probability distributions for predicted case incidence for class 3 substances is above the *de minimis* risk level for all outcomes, and this measure therefore does not distinguish the relative potential impact of SO_x, NO_x, and primary PM. Cumulative probability distributions are presented in Figure 26, Figure 27, and Figure 28 for predicted case incidence from exposure to PM from SO_x, PM from NO_x, and primary PM at the hypothetical refinery. Results for each of the four health outcomes considered by HEIDI II are included.


Predicted incidence for mortality for PM (SOx) at the Hypothetical Worst-case refinery

Predicted incidence for chronic bronchitis for PM (SOx) at the Hypothetical Worst-caserefinery

Predicted incidence for asthma hospitalizations PM (SOx) at the Hypothetical Worst-caserefinery

Predicted incidence for asthma ER visits PM (SOx) at the Hypothetical Worst-case refinery

Figure 26: Cumulative probability for predicted case incidence of each outcome associated with exposure to $PM_{2.5}$ from SO_x

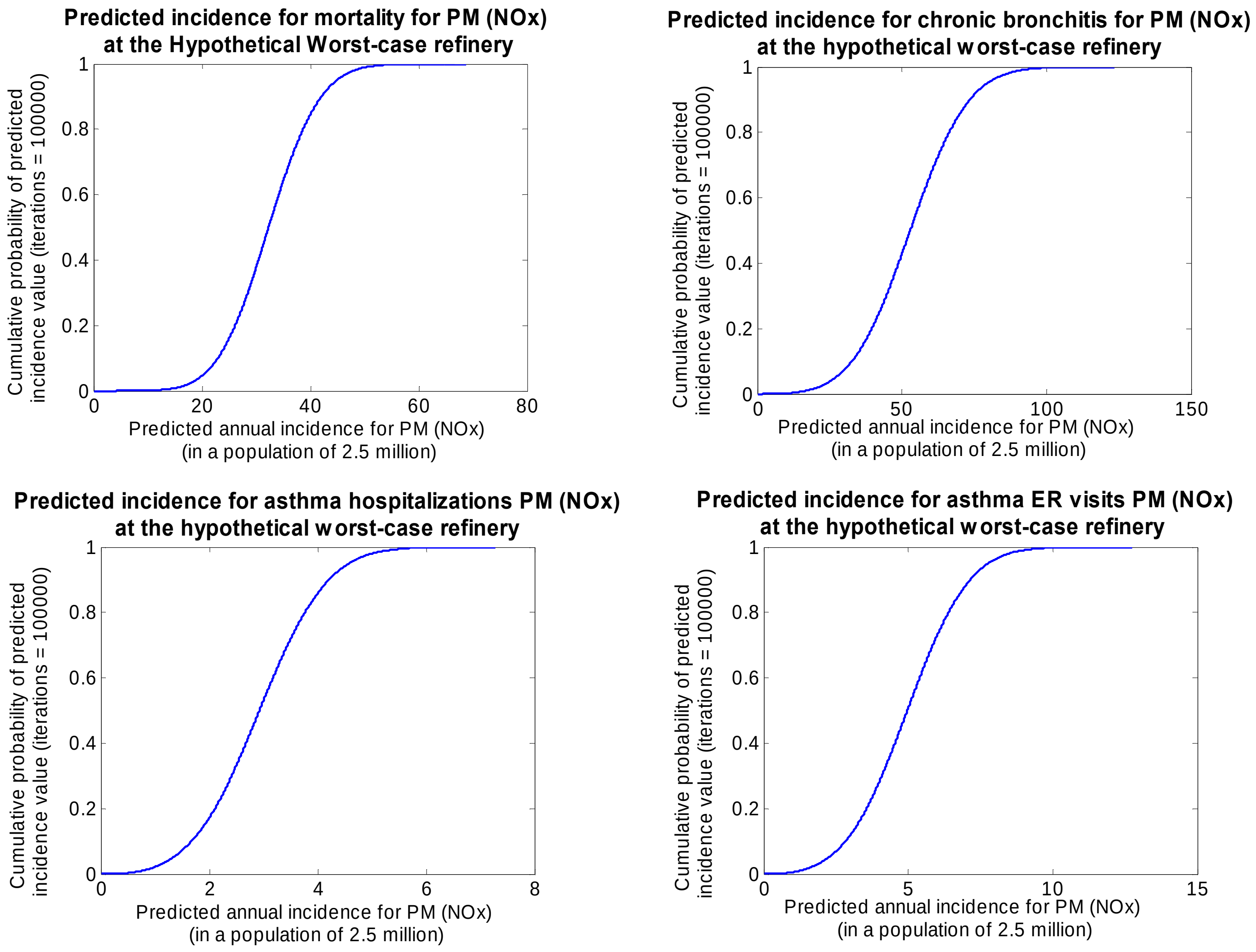
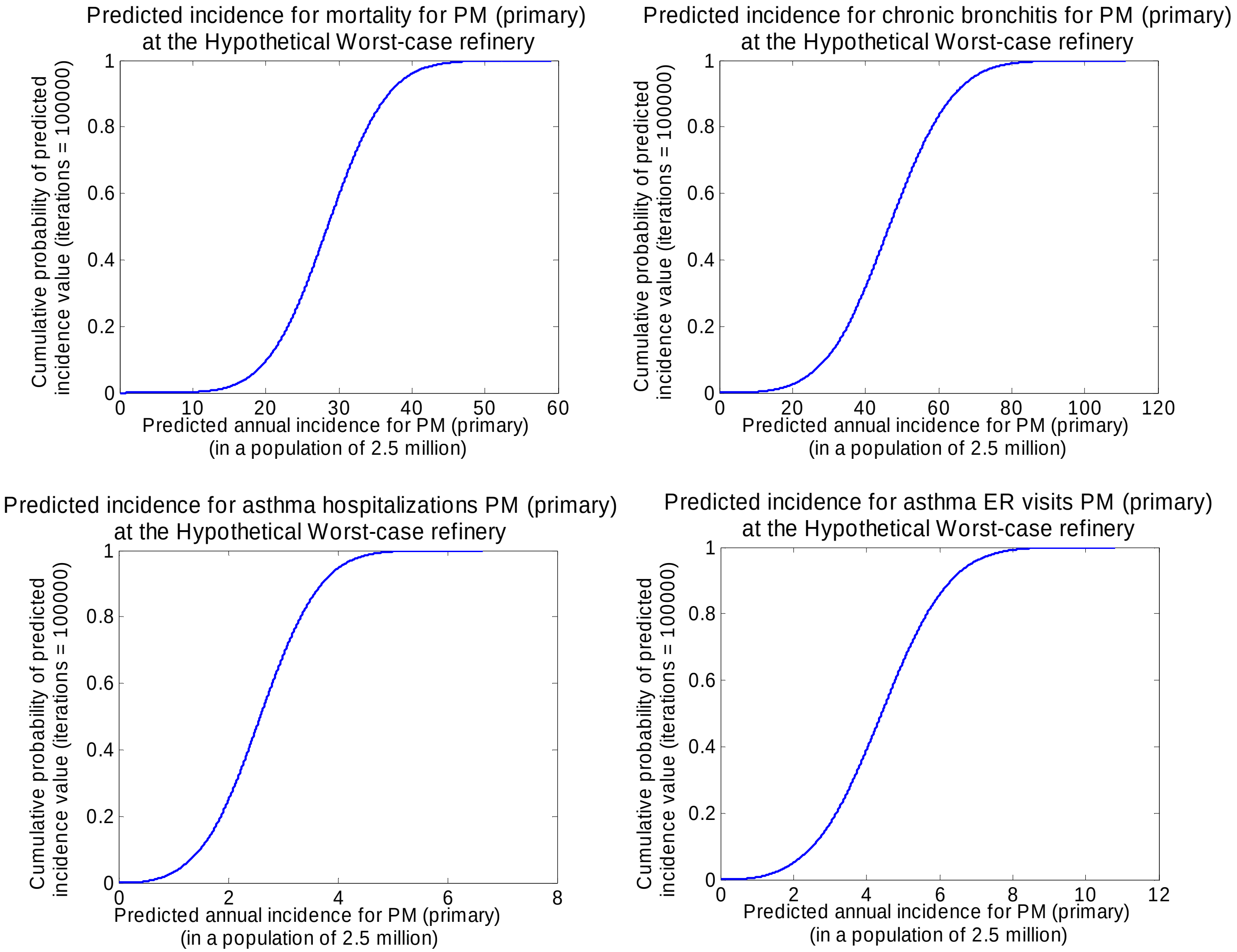


Figure 27: Cumulative probability for predicted case incidence of each outcome associated with exposure to $PM_{2.5}$ from NO_x


Predicted incidence for mortality for PM (primary) at the Hypothetical Worst-case refinery

Predicted incidence for chronic bronchitis for PM (primary) at the Hypothetical Worst-case refinery

Predicted incidence for asthma hospitalizations PM (primary) at the Hypothetical Worst-case refinery

Predicted incidence for asthma ER visits PM (primary) at the Hypothetical Worst-case refinery

Figure 28: Cumulative probability for predicted case incidence of each outcome associated with exposure to primary $PM_{2.5}$

The probability distributions for predicted case incidence from PM were normal in character. These cumulative distribution functions (CDFs) suggest that significant morbidity and mortality may be associated with PM emissions from Canadian refineries at nearby locations. Table 22 describes the distributions predicted for the hypothetical refinery.

Table 22: Predicted case incidence for mortality, chronic bronchitis, asthma hospitalization and asthma ER visits for the hypothetical worst-case refinery (population ~2.5 million).

Substance	**5th percentile**	**Mean**	**95th percentile**	**Mean (predicted) cases per person annually**
Refinery: Hypothetical Worst-Case (population = 2 612 269)				
PM from SOx - Mortality	35	350	660	1.3E-04
Chronic bronchitis	71	710	1300	2.7E-04
Asthma hospitalizations	3.8	38	72	1.4E-05
Asthma ER visits	6.5	65	120	2.5E-05
PM from NOx - Mortality	3.3	33	63	1.3E-05
Chronic bronchitis	6.5	65	120	2.5E-05
Asthma hospitalizations	0.4	3.8	7.2	1.5E-06
Asthma ER visits	0.6	6.5	12	2.5E-06
Primary PM - Mortality	2.8	28	53	1.1E-05
Chronic bronchitis	5.4	54	100	2.1E-05
Asthma hospitalizations	0.3	3.2	6.2	1.2E-06
Asthma ER visits	0.6	5.5	11	2.1E-06

For each outcome and PM combination, the mean rate of annual predicted case incidence exceeded 10^{-6}. Exposure to SO_x is associated with the highest rates of predicted case incidence. The upper 95th percentiles of predicted case incidence are associated with exceptionally high numbers of predicted cases of mortality and respiratory morbidity.

These probability distributions were created under the assumption of no threshold for health impact from PM. To date, large-scale studies have not been able to identify a specific threshold for the health impacts of $PM_{2.5}$, but the possible existence of such a threshold is still contentious (World Health Organization (WHO) 2004).

It is not practical to compare the exposures to CACs from refineries to any kind of "policy-based" threshold[21]. In Canada, Canada-wide standards are set at 30 μg/m^3, and apply to ambient levels of $PM_{2.5}$ contributed from all sources. Inspection of the delivered concentrations predicted by HEIDI II reveals that the concentration of PM delivered by

---

[21] Because the dose-response function for CACs is linear, the effect of introducing any kind of threshold into the model is easily predicted: it reduces the predicted case incidence by the amount predicted using the threshold alone. For example, applying an arbitrarily selected threshold of 1μg/m^3 has the expected effect of narrowing and shifting the cumulative probability distributions for predicted case incidence to the left.

the refineries to any given quadrant around them is predicted not to reach even half that value.

2.2.3 Predicted case incidence at actual refineries in Canada

The actual emissions from "real" Canadian refineries differ at each location in terms of which substances are emitted, and in what quantities. As well, the number and geographic dispersion of people potentially affected differs at each refinery. Although (as the disclaimer prior to the methods chapter explains) predicted case incidence cannot be taken at a true estimate of the annual number of cases at each refinery, comparing the distributions of predicted case incidence values for different emissions still facilitates identification of (i) which substances are typically of concern at refineries across Canada using data relevant for individual communities, (ii) which refineries emit multiple substances of concern, and (iii) whether there is a meaningful difference between predicted incidence values that are associated with adjacent ranks.

2.2.3.1 Class 1 and 2 substances

Table 23 indicates that predictions of incidence above the *de minimis* risk level were consistently associated with a limited set of substances. The table identifies only emitted substances where a portion of the cumulative probability distribution exceeded the *de minimis* risk level of 10^{-6} at each refinery. These include PAH, Nickel, BTEX, Sulphuric acid, hydrogen sulphide, and vanadium. The relevant human health outcomes for each of these substances are disparate, encompassing lung cancer, CNS neurotoxicity, nose irritation and benign nasal and upper airway tumors, and upper airway irritation. These outcomes are clearly not directly comparable.

The Imperial Sarnia refinery is associated with predictions of incidence above the *de minimis* level for the highest number of substances (6). This may be of particular concern since there are other refineries located nearby, all of which contribute to exposure of the same population. This includes the Shell Sarnia refinery, which emits four substances of concern. The Petro Canada refinery in Montreal also has four emissions of concern, while the rest have either three, two, or one.

Table 23: Class 1 and class 2 substances emitted from each refinery for which the proportion of predicted case incidence above the *de minimis* risk level was greater than zero. A complete list including all substances and all refineries can be found in Appendix I.

Refinery	Substance	Proportion of predicted case incidence above 10^{-6}	Relevant outcome (for reference)
Chevron-Burnaby	BTEX	0.20	CNS neurotoxicity
	Vanadium	0.14	Nasal and upper airway irriatation
Consumer's Co-operative	BTEX	0.10	CNS neurotoxicity
	Hydrogen Sulphide	0.04	Nose irritation
Prince George	BTEX	0.09	CNS neurotoxicity
Imperial Dartmouth	BTEX	0.09	CNS neurotoxicity
	Sulphuric Acid	0.22	Benign nasal and upper airway tumors
Imperial Nanticoke	BTEX	0.09	CNS neurotoxicity
	Hydrogen Sulphide	0.01	Nose irritation
	Sulphuric Acid	0.17	Benign nasal and upper airway tumors
Imperial Sarnia	Nickel	0.50	Lung cancer
	PAH (using Benzo[a] pyrene)	0.08	Lung cancer
	BTEX	0.09	CNS neurotoxicity
	Hydrogen Sulphide	0.01	Nose irritation
	Sulphuric Acid	0.39	Benign nasal and upper airway tumors
	Vanadium	0.55	Nasal and upper airway irriatation
Imperial Strathcona	BTEX	0.20	CNS neurotoxicity
	Sulphuric Acid	0.19	Benign nasal and upper airway tumors
Irving Saint John	Nickel	0.01	Lung cancer
	BTEX	0.09	CNS neurotoxicity
North Atlantic Refining	Nickel	0.36	Lung cancer
	BTEX	0.10	CNS neurotoxicity
	Vanadium	0.44	nasal and upper airway irritation
Nova Corunna	BTEX	0.10	CNS neurotoxicity
	Sulphuric Acid	0.24	Benign nasal and upper airway tumors
Parkland Bowden	BTEX	0.09	CNS neurotoxicity
Petro-Canada - Edmonton	BTEX	0.20	CNS neurotoxicity
	Sulphuric Acid	0.14	Benign nasal and upper airway tumors
	Vanadium	0.01	Nasal and upper airway irriatation
Petro-Canada - Mississauga	BTEX	0.09	CNS neurotoxicity
	Sulphuric Acid	0.05	Benign nasal and upper airway tumors
Petro-Canada - Montreal	Nickel	0.40	Lung cancer
	BTEX	0.20	CNS neurotoxicity
	Sulphuric Acid	0.16	Benign nasal and upper airway tumors
	Vanadium	0.19	Nasal and upper airway

			irritation
Petro-Canada - Oakville	PAH (using Benzo[a] pyrene)	0.34	Lung cancer
	BTEX	0.20	CNS neurotoxicity
	Sulphuric Acid	0.20	Benign nasal and upper airway tumors
	Vanadium	0.12	Nasal and upper airway irritation
Shell-Montreal	BTEX	0.20	CNS neurotoxicity
	Sulphuric Acid	0.16	Benign nasal and upper airway tumors
Shell Sarnia	Nickel	0.22	Lung Cancer
	BTEX	0.10	CNS neurotoxicity
	Sulphuric Acid	0.38	Benign nasal and upper airway tumors
	Vanadium	0.33	Nasal and upper airway irritation
Shell Scotford	PAH (using Benzo[a] pyrene)	0.04	Lung Cancer
	BTEX	0.20	CNS neurotoxicity
Sunoco	BTEX	0.09	CNS neurotoxicity
	Sulphuric Acid	0.17	Benign nasal and upper airway tumors
Ultramar St. Romuald	BTEX	0.09	CNS neurotoxicity
	Sulphuric Acid	0.07	Benign nasal and upper airway tumors

2.2.3.2 Class 3 substances

Predicted case incidence for class 3 substances was determined for four separate outcomes per substance. For brevity, results are presented in Table 24 only for the Shell Montreal refinery, which was associated with the highest total predicted cases overall, and the Shell Scotford refinery, which was among the refineries with the lowest predicted case incidence from PM emissions. These results suggest that a significant health impact is associated with PM emissions from some refineries in Canada. They also suggest that total number of cases predicted is heavily influenced by the total population exposed: while there are about 2.6 million people living within 25 km of the Montreal refinery, there are only ~62 000 people living near the Scotford refinery. The predicted incidence per person may be a better metric that total incidence to assess the implications of emissions at any particular site. A table containing predictions for all refineries can be found in Appendix J.

Table 24: Predicted case incidence from exposure to primary and secondary PM at the Shell Montreal refinery (where highest impact was predicted) and Shell Scotford refinery (where lowest impacts were predicted)

Substance	**5th percentile**	**Mean**	**95th percentile**	**Mean (predicted) cases per person annually**
Refinery: Shell Montreal (population = 2 612 269)				
PM from SOx - Mortality	8.7	87	165	3.3E-05
Chronic bronchitis	16	160	310	6.2E-05
Asthma hospitalizations	1.1	11	21	4.3E-06
Asthma ER visits	1.6	17	31	6.3E-06
PM from NOx - Mortality	2.5	25	47	9.4E-06
Chronic bronchitis	4.5	45	85	1.7E-05
Asthma hospitalizations	0.3	2.6	5.0	1.0E-06
Asthma ER visits	0.4	4.4	8.4	1.7E-06
Primary PM - Mortality	1.5	15	28	5.7E-06
Chronic bronchitis	2.5	26	48	9.6E-06
Asthma hospitalizations	0.2	1.5	2.9	5.8E-07
Asthma ER visits	0.3	2.6	4.9	9.9E-07
Refinery: Shell Scotford (population = 31 231)				
PM from SOx - Mortality	0.0	0.0	0.1	8.8E-07
Chronic bronchitis	0.0	0.0	0.1	1.6E-06
Asthma hospitalizations	0.0	0.0	0.0	1.2E-07
Asthma ER visits	0.0	0.0	0.0	1.8E-07
PM from NOx - Mortality	0.0	0.1	0.2	2.5E-06
Chronic bronchitis	0.0	0.2	0.3	5.0E-06
Asthma hospitalizations	0.0	0.0	0.0	3.1E-07
Asthma ER visits	0.0	0.0	0.0	5.5E-07
Primary PM - Mortality	0.0	0.0	0.0	3.1E-07
Chronic bronchitis	0.0	0.0	0.0	5.5E-07
Asthma hospitalizations	0.0	0.0	0.0	4.0E-08
Asthma ER visits	0.0	0.0	0.0	6.2E-08

Large differences in predicted cases per million people are observed when comparing across refineries and likely stem mainly from the amount of emissions at each individual refinery. However, the geographic distribution of people relative to the refinery is also important. The northeast quadrants are subject to the highest predicted exposures as a result of the generic meteorology scenario used throughout HEIDI. As Table 25 shows, the Imperial Sarnia refinery seems to have especially high rates of annual predicted case incidence for all outcomes – as high as one in 1000 for mortality from SO_x. Imperial Sarnia has the highest PM emissions of all the Canadian refineries, and as Figure 29 shows, the majority of the population density is located to the northeast of the refinery, the quadrant that would be subject to the highest exposure given the meteorology used (which includes winds predominantly from the southwest).

Table 25: Predicted case incidence – annual rates per person at the Imperial Sarnia Refinery

Outcome	*PM from SOx*	*PM from NOx*	*Primary PM*
Mortality	1.0E-04	1.1E-05	2.0E-05
Chronic bronchitis	2.0E-04	2.0E-05	3.7E-05
Asthma hospitalizations	1.2E-05	1.2E-06	2.2E-06
Asthma ER visits	2.0E-05	2.0E-06	4.2E-06

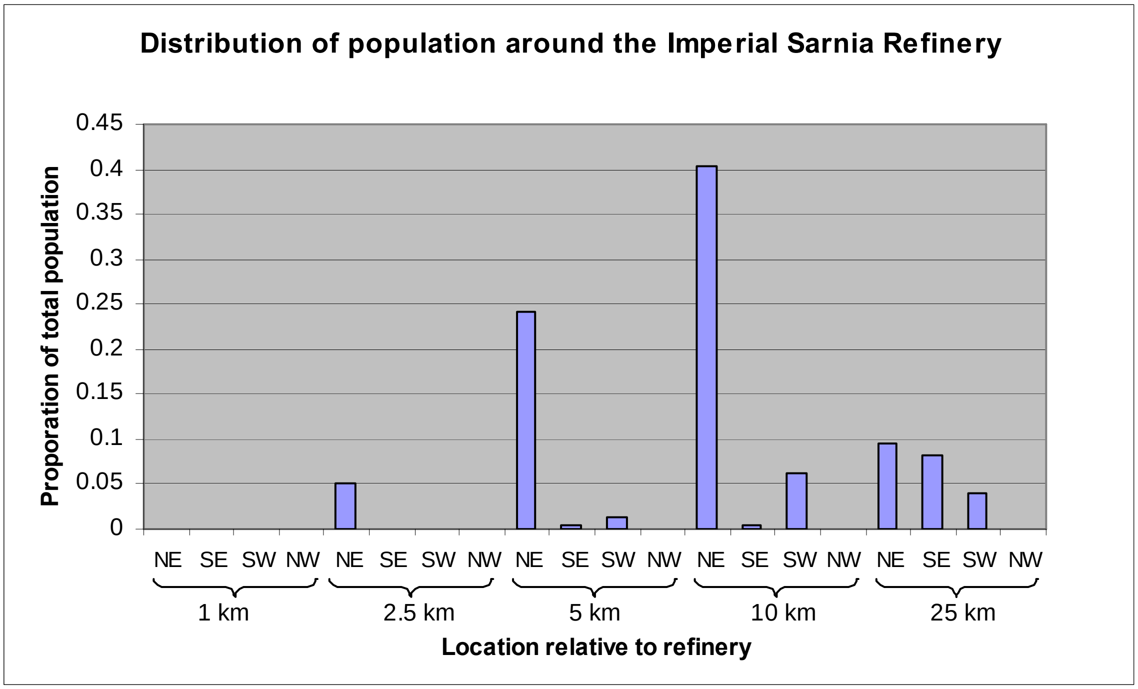


Figure 29: Distribution of population in each of 20 "quadrants" around the Imperial Sarnia Refinery

Different demographic composition of the populations in each area could also affect predicted rates of incidence - high rates would be observed where more of the population is “at-risk” (i.e, a greater proportion of adults and seniors relative to children puts a greater proportion of the population at risk for mortality from PM exposure, which HEIDI II assumes to be relevant for only adults and seniors).

2.2.4 HEIDI II as a Ranking Tool

HEIDI II was developed as a screening tool and is intended to be used to identify those refinery emissions associated with the greatest health impacts. The output of the deterministic model was a rank ordering of substances where a high rank indicated greater health impacts. The ranking information, however, did not provide any information about the absolute difference between impacts of different substances – an issue which may be important for policy decisions.

As part of the Monte Carlo simulation, a rank was generated at each iteration for each substance, allowing construction of a probability distribution for "rank" for each emission from the refinery. The distributions of rank provide insight about the level of separation that exists between ranked substances – information that is not available when using the ranks from the deterministic version of HEIDI II. However, there are some difficulties in interpreting probabilistically generated ranks when there is overlap in the CDFs for the health impact outputs.

2.2.4.1 Ranks within classes – Hypothetical Refinery

Because predicted case incidence was calculated differently for each class of substances (i.e., as a result of the concentration-response functions used), ranks are most valid when examined on a within-class basis.

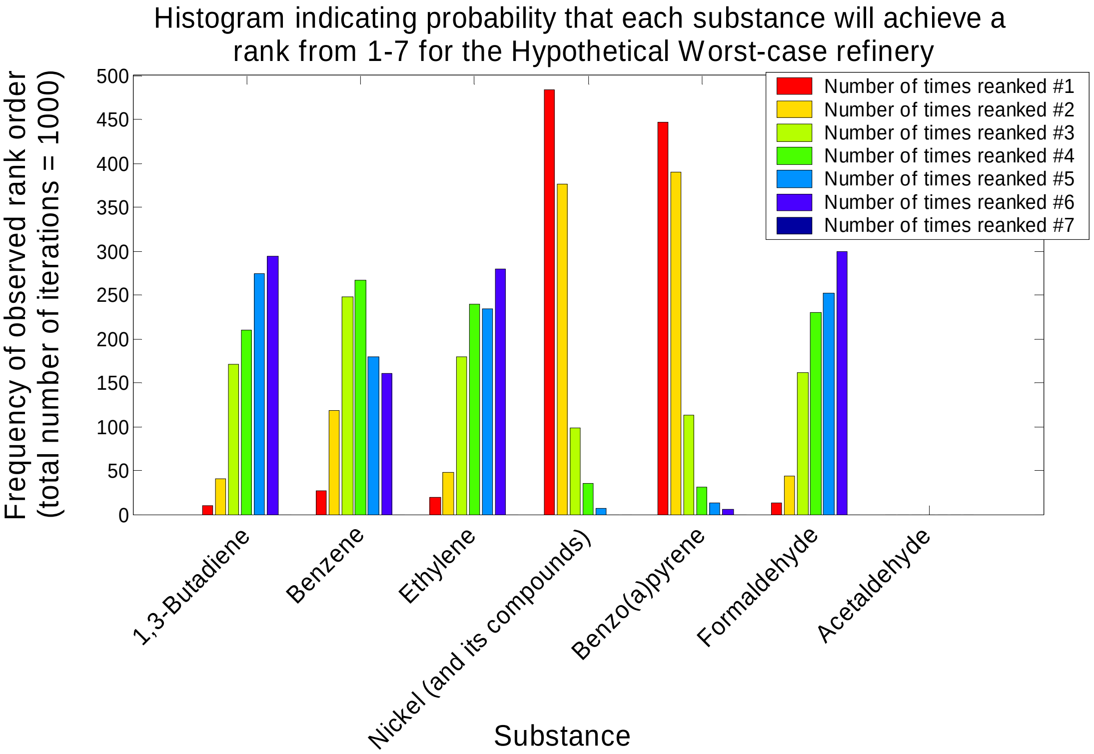


Figure 30: Probability that class 1 substances will be assigned a rank from 1-7 based on predicted incident cases. Nickel and PAH are most likely to be ranked as having the greatest health impact .

Figure 30 shows the distribution of ranks for class 1 substances based on predicted case incidence, showing how often each of the seven class 1 substances was assigned each possible rank (from 1-7). (Although acetaldehyde is included in the figure, no emissions were actually recorded for acetaldehyde at any Canadian refineries, so there was no data available to rank.) The figure clearly identifies Nickel and PAH as being priorities based on predicted health incidence, as they are most frequently ranked as the first or second priority among class 1 substances. Identifying a predominant rank for 1,2-butadiene, ethylene, and formaldehyde is particularly difficult from this figure, as they all appear to fall within the same level of priority. This suggests that there is probably not much distinction between the predicted case incidence probability distributions for these substances.

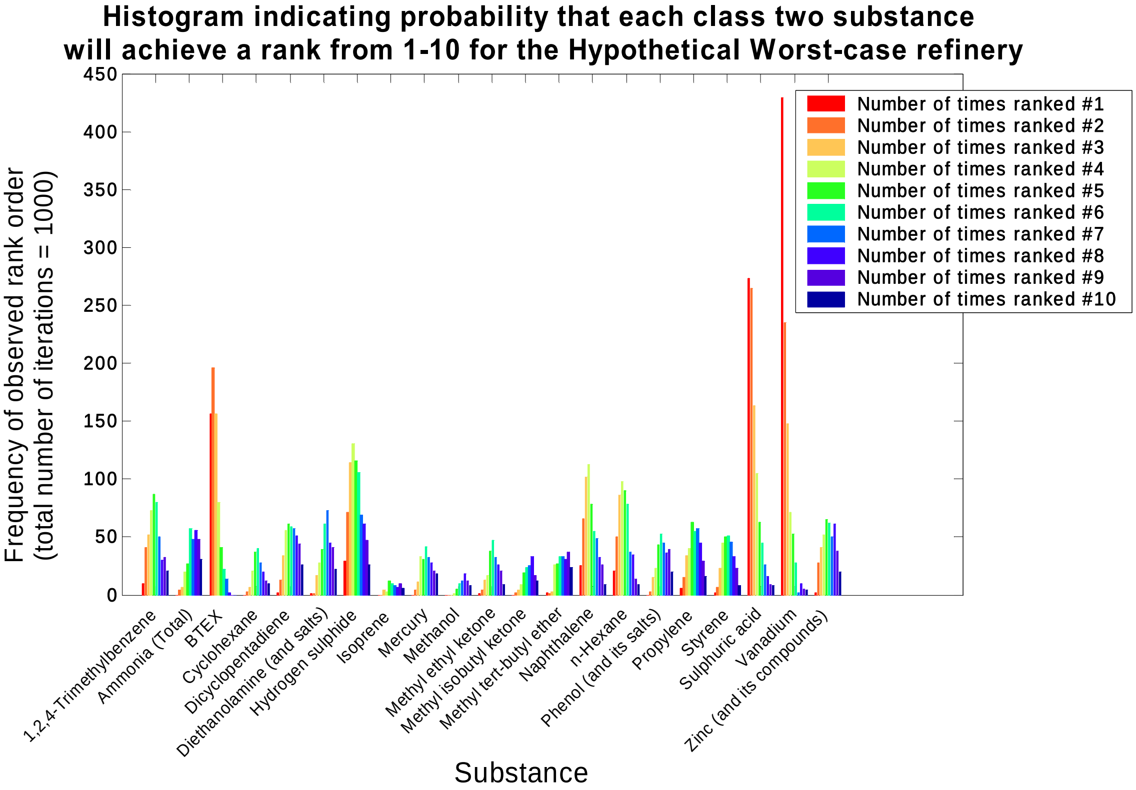


Figure 31: Probability that class 2 substances will be assigned a rank from 1-10 based on predicted incident cases. Vanadium is usually highest priority, followed by sulphuric acid and BTEX (ranks 11-25 are omitted for clarity).

Figure 31 indicates that of the class 2 substances, Vanadium, Sulphuric Acid, and BTEX are most often accorded the highest priority based on predicted case incidence. In this figure only the top ten ranks are presented for clarity, although there are a possible 25 ranks. As a result, the total frequency across all rank orders is unequal for each substance. Those substances with “short” frequency bars for all ranks are thus primarily associated with ranks of 10 or higher. Including all 25 ranks indicates that most often the ranks greater than 10 are ranks of 25, which would result from zero predicted case incidence (and could therefore occur coincidentally among multiple substances in any iteration).

These figures showing probabilistic ranks provides immediate visual information about which substances are generally related to higher predicted case incidence relative to the others, and about the relative difficulty of distinguishing priority orders for substances. These figures may be a useful way to present the results from HEIDI II to policy makers in a way that characterizes the uncertainty in the predictions.

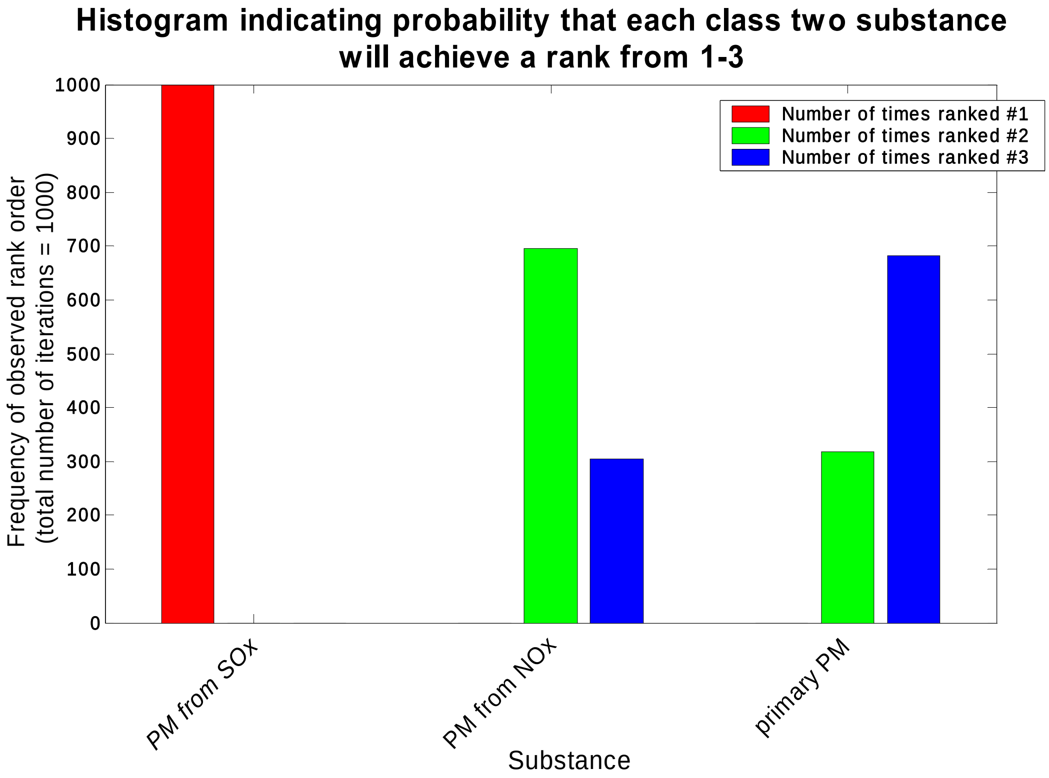


Figure 32: PM from SOx is always ranked as having the greatest impact on health effects based on predicted case incidence. PM from NOx is more likely to be ranked as the second-most important in terms of health impacts, and primary PM usually falls into third place

Figure 32 indicates that there is little ambiguity about which class of PM is associated with the greatest total predicted case incidence: PM from SO_x. This is a reflection of the greater amount of SO_x delivered to most quadrants around each refinery. The relative rankings of secondary PM from NO_x and primary $PM_{2.5}$ is highly dependent on the relative amounts of NO_x and $pM_{2.5}$ emitted from the refinery – alternate scenarios using emissions data from different years show that PM from NO_x can sometimes be ranked third.

2.2.4.2 Ranking probabilistic data – overlapping CDFs

Some difficulties arise when prioritizing parametric outputs where the distributions overlap. In the case of HEIDI II, the distributions of predicted case incidence overlap significantly in some cases, which means that the rank order assigned to each substance (which is intended to convey relative importance of the substance for health impacts in the population surrounding the refinery) could change with each iteration of the model. As well, the ranks are interdependent: in any given iteration, each rank order can only occur once, which means that any change in rank by one substance necessitates a change in rank for at least one other substance.

In order to properly communicate the prioritization results, it is important to specify which rank a substance achieves most often (i.e., the most probable rank) and whether the rank can be thought of as distinct from other substances (i.e., how much do the output distributions overlap) - both of these pieces of information inform any declaration about which substances are “higher priority”.

Figure 33 indicates why different ranking methods might result in different rank orders when comparing incidence. BTEX, sulphuric acid, and Vanadium were frequently among the top three ranked class 2 substances based on predicted case incidence. At the *de minimis* level and above, the ranks for these substances are distinct. However, Figure 33 suggests that extrapolation down to predited incidence for probabilities below ~0.4, the order might change, with sulphuric acid becoming less important than BTEX[22].

---

[22] Limitations of the program do not allow easy extrapolation to lower probabilities: these distributions are based on binning predicted values from the Monte Carlo simulation, and most predicted values were observed at low predicted case incidence, and therefore fell into the first few bins, meaning that the first data point on the cumulative curve is at a relatively high probability. (This might be rectified in the code by using bins of unequal size for the frequency data – since most of the observations are falling into the first bin)

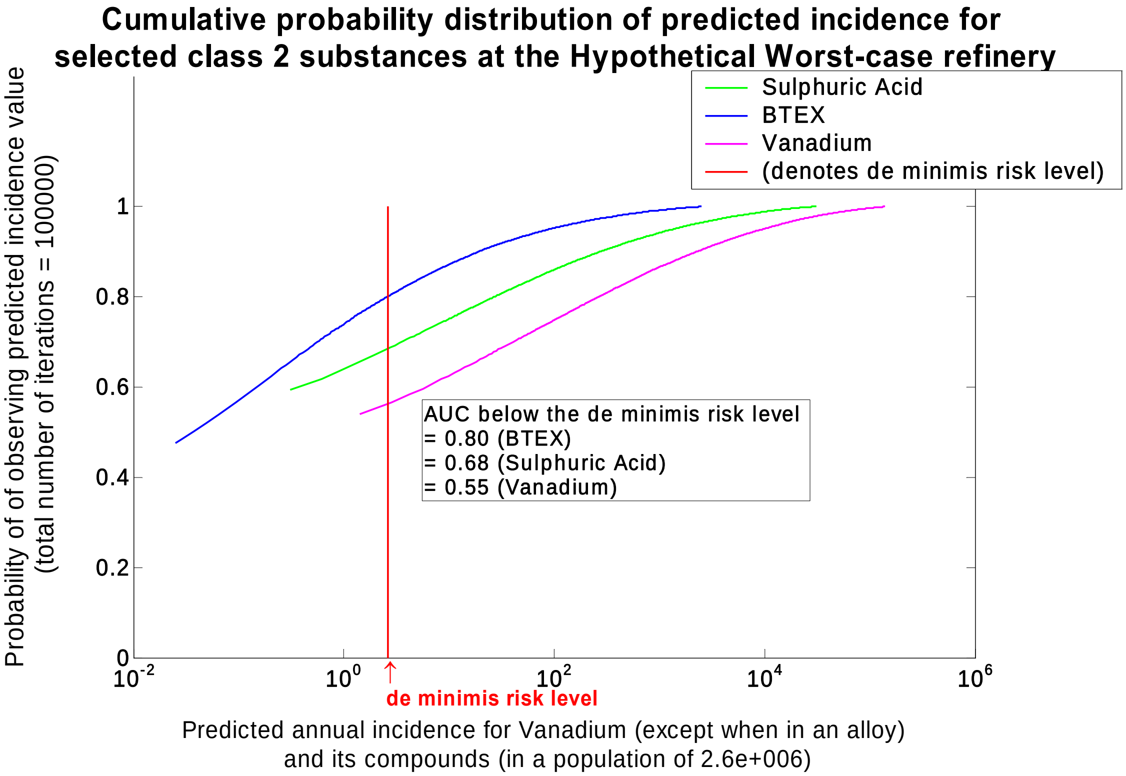


Figure 33: Cumulative probability for predicted case incidence of CNS neurotoxicity from BTEX, nasal irritation from Vanadium, and benign nasal tumors from sulphuric acid. The *de minimis* line crosses each curve at y = 0.80, 0.69, and 0.55 for each substance, respectively.

2.2.4.3 Health impact priorities – does application of DALYs alter the interpretation?

DALYs are intended to enable comparison of disparate health endpoints by accounting for the differences in the way each endpoint affects years of life lost and quality of life with disease of disability. It may therefore be more appropriate to conduct rankings on the basis of the DALYs incorporated in HEIDI, regardless of how unsophisticated the implementation of these values may be. Performing rankings this way may provide information on the utility of applying currently available DALYs in future health risk assessments.

Applying a measure of health impact such as DALYs does alter the interpretation of the cumulative probability distributions. Figure 34 indicates that using complex DALYs, BTEX is the highest priority substance at y=0.5 and below, and that at no point would sulphuric acid be considered a higher priority emission. Since sulphuric acid is related to benign nasal and upper airway tumors while BTEX is related to CNS neurotoxicity, a more severe outcome, this shift makes sense. Vanadium does not become relatively more important; this is expected since its health effects are relatively mild.

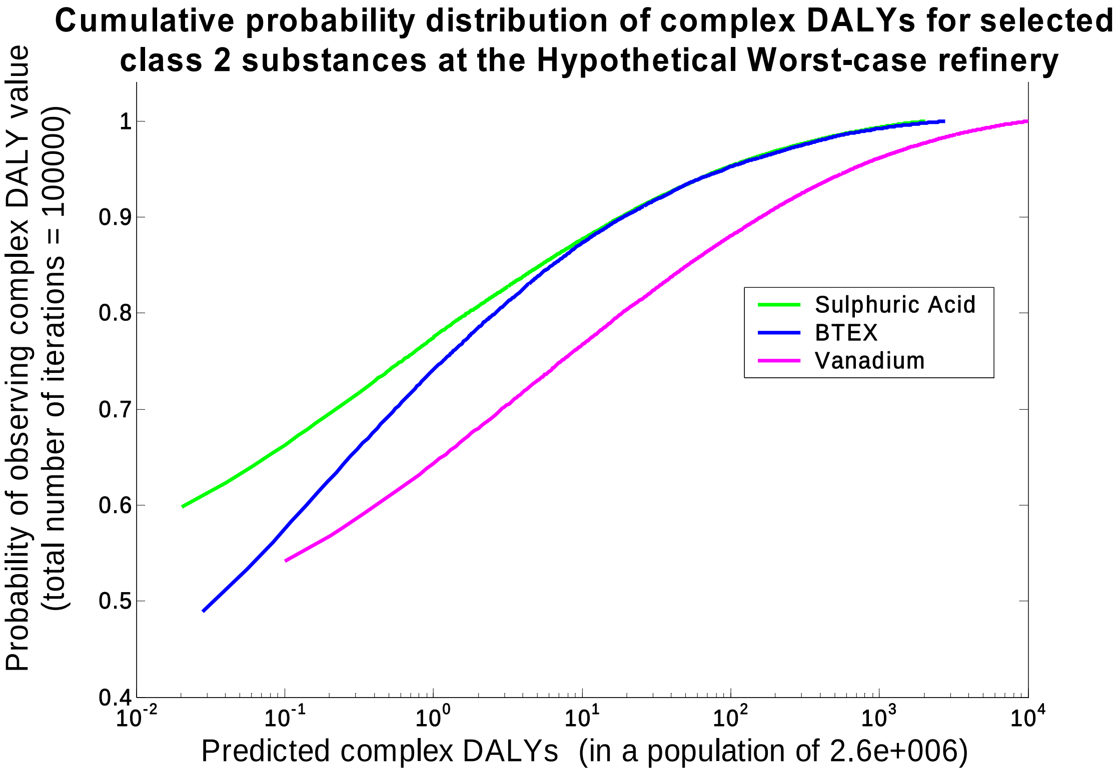


Figure 34: Applying DALY values to the predicted case incidence numbers changes the perception of which substance is "high priority".

2.2.4.4 Ranks across Classes

Because of the way the data was generated and the types of health endpoints, it may not be appropriate to compare outcomes across classes using predicted case incidence. However, a comparison using DALYs was attempted to determine whether specific substances or any class generally is consistently identified as being high priority.

Figure 35 shows that distinguishing the probability distributions for predicted health impact (calculated using the complex DALYs formulation) is not straightforward. The narrow distribution predicted for primary PM and 1,3 butadiene illustrates that there is less uncertainty associated with predicting health impact of class 1 and class 3 substances as compared with class 2 substances. However, the overlapping nature of all of the distributions, particularly around the mean values (i.e., between y=0.4 and y=0.6) precludes identification of a clear “priority substance”.

The figure suggests that it may be difficult to rank health impacts predicted by HEIDI II across classes, even using DALYs. This may be partially a function of the different types of outcomes: class 1 substances are associated with cancer development – a rare but severe health outcome. In contrast, vanadium emissions are associated with upper airway and nasal irritation – a far milder, but potentially more common, health effect. The overlapping and different shapes of CDFs in Figure 35 likely result from uncertainty in the toxicity values coupled with a lack of certainty about how to compare disparate endpoints.

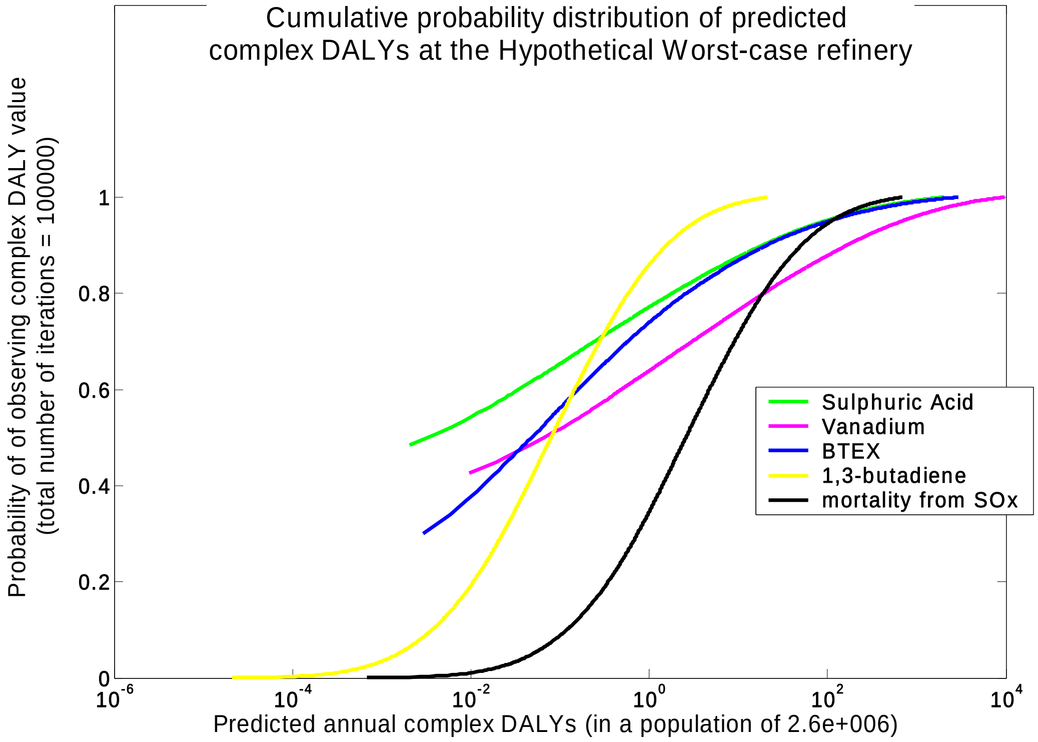


Figure 35: Comparing probability distributions for predicted health impact across classes

2.2.4.5 Numerical approaches to ranking probabilistic data

Visual inspection of the CDFs for predicted case incidence or predicted health impact (such as those presented above) can sometimes identify substances which generally have greater health impact at a specific refinery. The approach has been used before: a group prioritizing groundwater management strategies (Lytton, Howe et al. 2003) found that plotting risk and uncertainty on the same histogram allowed classification of outputs into three categories for prioritizing. However, numerical methods are also available and may be more informative in cases such as those depicted in Figure 35, where several CDFs overlap at a cumulative probability of around 0.5, and where arbitrary choice of a “point of comparison” along the x-axis or along the y-axis could result in several alternative rank orders. Duchesne et al (Duchesne, Beck et al. 2001) suggest four potential ranking methods: (i) using the lowest mean predicted after running a Monte Carlo Simulation, (ii) Using the lowest maximum value obtained after running a Monte Carlo Simulation, (iii) using the sum of the lowest mean and the standard deviation obtained over all simulations, or (iv) using tests of stochastic dominance. The first-degree stochastic dominance test checks whether the CDF of a given probability distribution is higher than another for all input values. For example, in Figure 35, SO_x meets this criterion for dominance over 1,3-butadiene. The second-degree test of stochastic dominance addresses instances where CDFs may cross within the range of possible input values. This test calculates the difference in value between two alternative CDFs (say i-j) across all input values. If the cumulative difference is positive, it suggests that the CDF for option i is dominant and should be ranked more highly. Steen (Steen 1997) offers a similar interpretation, suggesting that creating a cumulative distribution of the difference between two options can identify the probability with which each is likely to be the better alternative.

Table 26 compares the within-class rank orders that are predicted by HEIDI II under a variety of ranking approaches, using three different impact measures: I = incidence, S = simple DALYs, and C = complex DALYs.

Table 26: Comparing (within-class) ranks for substances using different ranking methods. Rank is based on predicted case incidence, simple DALYs, or complex DALY. Low rank numbers indicate high priority. Emissions from the hypothetical worst-case refinery default scenario are used. Multiples of the same rank order indicate that the health impact was predicted to be zero for more than once substance in the class. Top three ranks are highlighted in pink, yellow, and green.

Substance	Rank from deterministic model			Rank based on mean[23] value predicted in Monte Carlo Simulation			Test of stochastic dominance (second-degree)			Rank based on proportion of predicted case incidence probability distribution exceeding 10^{-6}
Class 1	**I[24]**	**S[24]**	**C[24]**	**I**	**S**	**C**	**I**	**S**	**C**	**Incidence**
1,3-Butadiene	5	5	5	6	5	6	5	6	5	4
Benzene	3	3	3	3	3	3	3	3	3	3
Ethylene (as oxide)	4	4	4	4	6	5	6	4	6	6
Nickel (and its compounds)	1	1	1	1	1	1	1	2	1	1
PAH (as benzo(a)pyrene)	2	2	2	2	2	2	2	1	2	2
Formaldehyde	6	6	6	5	4	4	4	5	4	5
Class 2										
1,2,4-Trimethylbenzene	11	11	11	7	10	8	9	8	11	19
Ammonia (Total)	10	10	10	18	19	19	18	20	19	18
BTEX	3	3	3	1	1	1	1	1	1	3
Cyclohexane	11	11	11	16	15	14	19	17	13	9
Dicyclopentadiene	11	11	11	11	8	10	8	10	7	15
Diethanolamine (and its salts)	11	11	11	12	12	12	11	13	18	14
Hydrogen sulphide	5	6	6	4	5	6	4	5	5	4
Isoprene	11	11	11	20	21	21	20	18	20	7
Mercury (and its compounds)	7	4	4	6	4	4	5	4	4	10
Methanol	11	11	11	21	20	20	21	21	21	6
Methyl ethyl ketone	11	11	11	13	17	13	15	19	17	10
Methyl isobutyl ketone	11	11	11	19	16	15	17	15	14	8
Methyl tert-butyl ether	11	11	11	17	18	18	16	16	16	13
Naphthalene	9	9	9	5	7	7	6	7	6	20
n-Hexane	8	8	8	8	6	5	7	6	8	5
Phenol	4	5	5	15	14	16	14	14	10	10
Propylene	11	11	11	10	9	9	10	9	12	17
Styrene	11	11	11	14	13	11	13	11	9	16
Sulphuric acid	2	2	2	3	3	3	3	3	3	2

---

[23] The median would provide a better sense of where most of the predicted values lie along the distribution, while the mean value can be highly influenced by skew of a distribution, and may better reflect the potential for high values of predicted health impact.

[24] I = rank based on predicted case incidence; S = rank based on predicted simple DALYs; C = rank based on predicted complex DALYs

Vanadium and its compounds	1	1	1	2	2	2	2	2	2	1
Zinc (and its compounds)	6	7	7	9	11	17	12	12	15	21
Class 3										
PM from SO_x	1	1	1	1	1	1	1	1	1	N/A entire distribution is above 10^{-6}
PM from NO_x	2	2	2	2	2	2	2	2	2	
Primary PM	3	3	3	3	3	3	3	3	3	

These hypothetical refinery results indicate that for class 1 substances, the top priority substances are consistently identified as being Nickel, PAH, and benzene, regardless of ranking approach. For class 2 substances, BTEX, Vanadium, and sulphuric acid are consistently identified as the three most important substances. Rank order for the other substances fluctuates somewhat as a result of various ranking approaches, but the general trend of priorities is relatively consistent. For class 3 substances, the order of priority is clear: it is consistently the same cross each possible ranking method.

Table 27 shows that there is high correlation for the ranks achieved by each substance across ranking approaches. The results of Table 26 and Table 27 together suggest that the (much simpler) deterministic version of HEIDI II might be sufficient to obtain good ranking information.

Table 27: Correlation coefficients between different ranking methods for within-class rankings. The test of using the proportion of the cumulative incidence curve beyond 10^{-6} does not correlate well with the other ranking methods for class 2 substances.

		Using rank from deterministic model			**Using rank based on mean value predicted in Monte Carlo Simulation**			**Using test of stochastic dominance (second-degree)**			**Using the Exceeding 10^{-6} test**
Class 1		**I**	**S**	**C**	**I**	**S**	**C**	**I**	**S**	**C**	**Incid.**
Rank from deterministic model	I	1.00	1.00	1.00	0.83	0.83	0.94	0.83	0.66	0.77	0.83
	S	1.00	1.00	1.00	0.83	0.83	0.94	0.83	0.66	0.77	0.83
	C	1.00	1.00	1.00	0.83	0.83	0.94	0.83	0.66	0.77	0.83
Rank based on mean value predicted in Monte Carlo Simulation	I	0.83	0.83	0.83	1.00	1.00	0.77	1.00	0.83	0.77	0.83
	S	0.83	0.83	0.83	1.00	1.00	0.77	1.00	0.83	0.77	0.83
	C	0.94	0.94	0.94	0.77	0.77	1.00	0.77	0.77	0.89	0.77
Test of stochastic dominance (second-degree)	I	0.83	0.83	0.83	1.00	1.00	0.77	1.00	0.83	0.77	0.83
	S	0.66	0.66	0.66	0.83	0.83	0.77	0.83	1.00	0.94	0.66
	C	0.77	0.77	0.77	0.77	0.77	0.89	0.77	0.94	1.00	0.60
Exceeding 10^{-6}	Incid.	0.83	0.83	0.83	0.83	0.83	0.77	0.83	0.66	0.60	1.00
Average correlation		0.87	0.87	0.87	0.87	0.87	0.86	0.87	0.78	0.81	0.80

coefficient											
Class 2											
Rank from deterministic model	I	1.00	0.99	0.99	0.79	0.83	0.76	0.82	0.79	0.76	0.68
	S	0.99	1.00	1.00	0.75	0.82	0.80	0.79	0.78	0.77	0.69
	C	0.99	1.00	1.00	0.75	0.82	0.80	0.79	0.78	0.77	0.69
Rank based on mean value predicted in Monte Carlo Simulation	I	0.79	0.75	0.75	1.00	0.97	0.80	1.00	0.93	0.85	0.37
	S	0.83	0.82	0.82	0.97	1.00	0.86	0.98	0.94	0.89	0.41
	C	0.76	0.80	0.80	0.80	0.86	1.00	0.83	0.95	0.97	0.54
Test of stochastic dominance (second-degree)	I	0.82	0.79	0.79	1.00	0.98	0.83	1.00	0.94	0.86	0.38
	S	0.79	0.78	0.78	0.93	0.94	0.95	0.94	1.00	0.97	0.48
	C	0.76	0.77	0.77	0.85	0.89	0.97	0.86	0.97	1.00	0.53
Exceeding 10^{-6}	Incid.	0.68	0.69	0.69	0.37	0.41	0.54	0.38	0.48	0.53	1.00
Average correlation coefficient		0.84	0.84	0.84	0.82	0.85	0.83	0.84	0.86	0.84	0.58

Table 28 shows the numerical rank results for an across-class comparison. Although the previously identified within-class priorities are consistently selected as higher-priority emissions in the across-class scenario, the order is not consistent across ranking approaches. BTEX and PM from SO_x are most frequently accorded the number one rank, with vanadium, primary PM, PM from NO_x, sulphuric acid or nickel following. Benzene and PAH are not identified as being among the top three overall priorities for emissions reduction. The lack of convergence among these results suggest that across-class rankings may not be appropriate, but that primary and secondary PM deserve special attention.

Table 28: Comparing across-class ranks for substances using different ranking methods. Low rank numbers indicate high priority. Emissions from the hypothetical worst-case refinery default scenario are used. Multiples of the same rank order indicate that the health impact was predicted to be zero for more than once substance in the class. Top three ranks are highlighted in pink, yellow, and green.

Substance	Rank from deterministic model			Rank based on mean value predicted in Monte Carlo Simulation			Stochastic dominance		
	I[24]	S[24]	C[24]	I	S	C	I	S	C
1,3-Butadiene	9	8	8	15	13	13	18	13	12
Benzene	6	6	6	12	10	10	13	10	10
Ethylene (as oxide)	8	7	7	17	11	11	17	12	11

Nickel (and its compounds)	4	2	2	7	6	7	8	6	6
PAH (as benzo(a)pyrene)	5	5	5	9	8	6	7	7	7
Formaldehyde	10	9	9	14	12	12	14	11	13
1,2,4-Trimethylbenzene	20	20	20	13	19	17	16	17	20
Ammonia (Total)	19	19	19	27	28	28	27	29	28
BTEX	12	12	12	1	1	1	1	1	1
Cyclohexane	20	20	20	25	24	23	28	26	22
Dicyclopentadiene	20	20	20	20	17	19	15	19	16
Diethanolamine (and its salts)	20	20	20	21	21	21	20	22	27
Hydrogen sulphide	14	15	15	8	14	15	9	14	14
Isoprene	20	20	20	29	30	30	29	27	29
Mercury (and its compounds)	16	13	13	11	9	9	10	9	9
Methanol	20	20	20	30	29	29	30	30	30
Methyl ethyl ketone	20	20	20	22	26	22	24	28	26
Methyl isobutyl ketone	20	20	20	28	25	24	26	24	23
Methyl tert-butyl ether	20	20	20	26	27	27	25	25	25
Naphthalene	18	18	18	10	16	16	11	16	15
n-Hexane	17	17	17	16	15	14	12	15	17
Phenol	13	14	14	24	23	25	23	23	19
Propylene	20	20	20	19	18	18	19	18	21
Styrene	20	20	20	23	22	20	22	20	18
Sulphuric acid	11	11	11	4	7	8	3	8	8
Vanadium and its compounds	7	10	10	2	3	3	2	3	3
Zinc (and its compounds)	15	16	16	18	20	26	21	21	24
PM from SO_x	1	1	1	3	2	2	4	2	2
PM from NO_x	2	3	3	5	4	4	5	4	4
Primary PM	3	4	4	6	5	5	6	5	5

2.2.5 Discussion

Ranks depend strongly on emissions. Thus the priorities identified for the hypothetical worst-case refinery do not necessarily apply to all refineries or emission years. For example, there are refineries where vanadium might not be considered the highest priority for reduction from among the class 2 substances. It is important to examine the rankings for refineries individually. However, there are similarities in priority substances across all refineries (nickel, PAH, BTEX, sulphuric acid, and vanadium), and these may be used in making general recommendations about refinery emissions of concern.

2.2.5.1 The high priority substances

Where nickel is emitted, it appears that a large proportion of the probability distribution is often above the *de minimis* level. Given the severity of the health outcome (lung cancer), this makes Ni a substance of concern. Ni emissions are reported in the NPRI for only 8 of the 20 refineries, suggesting that the source of the crude oil may have a large impact on its Ni content and subsequent emissions during refining. PAH was also identified as an important class 1 substance – also with an endpoint of lung cancer. These are two substances with the same endpoint: further analysis of the combined impact of the class 1 substances could be important.

While the deterministic version of HEIDI II ranked BTEX fairly low during across-class comparison, the stochastic version tended to rank it much higher. This is likely because the lognormal distributions used for each of the BTEX components increased the overall skewness of the distribution for the substances combined, meaning that there was a long tail at the upper end of the distribution. This may be an example of statistical compounding. The toxicity associated with each of the mixture components was assigned a probability distribution, and the toxicity for the mixture was based on values selected from those distributions during the simulations. It might have been more appropriate to use the individual toxicity estimates for each mixture component to estimate the toxicity of BTEX, and then assign a probability distribution to the mixture. For all class 2 substances where the ED05 was developed in the absence of epidemiological data, a GSD of 7.5 was selected (for rationale, see Appendix C). By assigning this GSD of 7.5 to the toxicity values of the individual components of BTEX rather than to the mixture as a whole, the distribution for BTEX toxicity may have become artificially skewed. However, each of the component substances could have a higher toxicity than is suggested by the point estimate for the (uncertain) ED05 value, in which case this approach may be appropriate. The potential for high predicted case incidence with exposure to BTEX at each of the Canadian refineries suggests that other groups of substances with similar health endpoints should be considered as mixtures. While this would require a detailed evaluation of whether the mechanisms of toxicity are similar, there are several outcomes that are associated with exposure to more than one substance, including developmental and neurotoxic effects.

Exposure to sulphuric acid has been associated with laryngeal cancer in an occupational setting (Soskolne, Jhangri et al. 1992; Sathiakumar, Delzell et al. 1997), and IARC has defined sulphuric acid when contained in strong inorganic mists as a suspected human carcinogen (International Agency for Research on Cancer 1997). Because sulphuric acid is repeatedly identified as a high priority substance from among the class 2 substances, the possibility that it should be treated as a class 1 substance was considered. However, regulatory agencies such as the EPA and Health Canada have not determined reference values for carcinogenicity from sulphuric acid. The health council of the Netherlands reviewed the genotoxocity and carcinogenicity of sulphuric acid in strong inorganic mists and concluded that it was a carcinogen in humans and that it acted by a non-stochastic genotoxic mechanism (Dutch Expert Committee on Occupational Standards 2003). This means that laryngeal cancer is probably related to regenerative cell proliferation that would occur after local irritation caused by exposure to sulphuric acid mists. Genotoxic effects (where damage to the DNA is involved) are assumed to play no (or a very minor) role. The Dutch Committee therefore recommended that a threshold approach to determining reference levels was more appropriate than the traditional linear no-threshold approach used for carcinogens (Dutch Expert Committee on Occupational Standards 2003). Given the lack of data about a potential threshold for carcinogenicity for sulphuric acid and the probability that it acts via a genotoxic mechanism, sulphuric acid is best treated as a class 2 substance in HEIDI II.

In HEIDI II, the critical endpoint identified for sulphuric acid is bronchial hyperplasia. According to a review by Agency for Toxic Substances and Disease Registry (ATSDR) (Agency for Toxic Substances and Disease Registry (ASTDR) 1998), ambient levels of sulphuric acid are also associated with respiratory effects including asthma admissions, airway obstructive disease and decreased respiratory function. Since sulphuric acid is frequently emitted in large quantities from Canadian refineries, the possibility that it may compound effects observed with PM should be considered.

Vanadium was often identified as a priority. There is high uncertainty associated with the toxicity data selected to represent Vanadium, especially since the NPRI – the source of emissions data - defines vanadium as “vanadium and its compounds (except when in alloy)”, which could include a variety of agents. Pentavalent vanadium appears to be more toxic than other forms, but it is unclear from the inventory data which forms are predominantly emitted by the refineries. The toxicity value used in HEIDI II was for pentavalent vanadium – which may be a very conservative estimate. The priority ranking must be considered within the limitations of this toxicological data.

2.2.5.2 Issues about looking at the absolute predictions for incidence

The limitations of using the absolute values of predicted incidence generated by HEIDI II are explained elsewhere. However, looking at the values may be useful in broadly characterizing the model result and in planning future research.

The absolute predictions of incidence at the hypothetical refinery and at several refineries for several substances – especially the CACs - are worrying. Many of the limitations of HEIDI II have been identified in previous sections of this document. Given those limitations, to what extent should these predictions be considered representative of the possible effects of refinery emissions? HEIDI II is intended to be used as a screening tool in conjunction with other methods to set priorities. The results suggest that CACs should be high priority for emissions reduction and that a more thorough assessment of the health effects of CACs emitted from Canada's refineries may be warranted. If any results from HEIDI II were to be reported, those in southwest Ontario would have the most validity since the meteorology should be appropriate to that region.

Secondary PM is generated as the nitrate and sulphate pollutants travel away from the point source (stack). A 2003 analysis of power plants in the U.S. showed that using even a 500 km radius significantly underestimated population exposure and risks from $PM_{2.5}$ (Levy, Wilson et al. 2003). Although power plants typically have higher stacks than refineries (which would induce emissions to travel further from the source), this implies that the mortality and morbidity predicted by HEIDI II may represent only a small portion of the health impacts of primary and secondary PM emitted from refineries. This issue is of particular importance for refineries located in southern Ontario, where the population density is consistently high over a large extent of the geography. HEIDI II currently estimates effects only within 25 km of each refinery, but a large number of people would be expected to be exposed to secondary PM formed beyond 25 km from each refinery.

PM is emitted from many point and mobile sources including other industry such as coal-fired power plants and vehicles. Because PM is usually considered as a nonthreshold-acting substance, additional emissions from any sector add to the health burden of exposed populations.

2.2.5.3 Issues about ranking

The frequency histograms comparing the number of times each substance achieved a particular rank during a simulation appear to be a useful way to visually represent information about which substances are important and the extent to which the impacts of various substances are distinct. This type of analysis might be most appropriate for presenting information to policy and decision-makers, who may have less familiarity with probability distributions than many scientists.

Using the proportion of the probability distribution that is below the *de minimis* level is another useful prioritization measure, as it provides a sense of how often an unacceptable (by typical regulatory standards) number of cases are predicted. However, the proportion of the distribution likely to exceed the *de minimis* risk level is directly associated to the input distributions used to characterize uncertainty and variability in the inputs, especially for the C-R relationships. The GSD selected to represent the C-R data is itself uncertain. A value of 7.5 was used for class 2 threshold data, but values of up to 11 have been proposed. If a GSD of 11 had been used, the overall distributions would have been broader, and a greater proportion of the predicted case incidence may have been above the *de minimis* risk level for substances that were associated with predicted case incidence>0.

Comparing impacts across classes may have limited validity; however, the implications of the overlapping distributions presented in Figure 35 should be considered. The figure suggests that the health impacts of several high-priority substances that are emitted from Canadian refineries may have similar extent of impact on the surrounding population; that attempting to identify priority substances may not be possible. Several alternate emissions reductions strategies are suggested by this figure. Emissions reduction for all substances deemed “high-priority” could be undertaken, but this would require some arbitrary definition of “high priority” – for example, “top three”, and does not consider cost of reduction. Alternately, reduction of the priority emissions most easily/cheaply reduced could be unertaken, since no single substances appears to be dramatically more harmful. However, the issue of communication with stakeholders should also be considered. They may respond more favorably towards reduction of the emission with the most severe health effect, even if the estimated total benefit is the same as for a lesser reduction of emissions of a different substance.

A disadvantage of using a prioritization approach is that ranks do not communicate about absolute impact. While a substance may be listed as high priority, the impact may actually be predicted to be incidence less than the *de minimis* risk level (i.e., if all emissions from a particular refinery are low). In this case it may not be appropriate to take action to reduce emissions of the substance. Ranks also do not inform about the benefits of reducing emissions. Cost-benefit of emissions reductions is an important consideration from both a technological and public health standpoint. A similar reduction in mass of emissions for two distinct substances may result in different extent of benefits.

2.2.5.4 Limitations

The different patterns of predicted case incidence according to population distribution indicate that consideration of the local meteorology is important for decisions regarding siting of refineries. In general, refineries should be sited downwind from the majority of the population to minimize health impacts. HEIDI II uses a generic meteorology which does not apply to all locations across Canada - the predicted impacts at most real refinery locations are therefore inaccurate; the predicted case incidence values should in no way be taken literally, especially for locations outside Southern Ontario.

The generic meteorology used in HEIDI II is one reason that ground-truthing of the predictions was not carried out. Another is that it would be very difficult to distinguish cases due to refinery emissions from cases due to other emissions in communities near to refineries.

The ranks produced by HEIDI II are particular to each refinery. This is inappropriate for regions such as Sarnia which have several refineries in close proximity to each other. A better approach might be to determine the impact of the cumulative emissions from all of the refineries in the region on the local population.

The analysis of the Imperial Sarnia refinery showed that high impacts are expected where most people live (to the northeast of the refinery). The northeast quadrants were also associated with greatest delivered concentration as a result of the meteorology selected. This also suggests that the worst-case scenario might have been better designed – it was chosen to maximize the total number of people living around the refinery, without considering where people were living relative to where the greatest exposures might be occurring.

2.2.5.5 Recommendations

Future prioritizations of health impacts from industries would benefit from including a valuation of reduction. The ranking alone is insufficient to determine whether a given substance is a health concern, or whether reducing emissions would result in a net public health benefit. Cost-benefit analysis of reducing emissions would be a welcome addition to any tool intended to identify priority substances for emissions reduction.

Unless the magnitude of emissions increases dramatically (unlikely), there are some substances for which the refinery contributions to the atmosphere are unlikely to ever pose a health risk to the public: these were identified as being associated with zero predicted case incidence in the hypothetical worst-case scenario.

Urban planners should consider information about population density and potential exposure, including predominant wind direction) when siting refineries, or planning for broadly residential and/or industrial areas. Refineries which are located upwind of densely populated areas are associated with much greater health impacts in the population, ultimately affecting individual quality and length of life. This could have downstream effect on economic productivity and social capital of the community.

2.2.5.6 Sarnia – another analysis required?

HEIDI II's predictions suggest that there may be a particular problem for refinery emissions in Sarnia. Sarnia is a highly industrial region, and there are four refineries in close proximity to one another in the area. Although HEIDI II does not account for it, each of the people living in the area may be subject to exposures from all four refineries. The combined predicted impacts may therefore be much higher that those from each refinery alone. The analyses suggest that in Sarnia, there are two refineries where predicted case incidence for six (Imperial Sarnia) and four (Shell Sarnia) of the class 1 and class 2 emissions exceeds the *de minimis* level at least occasionally. The Imperial Sarnia refinery has the most CAC emissions of all refineries included in HEIDI II – which were associated with some of the highest rates of predicted mortality (up to 10^{-4}) and morbidity.

HEIDI II does not appropriately assess exposure or health impact from refinery emissions for this population; a more complex analysis incorporating emissions from all refineries and the geographic distribution of people relative to each of the refineries would be required. Assigning priorities for reduction at each refinery would be fraught with difficulties however, as assigning responsibility to each refinery for a portion of health impacts – particularly for impacts above a threshold level, would be technically (and politically!) difficult.

2.3 Further Analysis – what else can HEIDI II do or tell us?

2.3.1 Impact Equivalents

In order to examine predicted health impact in a relative sense, values for predicted incidence and predicted DALYs were converted into benzene equivalents (for class 1 substances) and mercury equivalents (for class 2 substances)[25]. These two substances have been well-characterized in terms of their toxicity which allows them to be useful as a basis for comparison. For anyone familiar with the toxicity/potential health impacts of benzene and mercury exposure, the values below provide a sense of the importance of other refinery emissions. (Because the class 3 substances are not treated using toxicologic data, and the predicted values from each CAC are of similar magnitudes, this exercise was not completed for class 3 substances.)

The simple calculation was based on each health impact measure, i.e., (i) predicted incidence, (ii) predicted simple DALY, (iii) predicted complex DALY. Table 29 indicates that nickel and PAH have a much greater impact than most other class 1 substances emitted from the hypothetical refinery.

Table 29: Class 1: benzene equivalent = (substance-specific predicted health impact score) / (predicted benzene impact score). TRACI characterization factors are provided for comparison, although they are not directly analogous: TRACI's factors are per mass of emissions, while impacts from HEIDI II depend on the amount emitted.

NPRI substance	**Equivalent human endpoints**	**Predicted population health impact in Benzene equivalents**			**TRACI characterization factor**
	primary human endpoint	*predicted incident cases*	*simple DALYs total*	*complex DALYs total*	*(kg benzene eq /kg)*
1,3-Butadiene	leukemia	0.21	0.21	0.21	0.41
Benzene	***leukemia***	***1.00***	***1.00***	***1.00***	1.00
Ethylene (as oxide)	leukemia	0.45	0.45	0.45	11.02
Nickel (and its compounds)	lung cancer	240	240	150	1.51
PAH (as benzo(a)pyrene)	lung cancer	11	11	7.2	914
Formaldehyde	nasal and lung cancer	0.25	0.25	0.16	0.00
Acetaldehyde	nasal and lung cancer	0.02	0.02	0.01	0.00

---

[25] TRACI, a popular screening tool developed by the EPA ((Bare, Norris et al. 2003) uses toluene equivalents rather than mercury equivalents, but because the toluene values are "wrapped up" into BTEX in HEIDI II, toluene equivalents are not appropriate here.

Table 30: Class 2: Mercury equivalent = (substance-specific predicted health impact score)/(predicted mercury impact score)

NPRI substance	equivalent human endpoints	predicted population health impact (Mercury equivalents)		
	primary human endpoint	*predicted incident cases*	*simple DALYs total*	*complex DALYs total*
1,2,4-Trimethylbenzene	moderate anemia	0.00	0.00	0.00
Ammonia (Total)	skin and nose irritation	8.58E-06	8.58E-08	5.25E-08
Benzene (as BTEX component)	moderate CNS neurotoxicity	*See BTEX Mixture*	*See BTEX Mixture*	*See BTEX Mixture*
BTEX	moderate CNS neurotoxicity	8.82	8.82	7.46
Cyclohexane	reduced bodyweight	0.00	0.00	0.00
Dicyclopentadiene	chronic renal disease	0.00	0.00	0.00
Diethanolamine (and its salts)	throat irritation	0.00	0.00	0.00
Ethylbenzene (as BTEX component)	moderate CNS neurotoxicity	*See BTEX Mixture*	*See BTEX Mixture*	*See BTEX Mixture*
Hydrogen sulphide	nose irritation	8.99E-01	8.99E-03	5.50E-03
Isoprene	benign lung tumours	0.00	0.00	0.00
Mercury (and its compounds)	***severe CNS neurotoxicity***	***1.00***	***1.00***	***1.00***
Methanol	physical teratogenesis	0.00	0.00	0.00
Methyl ethyl ketone	developmental retardation	0.00	0.00	0.00
Methyl isobutyl ketone	developmental retardation	0.00	0.00	0.00
Methyl tert-butyl ether	PNS neurotoxicity	0.00	0.00	0.00
Naphthalene	benign lung tumours	7.02E-04	7.02E-05	7.90E-05
n-Hexane	PNS neurotoxicity	1.67E-03	1.67E-04	1.05E-04
Phenol	mild CNS neurotoxicity	2.39E-01	2.39E-02	2.02E-02
Propylene	benign nasal & upper airway tumours	0.00	0.00	0.00
Styrene	mild developmental retardation	0.00	0.00	0.00
Sulphuric acid	benign nasal & upper airway tumours	8.60E+03	86	53
Toluene (as BTEX component)	moderate CNS neurotoxicity	*See BTEX Mixture*	*See BTEX Mixture*	*See BTEX Mixture*
Vanadium and its compounds	nasal and upper airway irritation	2.02E+07	2.02E+05	1.24E+05
Xylene (as BTEX component)	moderate CNS neurotoxicity	*See BTEX Mixture*	*See BTEX Mixture*	*See BTEX Mixture*
Zinc (and its compounds)	moderate anemia	2.16	2.16E-02	2.27E-03

As with the base model, the values presented in Table 29 and Table 30 depend strongly on the emissions chosen. These values were created using the "hypothetical worst-case" refinery, but if a different refinery (with a different set of emissions) were chosen, different health impacts would be predicted. For example, many refineries do not have substantial nickel emissions and so for those cases, nickel would not appear to be as important as it does above. Note also that this method of comparison will not work for refineries where either benzene or mercury are not emitted (i.e., mercury is not a reported emission for the Chevron-Burnaby refinery).

2.3.2 Several refineries in one area

In Sarnia, the population is exposed to emissions from four separate petroleum refineries. HEIDI II was used to model a "composite" refinery where the emissions from the four individual refineries were summed, and the population distribution was created by averaging the population distributions around each of the four individual refineries. (A comparison of the populations living within 25 km of each individual refinery with the "average population" determined for the "composite" indicated that approximately the same urban population of the region is captured in each case).

Table 31 shows that using the deterministic version of HEIDI II, the predicted cumulative impacts of the four refineries is much greater than the impact of any individual refinery. The table also highlights the main problem with using a "composite" refinery: the location of the population relative to the refinery and the dispersion of emissions is incorrect. If the location of the population was properly accounted for, the sum of all the DALYs from the class 1 and three substances should be the same as the DALYs predicted by the composite (since the concentration-response function used is linear). This suggests that a summed value for class 1 and class 3 substances (which were modeled as "non-threshold") is probably more reliable than that of the composite. The results also suggest that emissions from the Imperial refinery have a strong influence on the total health impact of petroleum refineries in the area.

Table 31: Comparison of simple DALYs predicted for individual refineries in Sarnia, the sum of the individual effects, and predicted impacts from a "composite" refinery where the emissions input was the sum of emissions from the four refineries.

Health impact score	**Imperial Sarnia**	**Nova Corunna**	**Shell Sarnia**	**Sunoco**	**Sum of impacts from all four individual refineries**	**Sarnia composite – using summed emissions**
Class 1 DALYs	28	0.1	3.9	0.1	*32*	23
Class 2 DALYs	1.2E-03	9.4E-10	1.7E-05	4.4E-11	*1.2E-03*	1.7E-03
Class 3 DALYs	120	No emiss. data	6.3	16	*140*	210
Total DALYs	*150*	*0.1*	*10*	*16*	*170*	240

For class 3 substances, predictions were much lower at the Sarnia facility, mainly because of the much smaller at-risk population. The following comparison was made using the deterministic version of HEIDI II.

Table 32: Predicted health impact at the hypothetical worst-case refinery as compared to the hypothetical Sarnia refinery. Recall that the Sarnia hypothetical refinery uses the summed emissions from all the refineries in the region. Note that the impacts are similar to those predicted for the worst-case scenario. I = impact based on predicted case incidence; S = impact based on predicted simple DALYs; C = impact based on predicted complex DALYs

	Hypothetical Worst-Case			**Sarnia Composite**		
	I	S	C	I	S	C
1,3-Butadiene	5.8E-02	3.9E-01	1.4	3.0E-03	2.0E-02	7.1E-02
Benzene	1.9E-01	1.3	4.4	2.1E-02	1.4E-01	5.0E-01
Ethylene (as oxide)	6.7E-02	4.5E-01	1.6	4.2E-03	2.8E-02	9.7E-02
Nickel (and its compounds)	5.2E+01	3.5E+02	7.6E+02	3.3	2.2E+01	4.9E+01
PAH (as benzo(a)pyrene)	1.2	8.2	1.8E+01	5.8E-02	3.9E-01	8.5E-01
Formaldehyde	5.7E-02	3.8E-01	8.3E-01	N/A	N/A	N/A
Acetaldehyde	5.5E-03	3.7E-02	8.0E-02	N/A	N/A	N/A
1,2,4-Trimethylbenzene	0.0	0.0	0.0	4.6E-15	3.1E-16	5.5E-17
Ammonia (Total)	1.8E-14	1.2E-15	1.2E-15	7.6E-17	5.1E-18	5.3E-18
BTEX	2.9E-07	2.0E-07	2.8E-07	3.7E-08	2.5E-08	3.6E-08
Cyclohexane	0.0	0.0	0.0	5.9E-25	4.0E-25	8.3E-25
Dicyclopentadiene	0.0	0.0	0.0	7.4E-17	4.9E-17	7.0E-17
Diethanolamine (and its salts)	0.0	0.0	0.0	7.3E-19	4.9E-20	5.1E-20
Hydrogen sulphide	4.6E-09	3.1E-10	3.2E-10	1.6E-11	1.1E-12	1.1E-12
Isoprene	0.0	0.0	0.0	9.3E-32	6.2E-32	8.8E-32
Mercury (and its compounds)	4.1E-09	2.8E-08	4.7E-08	1.0E-09	6.8E-09	1.2E-08
Methanol	0.0	0.0	0.0	2.6E-18	1.8E-17	9.1E-17
Methyl ethyl ketone	0.0	0.0	0.0	6.1E-22	4.1E-22	8.5E-22
Methyl isobutyl ketone	0.0	0.0	0.0	3.2E-25	2.1E-25	4.4E-25
Methyl tert-butyl ether	0.0	0.0	0.0	N/A	N/A	N/A
Naphthalene	2.8E-12	1.9E-12	3.7E-12	1.4E-12	9.1E-13	1.8E-12
n-Hexane	5.6E-12	3.8E-12	4.0E-12	4.1E-14	2.8E-14	3.0E-14
Phenol	7.9E-09	5.3E-09	7.6E-09	4.8E-10	3.2E-10	4.7E-10
Propylene	0.0	0.0	0.0	5.8E-17	3.9E-18	4.1E-18

Styrene	0.0	0.0	0.0	2.3E-20	1.6E-20	3.3E-20
Sulphuric acid	5.8E-04	3.9E-05	4.1E-05	3.8E-03	2.6E-04	2.7E-04
Vanadium and its compounds	1.0E-01	7.0E-03	7.3E-03	2.1E-02	1.4E-03	1.5E-03
Zinc (and its compounds)	4.4E-09	2.9E-10	5.2E-11	1.1E-08	7.4E-10	1.3E-10
PM from SOx	950	2600	3800	58	160	240
PM from NOx	93	250	380	9	24	36
Primary PM	82	220	330	11	30	45

As shown in Table 33, the comparison of the summed emissions from the four refineries in the Sarnia area to the hypothetical worst-case scenario revealed that the prioritization order for the emitted substances was identical for class 1 substances and for the first four class 2 substances and very similar for subsequent emissions for class 2 substances. For class 3 substances there is a switch in priority, where primary PM becomes more important than NOx at the composite Sarnia refinery. In this contrived scenario, this is likely due to the relative emissions of primary $PM_{2.5}$ and NOx. In reality, the dispersion patterns would have to be considered more carefully: the emissions from the four refineries do not actually originate at one location, and the true dispersion pattern in Sarnia is likely to be much more complex.

Table 33: Predicted priority (within-class rankings) of health impact from emissions at the hypothetical worst-case refinery as compared to the composite Sarnia refinery. Recall that the Sarnia composite refinery uses the summed emissions from all the refineries in the region. Priority order is similar in each case. ("N/A" indicates no reported emissions at any of the Sarnia facilities). I = rank based on predicted case incidence; S = rank based on predicted simple DALYs; C = rank based on predicted complex DALYs

	Hypothetical Worst-Case			Sarnia Composite		
	I	S	C	I	S	C
1,3-Butadiene	6	6	5	5	5	5
Benzene	3	3	3	3	3	3
Ethylene (as oxide)	4	4	4	4	4	4
Nickel (and its compounds)	1	1	1	1	1	1
PAH (as benzo(a)pyrene)	2	2	2	2	2	2
Formaldehyde	5	5	6	N/A	N/A	N/A
Acetaldehyde	7	7	7	N/A	N/A	N/A
1,2,4-Trimethylbenzene	11	11	11	10	10	12
Ammonia (Total)	10	10	10	11	13	13
BTEX	3	3	3	3	3	3
Cyclohexane	11	11	11	18	18	18
Dicyclopentadiene	11	11	11	12	11	11
Diethanolamine (and its salts)	11	11	11	15	15	15
Hydrogen sulphide	6	7	6	7	7	8
Isoprene	11	11	11	20	20	20
Mercury (and its compounds)	5	4	4	5	4	4
Methanol	11	11	11	14	12	10
Methyl ethyl ketone	11	11	11	17	17	17
Methyl isobutyl ketone	11	11	11	19	19	19

Methyl tert-butyl ether	11	11	11	N/A	N/A	N/A
Naphthalene	9	9	9	8	8	7
n-Hexane	8	8	8	9	9	9
Phenol	7	5	5	6	6	5
Propylene	11	11	11	13	14	14
Styrene	11	11	11	16	16	16
Sulphuric acid	2	2	2	2	2	2
Vanadium and its compounds	1	1	1	1	1	1
Zinc (and its compounds)	4	6	7	4	5	6
PM from SOx	1	1	1	1	1	1
PM from NOx	2	2	2	3	3	3
Primary PM	3	3	3	2	2	2

2.3.3 Using other models to predict priorities for petroleum emissions

TRACI is a stand-alone, windows-based tool that was developed by the U.S. EPA (Bare, Norris et al. 2003). It uses a run-time version of Microsoft Access to characterize the potential impacts of a variety of environmental stressors, including human health cancer effects, human health noncancer effects, and human health criteria-related effects(Bare, Norris et al. 2003).

The within-class priorities identified in the deterministic version of HEIDI II were compared to the predictions that result from application of TRACI’s characterization factors to the emissions used for the hypothetical worst-case refinery. The characterization factors were applied to emissions to predict impacts, which were then ranked within and across classes. The class 1 substances were compared to the rankings that resulted from applying TRACI’s HH (human health) cancer air characterization factors, the class 2 substances were compared based on the ranking that resulted from applying TRACI’s HH noncancer air characterization factors, and the class thee substances were compared based on the rankings that resulted from applying TRACI’s HH criteria – air point source characterization factors.

2.3.3.1 Within-class comparisons based on rank

Regardless of the ranking method or metric used with HEIDI II, the top priority substances for class 1 are consistently identified as being nickel, PAH, and benzene. This is consistent with the results from TRACI shown in Table 34.

Table 34: Rank order resulting from application of TRACI's characterization factors to class 1 substances at the hypothetical worst-case refinery.

Rank	Order from Deterministic version of HEIDI II (using simple DALYs)	Order from TRACI based on HH cancer air
1	Nickel	PAH (as benzo(a)pyrene)
2	PAH (as benzo(a)pyrene)	Benzene
3	Benzene	Nickel
4	Ethylene (as oxide)	Ethylene (as oxide)
5	Formaldehyde	1,3-Butadiene
6	1,3-Butadiene	Formaldehyde

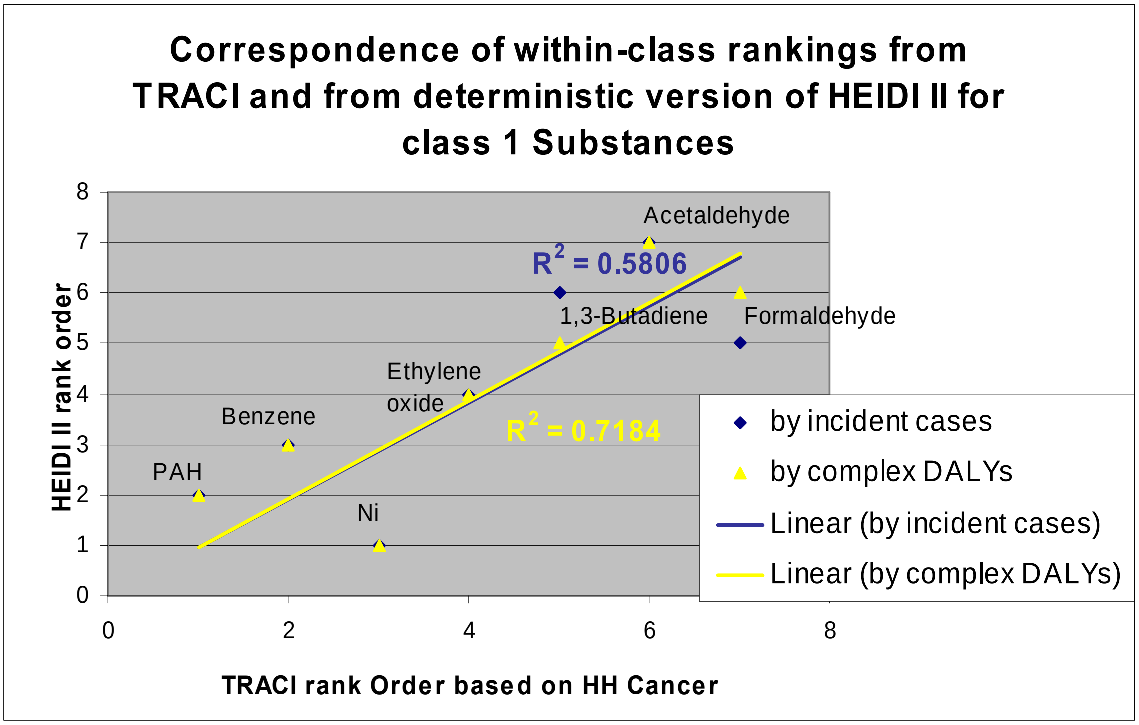


Figure 36: Rankings for class 1 substances obtained from HEIDI II and TRACI correspond relatively well. (Only two trendlines are shown since the rank order for indicent cases and simple DALYs are identical)

For class 2 substances, the top-ranked substances in HEIDI II were consistently vanadium, BTEX, and sulphuric acid, regardless of ranking method used. As shown in Table 35, TRACI also ranks vanadium as a top priority in terms of health impacts. However, TRACI does not evaluate BTEX as a mixture, and does not include a characterization factor for sulphuric acid. The individual components of BTEX are ranked, 3rd, 7th, 13th, and 20th, suggesting that unless the total impacts interact in an antagonistic way (unlikely), the minimum rank achieved by the mixture should be third, which is consistent with HEIDI II. Mercury and zinc both achieve relatively high prioritizations from the two models, and many of the same substances were ranked as being low priority (higher rank than 10). Class 2 substances for which the HEIDI II and TRACI rankings seemed divergent included diethanolamine, MIBK, and MEK which achieved ranks of 4, 6, and 8 with TRACI, but were associated with zero predicted incidence in HEIDI II and thus a last-place ranking.

Table 35: Rank order resulting from application of TRACI's characterization factors to class 2 substances at the hypothetical worst-case refinery

Rank	Order from Deterministic version of HEIDI II (using simple DALYs)	Order from TRACI based on HH noncancer air
1	Vanadium	Vanadium
2	Sulphuric Acid	Zinc
3	BTEX	Benzene
4	Mercury	Diethanolamine
5	Phenol	Mercury
6	Zinc	MIBK
7	Hydrogen Sulphide	Toluene
8	n-hexane	MEK
9	Naphthalene	1,2,4-trimethylbenzene
10	Ammonia	Naphthalene
11	1,2,4-trimethylbenzene, cyclohexane, dicyclopentadiene, diethanolamine, isoprene, methanol, methyl ethyl ketone, methyl isobutyl ketone, methyl tert-butyl ether, propylene, styrene	Ammonia
12		n-hexane
13	**All substances ranked in 11th place were associated with predicted incidence of zero	MTBE
14		Xylene
15		Methanol
16		Hydrogen Sulphide
17		Cyclohexane
18		Propylene
19		Phenol
20		Styrene
21		Isoprene, Ethylbenzene
Unranked	Benzene, Toluene, Ethylbenzene, Xylene as individual substances	Dicyclopentadiene. Sulphuric acid, BTEX as a group (no data in TRACI)

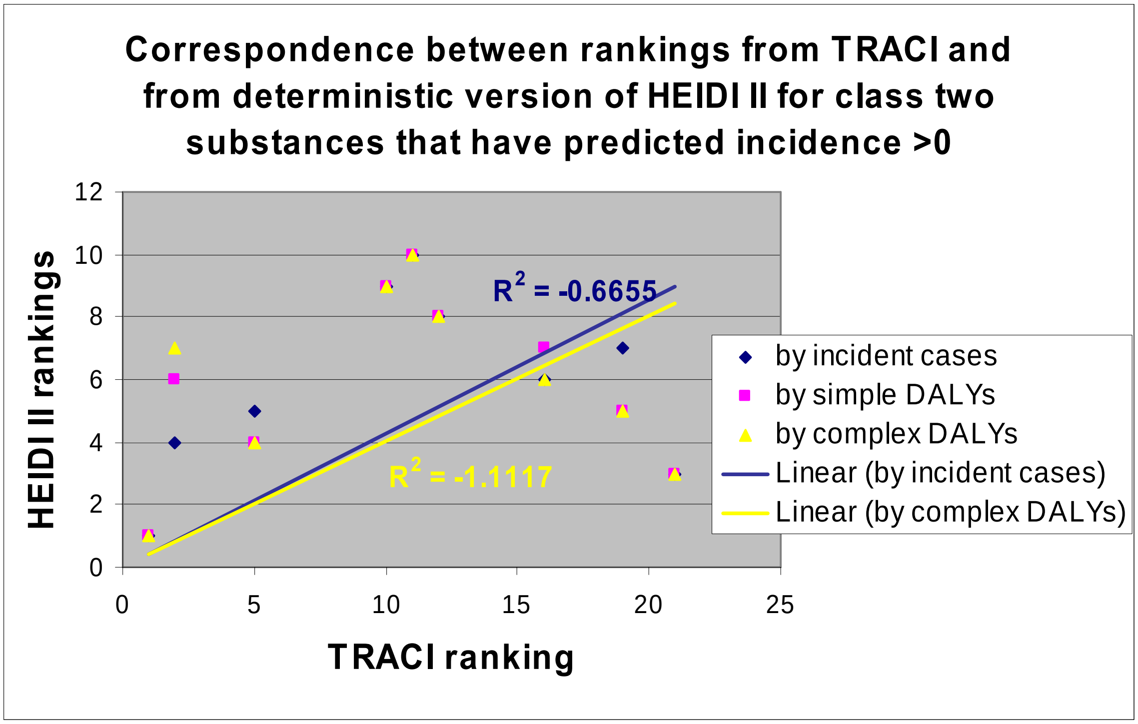


Figure 37: Rankings for class 2 substances obtained from HEIDI II and TRACI do not correspond well. Only substances with predicted indience (in HEIDI II) greater than zero were included to avoid multiple substances being given the same rank. (Only two trendlines are shown since the rank order for indicent cases and simple DALYs are identical)

Table 36: Rank order resulting from application of TRACI's characterization factors to class 3 substances at the hypothetical worst-case refinery

Rank	Order from Deterministic version of HEIDI II (using simple DALYs)	Order from TRACI based on HH criteria air contaminant-air point source
1	$PM_{2.5}$ from SOx	Primary $PM_{2.5}$
2	$PM_{2.5}$ from NOx	NOx
3	Primary $PM_{2.5}$	SOx

Table 36 indicates some divergence between priorities predicted by each of the models for class 3 substances. This is because TRACI provides characterization factors for SOx in the acidification category only and not in the human health criteria air contaminant impact category. There is an essential difference in what HEIDI II is evaluating compared to TRACI: HEIDI II considers the potential transformation of SOx and NOx to PM, which TRACI apparently does not. Thus comparing results predicted by HEIDI II and TRACI is invalid.

2.3.3.2 Across-class comparisons

In order to maintain proper units for relative comparison in TRACI, the contributions from cancer, noncancer, and criteria air contaminants impacts must be considered for each substance. This is not equivalent to the way that HEIDI II ranked the substances: by considering only the critical endpoint, regardless of whether there might be multiple endpoints. Table 37 suggests that although some substances are consistently identified as having the highest health impacts (i.e., nickel, $PM_{2.5}$, ethylene oxide, and benzene), there is little overall consistency about which substances cause the greatest health impacts.

Table 37: rank order resulting from application of TRACI's characterization factors across classes (omitting class 3, for which comparison of ranking is invalid) at the hypothetical worst-case refinery

Rank	Order from Deterministic version of HEIDI II (using simple DALYs)	Order from TRACI based on HH cancer air+HH noncancer air + HH criteria air-point source
1	Nickel	Vanadium
2	PAH	Nickel
3	Benzene	Zinc
4	Ethylene oxide	Ethylene oxide
5	Formaldehyde	Benzene
6	1,3-butadiene	Diethanolamine
7	Acetaldehyde	Mercury
8	Vanadium	PAH
9	Sulphuric Acid	MIBK
10	BTEX	Toluene
11	Mercury	Formaldehyde
12	Phenol	MEK
13	Zinc	Acetaldehyde
14	Hydrogen Sulphide	1,2,4-Trimethylbenzene
15	n-hexane	Naphthalene
16	Naphthalene	Ammonia
17	Ammonia	n-hexane
18	1,2,4-trimethylbenzene, diethanolamine, dicyclopentadiene, cyclohexane, isoprene, methanol, MEK, MIBK, MTBE, propylene, styrene	1,3-butadiene
19	**All substances ranked in 18th place were associated with predicted incidence of zero	MTBE
20		Xylene
21		Methanol
22		Hydrogen Sulphide
23		Cyclohexane
24		Propylene
25		Phenol
26		Styrene
27		Ethylbenzene, Isoprene
Unranked	Benzene, Toluene, Ethylbenzene, Xylene as individual substances	Dicyclopentadiene, Sulphuric acid, BTEX as a group (no data in TRACI)

2.3.4 Applying HEIDI II in other contexts

To see whether HEIDI II could be easily adapted to other industrial contexts, an effort was made to use HEIDI II to prioritize emissions from the Nanticoke Power Generation facility near Toronto, Canada. Table 38 provides a list of tasks that had to be accomplished to adapt HEIDI II to prioritize emissions from Nanticoke, and commentary on the relative ease of accomplishing the tasks.

Adapting HEIDI II to a coal-fired power generation facility was relatively easy for modules two and three, but difficult for model one as a result of the “black-box” nature of the dispersion modeling. The Nanticoke example was particularly easy since the population data was already in place within HEIDI II and the meteorology implied by HEIDI II is appropriate for the geographic location of the facility.

The main difficulty in applying HEIDI II to the Nanticoke power generation facility resulted from the stack height. While stack heights available in HEIDI II were 5 metres, 15 metres, and 30 metres, the actual stack height at the Nanticoke power generation facility is 198 metres(Environment Canada 2005). The dispersion modeling in Module 1 of HEIDI II was applied through a series of transfer factors which are specific to the stack heights available in HEIDI II. Thus, a stack height of 200 metres could not be appropriately represented.

The full adaptation of HEIDI II was completed despite this restriction, using 30 metres as the stack height for the modeling predictions. This was done (i) to test the difficulty of applying modules 2 and 3 to another context, and (ii) since, in the context of a screening tool, the ranking results could still indicate substances which might warrant further investigation.

HEIDI II could not easily be adapted to any industrial emissions for which exposure is mainly through non-inhalation sources. Even if emissions occur to the air, this limitation includes any industry that emits mostly organic emissions or any other emissions that they partition easily into soil and vegetation. As well, the assumptions about data values included in the Nanticoke model for substances that were not originally a part of HEIDI II have not been vetted by a multistakeholder group, and may be incorrect or unacceptable to some stakeholders.

Table 38: Tasks involved in adapting HEIDI II to another industrial context

Task	Comments
Obtain annual emissions for Nanticoke	Relatively easy. They were obtained through the NPRI in the same way that the refinery emissions were obtained
Check whether data used for stack height in HEIDI II are relevant for power facilities.	HEIDI II uses stack heights of 5, 15, and 30 metres. The height of Nanticoke's stack is 198 metres (Environment Canada 2005). Thus the dispersion modeling transfer factors used in HEIDI II are unlikely to apply to dispersion of pollutants from the Nanticoke Power generation facility. However, all of the petroleum refinery stacks are actually higher than 30 metres as well (heights range from ~50-110 metres). Thus the application of HEIDI II was continued as a proof-of-concept to test its feasibility.
Check whether toxicity data was available in HEIDI II for any of the substances emitted at Nanticoke	Toxicity data was available in HEIDI II for only 9 out of 27 substances
Check for toxicity data from the major agencies (Health Canada, EPA)	<u>Air Toxics:</u> Toxicity data was readily available from either HC or EPA for 6 of the 14 air toxic substances with missing data; toxicity data was available for a further 6 of the air toxics from Cal OEHHA or RIVM. <u>CACs:</u> HEIDI handles SOx, NOx, and primary $PM_{2.5}$. Nanticoke also emits PM_{10} and total PM. Although epidemiological data is available for PM10 from the original source of information (C-R functions are available for PM_{10} and chronic bronchitis, hospital admissions for COPD and pneumonia, and ER visits from asthma), HEIDI II is intentionally designed not to estimate the dispersion of PM_{10}. Health effects from PM_{10} and $PM_{2.5}$ are highly correlated and including both would result in double-counting. <u>Summary:</u> Data is not easily available for the following substances: aluminum, copper, carbon monoxide, total PM, and "VOCs".
Make assumptions about substances and C-R data to include	The following substances were not included in the adaptation of HEIDI II to the Nanticoke coal-fired power generation emissions: • Aluminum: is a suspected toxin, but no chronic C-R data was available. The amount released is 266 tonnes annually. • Copper: is a suspected toxicant, no chronic C-R data could be found and the annual emissions are very small (1.07 tonnes annually) • Carbon monoxide appears to be mainly an acute toxicant. HEIDI II was designed to assess chronic toxicity, so CO was not evaluated

	• Total PM and PM10: HEIDI II is not able to predict the dispersion of these substances. The original PM and dispersion data came from an AERMOD model and was dropped into HEIDI II as a ”black box”. $PM_{2.5}$ was assumed to be representative of the health effects of all CAC emissions, which are highly correlated with each other (this includes emissions of gaseous co-pollutants). I.e., PM10 and total PM are emitted from refineries as well and were not included in HEIDI II. They are excluded here for similar reasons. • “VOCs” -: toxicity is suspected but not confirmed. VOCs were included as harmful based mainly on their ability to cause ozone formation. Ozone was omitted from the original HEIDI II model and so is omitted again here. Additionally, VOCs are likely to partition quickly into organic media such as vegetation and soil, and so inhalation is likely to be a minor route of exposure.
Check for population data	In the case of the Nanticoke power generation facility, it is within the same postal code as the Imperial Oil Nanticoke refinery, so the population data for the facility is already available within HEIDI II.
Check for background data	Difficult for substances that were not included in HEIDI II; background data for most substances is not readily available from Environment Canada or Ontario Ministry sources; values were derived based on those cited in federal or provincial documents, or in some cases were assumed to be zero. For metals, ambient levels where available often refer to the amounts bound to PM rather than gas-phase concentrations, suggesting that metals may be more properly treated as components of the PM phase, or class 3 substances.
Check for DALY Data	Moderately easy. Given the relative crudeness of the DALYs already being used in HEIDI II, it was possible to follow up on the references used during development of HEIDI II and substitute appropriate DALY values in most cases
Recode in Excel	Time required for someone experienced in Excel: one day. Major tasks were replacing the substance and data lists that feed into the formulas. Many sheets were deleted which simplified the overall model.
Identify probabilistic data for each variable	Moderately difficult: sources used to derive distributions for HEIDI II were well-documented and typically provided data for substances not previously included in HEIDI II. The exception was for the Background variable, which had relied on data from several locations to develop a distribution. In this case, a simple standard deviation equivalent to 10% of the mean value was implemented
Recode in Matlab	Straightforward for someone familiar with the original HEIDI II code.

2.3.4.1 Predictions for Nanticoke Power Generation Facility

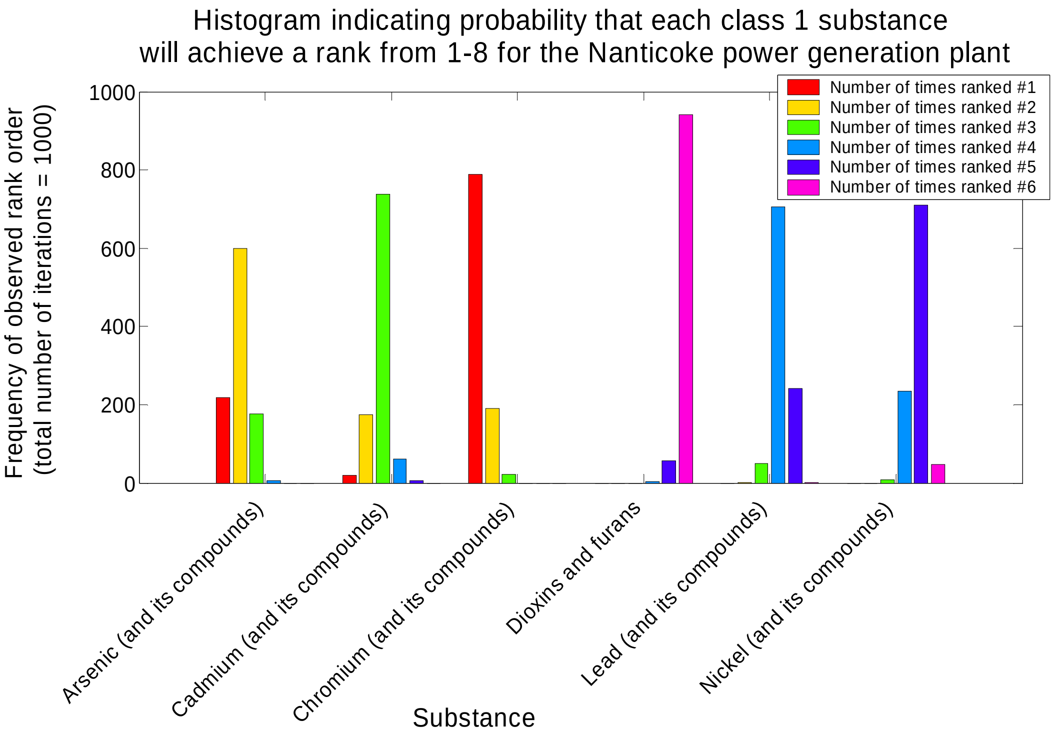


Figure 38: Frequency with which each class 1 substance achieved each possible rank during the Monte Carlo simulation. A fairly clear priority order is apparent from the simulation

Figure 38, Figure 39, and Figure 40 show the ranking results of the Monte Carlo simulation for the Nanticoke coal-fired power facility. The results from this analysis (which is based on predicted incidence) suggest that of the class 1 substances emitted from the Nanticoke facility, chromium and arsenic are of greatest concern, that of the class 2 substances, vanadium and selenium may be of concern, and that the order of priority for the three class 3 substances included in the model is clearly PM from SOx, PM from NOx, and then primary PM.

If desired, it should be possible to conduct further in-depth analysis for this facility, similar to the analyses conducted for HEIDI II.

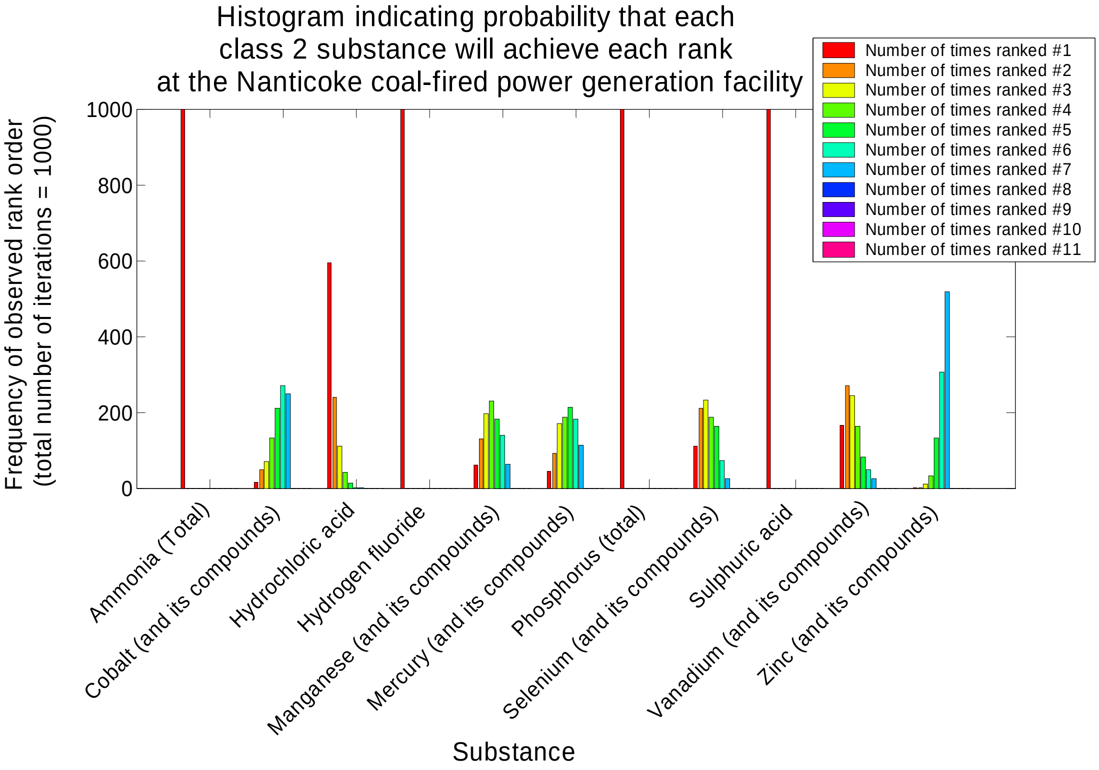


Figure 39: Frequency with which each class 2 substance achieved each possible rank during the Monte Carlo simulation. For some substances, zero incidence was predicted throughout the simulation – this is represented by a #11 rank.

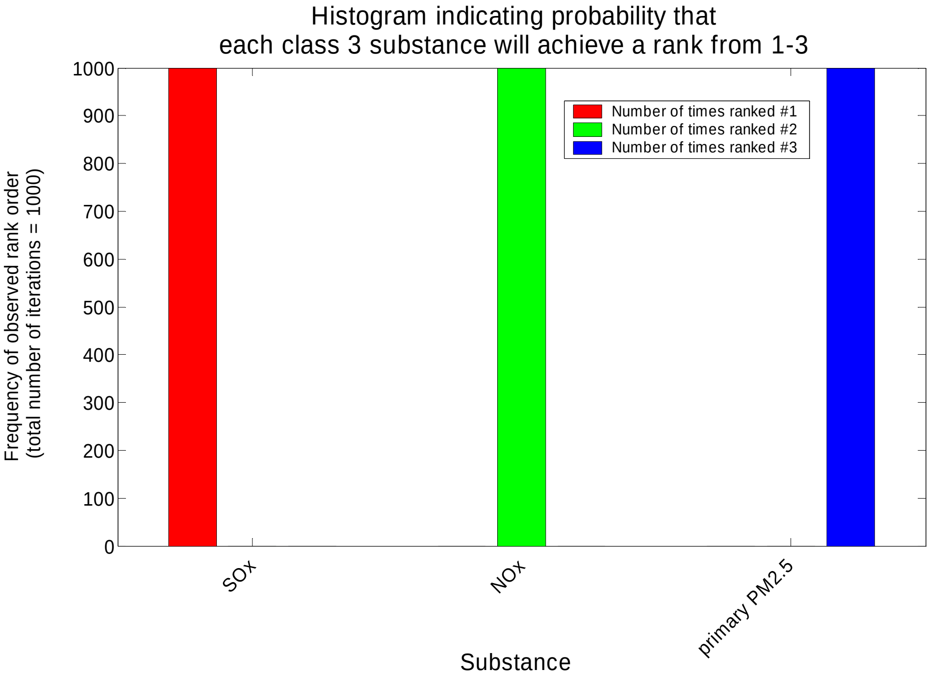


Figure 40: Frequency with which each class 3 substance achieved each possible rank during the Monte Carlo simulation. The order of priority for class 3 substances is clear.

2.3.5 Discussion

Use of a measure such as impact equivalents adds little to the current understanding of priority substances as predicted by HEIDI II, but may be a useful communications tool. Impact equivalents provide a sense of relative toxicity of emissions within a class, using well-known substances as a baseline. This allows easy comparison of substances across impact measures and straightforward identification of substances with relatively high impacts, such as nickel, PAH, BTEX, sulphuric acid, and vanadium (for the hypothetical refinery scenario). However, because any sense of absolute impact is lost, the impact equivalents must be presented with contextual information indicating whether the high values are of concern, perhaps relative to a standard risk level such as the *de minimis* risk. The values are also strongly dependent on the emissions selected by the HEIDI II model, and must be determined separately for each location.

The analysis of the refineries in Sarnia suggests that HEIDI II's approach of treating refineries in isolation is not appropriate for cases where the same population is exposed to emissions from multiple refineries. However, identifying emissions for reduction and responsibility, or "ownership" of these emissions becomes complex, particularly for class 2 substances, where there is assumed to be a level of exposure below which adverse effects will not occur.

Comparison of HEIDI's rankings to those which would be generated by TRACI suggested some correlation between priorities for class 1 and class 2 substances, with less concordance for class 2 substances. Comparing health impacts for class 3 substances was found to be invalid.

Analysis shows that it is technically not too difficult to adapt HEIDI II to other sets of emissions. However, the validity of making this adaptation must be assessed on a case-by case basis. HEIDI II could only be adapted to emissions that emanate from a point source. Only three stack heights are available within HEIDI II, and may not adequately represent emissions scenarios from other contexts. Additionally, HEIDI II assesses only exposure through inhalation. This is valid for HEIDI II by virtue of the specific emissions considered – none of which are expected to have significant persistence in the organic fraction. The exposure pathways for substances which are likely to partition into soil, vegetation and water would not be adequately represented by

HEIDI II. It would therefore be inappropriate to attempt to adapt HEIDI II to many other industries. Emissions from coal-fired power plants are similar to emissions from petroleum refineries in this way, which is why an effort was made to adapt HEIDI II to the Nanticoke coal-fired power generation facility. Additionally, Nanticoke is the largest coal-fired generating station in Ontario, and has been targeted by environmental groups as “Canada’s number 1 polluter”(Ontario Clean Air Alliance 2003). As with refineries, most public attention focuses on CAC emissions from power plants, rather than air toxics, but the analyses presented above suggests that HEIDI II can distinguish priorities within the air toxics classes.

3 Part 3: Discussion

3.1 Model Predictions

When the CCME initiated the National Framework for Petroleum Refinery Emission Reductions (NFPRER), its goal was to gather information that would aid jurisdictions in setting facility emissions caps for Canadian petroleum refineries. Development of a ranking model such as HEIDI was not an initial component of the framework, but was identified by the Health Prioritization Subgroup (HSP) as a potentially useful tool to inform jurisdictional decision-making about allowable emissions for local refineries. The HSP recommended that the HEIDI II model be used as one of a suite of information sources, including information about local concerns.

The predictions from HEIDI II suggest that air toxics emissions of concern at petroleum refineries across Canada include nickel, PAH, BTEX, hydrogen sulphide, sulphuric acid, and vanadium. Given the uncertainty and assumptions inherent in HEIDI II it is premature to suggest that efforts to reduce air toxics refinery emissions should target these particular substances and no others; however, further analysis of the potential for adverse health impacts from these emissions is warranted at refineries where they are emitted. Given the diverse types of health impacts that are predicted for the substances included in HEIDI II and the vastly different annual emissions associated with each refinery, a cost-benefit analysis might be appropriate to compare emissions on the basis of how much reduction can be achieved, the associated costs, and the associated health benefits.

In HEIDI II, vanadium and nickel were frequently co-identified as being emissions of concern. Nickel was treated as a carcinogen (lung cancer), and vanadium was treated as an upper respiratory tract irritant, based on occupational and environmental evidence (i.e., (WHO (World Health Organization) 2000)). However, the toxicity of vanadium is uncertain and pure vanadium is not distinguished from vanadium pentoxide. Transition metals have previously been associated with oxidative stress-related damage to DNA, suggesting a biological mechanism for carcinogenesis (Valko, Rhodes et al. 2006), and chronic irritation is known to generate oxidant stress in the lung and induce basal cell hyperplasia in chronic lung disorders. The low-level induction of respiratory tract irritation documented for vanadium could signal pre-carcinogenic activity. California listed vanadium pentoxide as a carcinogen for the purpose of drinking water safety in 2005 (Office of Environmental Health Hazard Assessment 2005), confirming that it is considered a carcinogen under other exposure conditions, and also suggesting that its characterization by regulators is in flux. This year, the IARC reviewed vanadium pentoxide and classified it as “possibly carcinogenic to humans” based on sufficient evidence for carcinogenicity in mice but insufficient evidence about its effects in humans (IARC (International Agency for Research on Cancer) 2006). They also note that vanadium pentoxide is rapidly absorbed when inhaled, which suggests that airborne sources may be of particular concern.

Both nickel and vanadium are impurities (less than 1 % of the mixture) frequently found in crude oils. However, whether or not the emissions concentrations of Ni and V are correlated depends on the source and composition of the crude oil refined at each refinery. The proportionality of vanadium to nickel is not consistent over all crude oils; it depends on the geographic origin of the crude (Lewan 1984). Typically rocks with high sulfur content expel crude with high vanadium to nickel ratios, while rocks with low sulfur content expel crude with a wide variety of V/(V+ Ni) ratios. Jurisdictions regulating refineries that process crude containing both impurities may choose to implement stringent emissions caps regarding transition metals as a precautionary strategy.

In general, the largest health effects appear to be attributable to particulates (both primary and secondary), which aligns well with the current federal regulatory focus on NO_x and SO_x as priority ambient pollutants for reduction (Bilateral Air Quality Committee 2004; Farnsworth 2005; Canadian Council for Ministers of the Environment 2006). HEIDI II does not analyse health impacts of O_3 or VOC emissions, both of which contribute to smog formation, a known risk factor for impaired cardiovascular and respiratory health (i.e., (Dockery, Pope et al. 1993; Pope, Thun et al. 1995; Brauer and Vedal 1999; Kunzli 2002; Dominici and Burnett 2003; World Health Organization (WHO) 2003; Cohen, Anderson et al. 2004)). The potential for smog formation from refineries emissions was not included in HEIDI II because of the problem of “double-counting”, where health impacts of emissions such as NO_x, O_3, and VOCs might be accounted for twice: as primary pollutants and as secondary pollutants. Instead, $PM_{2.5}$ was assumed to be an indicator of overall air quality, and the concentration-response functions used in HEIDI II were assumed to be representative of co-exposure of PM with gaseous pollutants (McColl, Gower et al. 2004).

Using time-series techniques, Burnett found that for co-exposure to PM and gaseous pollutants in 11 Canadian cities, improvements in health from reduction of some gaseous co-pollutants may be significantly greater than what would be predicted by $PM_{2.5}$ alone (Burnett, Cakmak et al. 1998). In a multipollutant model examining daily mortality in eight Canadian cities, exposure to $PM_{2.5}$ explained only 28% of variation, with the remaining effects accounted for by gases (Burnett, Brook et al. 2000). Canadian results suggest that substance-specific dose-response functions derived from multipollutant models are the most accurate method of estimating impacts such as respiratory and cardiac hospitalizations (Burnett, Smith-Doiron et al. 1999). Although time-series research is most relevant for short-term relationships between ambient air pollution and health outcomes, it is still considered valuable for demonstrating the adverse effects of pollution, identifying the toxic components, and providing indirect evidence of the plausibility of long-term health effects (European Centre for Environment and Health 2000; Bell, Samet et al. 2004). Although complex to implement, explicit consideration of the impacts of individual emissions from refineries that contribute to smog formation as well as the impacts of smog itself would improve HEIDI II.

The model also suggests that there are several emissions which are unlikely to be associated with significant health impacts even at the limit of uncertainty in worst-case scenarios. These substances can therefore be regarded as low priority for emissions reduction strategies unless new toxicological evidence emerges or there are dramatic changes in emissions.

3.1.1 Emissions reduction

Two distinct approaches to adjusting emissions profiles from point sources exist. *Proportional reduction* implies that the total mass emitted is reduced, with peak, average, and minimum concentrations being simultaneously and proportionally reduced. This approach would always be beneficial for reducing health effects of class 1 and class 3 emissions, where predicted incidence is directly related to delivered concentration.

However, since class 2 substances only initiate an effect above a particular threshold, and the magnitude of effects is not linearly related to delivered concentration, proportional reduction would be useful for class 2 substances only in cases where exposure above the threshold occurs. The extent of benefits achieved would depend on the extent to which emissions reduction reduced the gap between exposure and threshold concentration. As well, because HEIDI II predicts only chronic health effects, proportional reduction of emissions would really only be beneficial in cases where the emissions levels do not fluctuate significantly.

In the case of class 2 substances which exhibit large fluctuations in emissions levels over time, *peak-shaving* might be a more practical approach. This approach focuses on reducing emissions during periods of high release so that all (or most) emissions fall below the threshold level. Although this approach does not require a total emissions reduction (periods of minimum emission could theoretically simultaneously be adjusted upwards without exceeding the threshold), an ideal adjustment to the emissions profile would be part of a strategy to reduce emissions overall. For threshold-acting substances, emissions reduction is useful only if the toxicity threshold is being exceeded as a result of current emissions. The probability that this might occur depends on the relative proximity of (i) average annual emissions, (ii) peak emissions concentration (iii) threshold concentration.

Actual emissions reduction approaches used depend strongly on technologies available. Often, emissions reduction technologies can be implemented at varying points in the refining process, with varying results and costs (Baukal, Hayes et al. 2004). Some substances may be reduced in concordance with each other. Most emissions are a result of incomplete combustion, and advanced burner technologies appear to be a cost-effective solution for reducing some emissions including NO_x (Baukal, Hayes et al. 2004). Many emissions control technologies target specific emissions (such as SO_x). By implementing technologies to reduce SO_x losses at the fluid catalytic cracker and SO_x recovery unit as well as SO_x reduction additives, the Chevron Burnaby refinery has reduced its SO_x emissions by over 50% from 2002-2004 (Environment Canada 2006). This might be useful given the predictions of HEIDI II which suggest that several sulphur-containing agents may be harmful, including HS, H_2S, and SO_x.

3.1.2 Probability Distributions for Model Variables

Although most if not all model variables are subject to both variability and uncertainty, a single probability distribution was assigned to each in an attempt to capture the dominant source of variation pertaining to each parameter. A more sophisticated approach might have been to conduct a two-dimensional Monte Carlo Simulation, where the sensitivity of the model predictions resulting from variability and uncertainty of each input was separately assessed. Limitations in data availability prevented this, but the implications for the ranking output should be acknowledged. If the overlap in rankings was due primarily to uncertainty, better data might be able to resolve the area of overlap in rankings and thus clearly define priority substances. However, if inherent variability is responsible for the overlap in rankings, the implication is that substances with “adjacent” ranks might be of equal concern for protection of the most susceptible members of the population.

3.1.3 Characterizing PM exposure-response

HEIDI II used a linear nonthreshold dose-response function to predict health impacts from $PM_{2.5}$. While this form of the exposure-response relationship is broadly accepted and supported by research (Daniels, Dominici et al. 2000; Schwartz, Laden et al. 2002; Samoli, Analaits et al. 2005), the evidence base relies primarily on multicity analyses correlating daily PM levels with health outcomes, which are not ideally suited for assessing exposure-response for chronic outcomes (Pope 2000). Limited evidence for nonlinear exposure-response relationships does exist (Health Effects Institute 2000), and current regulatory approaches to PM imply the existence of a threshold, suggesting that the possibility of a threshold was worth exploring with HEIDI II.

Delivered concentrations of refinery emissions of primary or secondary PM were consistently predicted to be lower than the Canada-Wide Standard for $PM_{2.5}$ (30 $\mu g/m^3$) for zones within 25 km of any refinery. A sensitivity analysis that implemented a low threshold of 1 $\mu g/m^3$ indicated that the effect of including a threshold on the cumulative distribution for predicted incidence due to refinery emissions would be to narrow it and shift it to the left. Environment Canada data suggests, however, that fine PM is ubiquitous in most urban and industrial environments and that one third of Canadians were exposed to average concentrations of $PM_{2.5}$ above the CWS during 2001-2003

(Farnsworth 2005). If this is true then even if a threshold does exist for PM, it is probably consistently exceeded in jurisdictions containing refineries, even before the refinery emissions are considered.

The possibility that a threshold exists for any chemical emitted from multiple sources invokes thorny issues of responsibility. Combined emissions from multiple sources may clearly exceed the toxicity threshold for a particular agent, but any individual emitter contributing concentrations below the toxicological threshold may not feel compelled to reduce emissions as a result. Determining how emissions reductions should be regulated and implemented across sources in cases like this is complex. In the case of PM in particular, emissions result not only from various industries but also from privately-owned vehicles, meaning that "ownership" of the emissions is widely distributed across the affected population. Additionally, the ownership profile for emissions likely will not match the exposure profile for emissions across the affected population, leading to complicated issues of social and environmental justice.

3.1.4 Model structure and interesting questions of valuation, equality, fairness, and ethics

HEIDI II was designed with a particular purpose in mind and was not intended to address complex issues of valuation and ethics. The assumptions inherent in the model and the intended use of the model are clearly documented (McColl and Gower 2004; McColl, Gower et al. 2004). However, the structure of the model raises some interesting questions about scientific perceptions and valuation implied by the model design. These questions may appear to be beyond the scope of HEIDI II, but issues of perception and communication must also be considered by modellers. Air pollution and health is an important issue and the concerned public is a principal stakeholder. Even with extensive documentation, the possibility for misuse and misinterpretation of the model structure, intent and assumptions exists. Additionally, exploring the implications of the model form may identify issues of interest for future modeling efforts.

The predicted health impact value in HEIDI II depends on the number of people affected. Since the total number of people affected at a particular refinery is the same for each emission, this approach is useful for comparing emissions from an individual refinery. HEIDI II was not intended to be used for comparisons between refineries, but the method of valuation raises questions about how we perceive individual risk: this approach implies that a refinery in a rural area with high emissions could have less of an impact than a low-emissions refinery in a densely population area. Certainly the population health impact and direct and indirect economic costs are higher when more people are affected, but the individual-level risk may be a more important number to members of a community. Focusing emissions reduction strategies on large urban centres may convey to smaller centres that they are less important. The social costs of perceived inferiority and irrelevance are unclear.

An approach that suggests that the cumulative impact of refinery emissions is almost totally dependent on the number of people living nearby rather than the magnitude of emissions also has important implications for application of regulations. Does it mean that regulation should preferentially target refineries in densely populated areas? Would this affect competitive fairness in the refining sector?

Finally, this analysis evaluates individual refinery emissions at each location but does not look at the cumulative impact of living near a refinery. Generating a rank order suggests that sufficient protection may be offered to the public by reducing only those emissions with the greatest health impacts. Given that many of the substances included in HEIDI II were selected on the basis on their toxicity and biopersistence, the ethics of defining “harmful” vs. “harmless” seem important. Is this an ethical approach when there is evidence that all emissions could potentially cause harm? In scientific risk assessment, a *de minimis* risk level of 10^{-5} or 10^{-6} is usually applied to signify a “virtually safe” level. However a simple rank order does not communicate a sense of risk to a public user of HEIDI II and the HEIDI II documentation suggests that the predicted incidence values are not representative of reality. For users of HEIDI II trying to understand the level of risk in their community resulting from refinery emissions, the lack of “grounding” of the ranking information with either reliable predicted incidence values or cost-benefit analysis may cause undue concern – and perhaps constitutes an oversight in communication.

3.2 Limitations

Many limitations associated with characterizing variables in HEIDI II are identified and discussed in Appendix C. Although these limitations must be considered to understand the contexts for which HEIDI II is valid, not all points will be discussed here.

3.2.1 Stack heights

HEIDI II offers users three separate stack heights (5 m, 15 m, 30 m) to model dispersion of emissions away from petroleum refineries. This allows users flexibility in characterizing emissions. The 5 metre stack height in particular was intended to represent dispersion patterns for fugitive emissions. In reality, a single stack located in the centre of the refinery property does not represent the location or height of emissions. On most refinery properties, emissions originate from several stacks of varying heights and are combined with fugitive emissions. It may therefore be more appropriate to estimate an “average stack height” which is less than the actual stack height, to account for the contribution from fugitive emissions.

During the validation process, it was determined that the real stack heights of refineries across Canada are all 50 metres or higher (See Table 39). While a model stack height of 30 metres may appropriately represent an “average stack height” for some petroleum refineries (it is not possible to determine to what degree this is true, or for which refineries it would be most appropriate), it is certainly not uniformly applicable, and if this was the intended usage for the term “stack height”, it is not well-communicated to potential users.

Table 39: Stack heights for refineries in Canada as reported in the NPRI database for 2004(Environment Canada 2005).

Refinery	Stack height (metres). A range is provided where more than one stack is present.
Chevron Canada Limited - Burnaby Refinery	50.3
Consumer's Co-operative Refineries Ltd./NewGrade Energy Inc.	71.6-76.2
Husky Oil Operations Limited - Prince George Refinery	No longer operational (no data)
Imperial Oil - Dartmouth Refinery	50.9-61.9
Imperial Oil - Nanticoke Refinery	50-111.9
Imperial Oil - Sarnia Refinery Plan	61-106.7
Imperial Oil - Strathcona Refinery	45.7-108.8
Irving Oil Ltd - Irving Oil Ltd. - Refining	55.2-89

North Atlantic Refining - North Atlantic Refinery	50.3-76.2
Nova Chemicals (Ltd.) - Nova Chemicals (Canada) Ltd.	60.96-106.7
Parkland Refining Ltd. - Bowden Refinery	No longer operational (no data)
Petro-Canada - Edmonton Refinery	76.2-91.4
Petro-Canada - Mississauga Lubricant Center	121.9
Petro-Canada - Raffinerie de Montreal	60.96-100
Petro-Canada - Oakville Refinery	61-100
Produits Shell Canada - Raffinerie de Montreal-est	51.8-68.3
Shell Canada Products - Sarnia Manufacturing Centre	61-91.4
Shell Canada Products - Shell Scotford Refinery	61.2
Sunoco Inc. - Sarnia Refinery	60-99
Ultramar Ltee - Raffinerie St. Romuald	54.9-85

The height of the stack determines the dispersion pattern of emissions from the stack. Taller stacks typically result in dispersion to more distant locations. However, HEIDI II examines only populations within 25 km of the refinery. This suggests that for a real refinery with a tall stack, neither the population affected nor the dispersion pattern of pollution is appropriately represented in HEIDI II. This deficit means that exposure, and thus estimated health impact values are likely poorly estimated.

3.2.2 Geographic Zones selected for Evaluation

The geographic division of areas around each refinery modelled in HEIDI II is also problematic. HEIDI II only examines health impacts within 25 km of each refinery. This may be valid for the air toxics, most of which have half lives on the order of several hours (McColl, Gower et al. 2004) and so experience significant degradation within the first 25 km of dispersion away from the refinery. However, research suggests that long-range transport of secondary PM is significant, and that even in a catchment area of 500 km around a point source, total population exposure is unlikely to be accounted for (Levy, Wilson et al. 2003). For releases from Chicago area power plants (which have taller stacks than refineries), 40% of primary $PM_{2.5}$ exposure, 20% of exposure to $PM_{2.5}$ from sulfates and 25% of exposure to PM from nitrates occurred within 50 km of the source when a surrounding grid of 750 km^2 was used to calculate total exposure (Levy, Spengler et al. 2002). The health impacts from PM are already predicted to be significant in HEIDI II, but this suggests that most of the impacts have not been accounted for. This is particularly important for regions such as southwest Ontario, where the population is dense over a large geographic area, and is probably being simultaneously exposed to PM originating from several refineries.

Calculation of total exposure efficiency and exposure efficiency within-25 km intake fraction would be informative. This measure, sometimes called the “intake fraction” describes the proportion of PM emitted that is actually inhaled and describes the exposure efficiency of a particular source (Evans, Wolff et al. 2002). Its use would provide a sense of how much of the health impact of PM is actually captured by HEIDI II. A comparison of intake fractions for each of the emissions included in HEIDI II might also clarify the where potential reductions might be most beneficial.

3.2.3 Use of annual emissions data

HEIDI II uses annual emissions data for each refinery as reported to the NPRI. These values are usually modelled rather than measured and represent an estimated composite of point source, area, and volume emissions across the refinery property, and includes stack emissions, fugitive emissions, escape from containment, and evaporation from spills.

There is some evidence that the method used to calculate emissions (Canadian Association of Petroleum producers (CAPP)-sanctioned method) may be inaccurate. A relatively new method of measuring emissions, Differential Absorption Light Detection and Ranging (DIAL) uses laser technology to make a remote measurement of the amount of hydrocarbons in an emissions plume. It is often used in combination with gas-leak cameras, which use infra-red technology to identify existing hydrocarbon leaks. VOC emissions measured at an Alberta refinery using the technology were 9970 tonnes per year, while the CAPP method had estimated ~670 tonnes per year of releases (from combined sources of stack/point, storage/handling, fugitive, and spills) (Chambers 2004). Separate DIAL estimates for methane, VOCs and benzene at a gas processing plant in Alberta was 4 to 8 times higher than detailed CAPP estimates (Chambers 2006). The source of the differences at appeared to be mainly related to fugitive emissions: leaks at storage tanks, valve stem packings, unions, pipe thread fittings, tank vents and hatches and compressor packing vents. Emissions from flares were also underestimated by the CAPP method.

There is currently no remote technology sufficiently advanced to make remote measurements of airborne particulate concentrations. Additionally, some of the refinery emissions included in HEIDI II do not qualify as hydrocarbons (i.e., the metals). However, many of the emissions included in HEIDI II are organic.

These results are troubling: they suggest the possibility that all fugitive emissions are potentially being underestimated by the CAPP-sanctioned method. The 5-metre stack scenario suggests that this error would mainly affect people living closest to the refinery. A possible solution would be increased use of DIAL or similar technologies to detect fugitive emissions from petroleum refineries.

An explicit assumption in the deterministic version of HEIDI II was that emissions are continuous and uniform, but this assumption may be invalid and provides little sense of the most usual emissions level for each substance. It is possible that some emissions are not constant over time, but are periodic and fluctuate between peak levels and zero emissions. Others, emissions events, such as spills, may be one-time high-level releases that would be more properly associated with acute exposures. HEIDI II is not intended to address acute health impacts from refinery emissions, but understanding the extent to which fluctuations occur – and for which particular emissions – would be helpful.

For class 1 and 3 substances, where dose-response is modelled in a linear-nonthreshold manner, predicted health impact is not affected by periodic fluctuations in emissions as long as the total emissions are included in the model. However, for threshold-acting substances, adverse effects are only predicted by HEIDI II in cases where the average annual delivered concentration of the substance exceeds the threshold. This is problematic for the possible case where peak emissions are above the threshold but the annual average is below the threshold. If the threshold is exceeded for a portion of the year, it is possible that adverse health effects could result from the emission but not be predicted by HEIDI II. Additionally, in cases of fluctuating emissions, the background may be more important than it appears, “bumping” the delivered concentration over the threshold during periods when emissions are higher.

3.2.4 Exposure Model

HEIDI II determines the “delivered concentration” of each substance to twenty zones surrounding each refinery. This value, which accounts for dispersion and photodegradation of emissions and the ambient levels of pollutants in the region provides only a limited sense of the exposure of the population in the area. While it does account for the distribution of population relative to the predominant wind direction, the exposure of people affected is estimated based on residential address. In reality, people will move around the area, going to work, school, and recreational activities. As well, most people spend upwards of 90% of their time indoors, and the actual concentration reaching each person might depend on the degree to which pollutants are filtered out by building envelopes. Since filtration of chemicals into indoor environments depends on building construction, including age of the structure, ventilation, and presence of air conditioning, this may differ by neighbourhood, with people living or working in older buildings being more highly exposed. Children and elderly persons are assumed to be exposed to the same concentrations as adults, although activity patterns and amount of time spent outside depend on age. Additionally, since the dose-response function for class 1 and class 2 substances does not differentiate age groups, there is no accounting for potential accumulated exposure to air toxics in elderly persons.

The characterization of background levels may also be problematic: a single concentration was assigned to each refinery location, while in reality the background concentrations may vary over the geographic zones around the refinery depending on the presence and density of sources such as industry and automobiles. This issue is important for the class 2 substances where the ambient levels of pollutants affect whether or not the toxicity threshold might be exceeded as a result of added refinery emissions.

Finally, formation of photochemical smog from VOC emissions was not included in HEIDI II but could potentially be an important source of health impacts.

3.2.5 Dose-response Models

HEIDI II uses the USEPA’s IRIS (Integrated Risk Information System) database to access fully and consistently reviewed toxicological data for many substances. However, there is often a time lapse between availability of new information and its reflection in the database. Many toxicity scores in these databases are based on extrapolation from animal data. (Bailar and Bailar 1999) note that where comparable data exist for humans and animals, they often agree that risk does exist; however, significant uncertainties apply to extrapolating animal data to humans. Additionally, the extensive review process required means that not all chemicals are included. As well, values such as unit risk may differ by an order of magnitude between well-respected organizations such as the EPA and the WHO.

Characterizing impacts also requires decisions to be made about how specific substances are to be treated. Some substances, such as PAHs (polycyclic aromatic hydrocarbons) are often emitted together, and some assessors may opt to treat them as mixtures, applying only one toxicity score to the group, while others may treat them individually. Metals are also a source of difficulty, as their ionic state can affect properties such as toxicity. However, accounting for all the ionic states of different metals can increase the complexity of a model dramatically. Furthermore, toxicity scores are not available for all ionic species of all metals. The approach of HEIDI II was to treat PAH as one entity, and use the best available data for metals: toxicity data for the nearest ionic state of the most commonly emitted form of each metal was selected. HEIDI II also identified an additional mixture class: BTEX (benzene, toluene, ethylbenzene and xylene, which are frequently emitted together and whose critical health effects are similar), for which weighted concentration and toxicity values were derived.

The potential health impact of exposure to each substance was based on a critical endpoint for that substance. This was generally defined as the endpoint that would manifest at the lowest concentration. However, some substances may be related to multiple endpoints as concentrations increase. For example, the endpoint used for H_2S was nasal lesions/nose irritation but studies have also found that at high levels of exposure animals may exhibit CNS (motor activity) effects (Environmental Protection Agency (EPA) 2003). Local air quality standards for H_2S are being reviewed in Ontario because of this (Ontario Ministry of the Environment 2006). Toluene, generally associated with neurological deficits, has also been associated with respiratory tract irritation (Environmental Protection Agency (EPA) 2005).

Similarly, sulphuric acid has been proposed as a carcinogen, but because there is no good concentration-response data available for the substance on which to base cancer incidence predictions, it was treated as an irritant in HEIDI II. These endpoints are disparate and represent vastly diverging levels of impact on quality and length of life for an affected individual.

Finally, the dose-response model used for class 1 and class 2 substances does not discriminate by age group. Thus, children who are undergoing rapid development are assumed to respond to toxic exposures in the same way as adults.

3.2.6 Sensitivity Analysis

The sensitivity analysis was able to identify some variables that were important to predicting health impact – particularly the concentration-response / toxicity data. However, it was unable to evaluate the influence of the dispersion modelling approach the choice of meteorology or the choice of terrain. This was a major disadvantage since the dispersion model comprised all of module one. Because of the "black box" character of the dispersion model, there was no way to test how (or how much) changing the predominant wind direction or altering the geography could affect predictions of impact. Understanding these effects would be important for understanding the limitations of the model, but also for determining how policy might be made more relevant for specific locations.

If distinct distributions could have been chosen to characterize uncertainty vs. variability in input distributions, two dimensional Monte Carlo simulations could have been conducted to identify which was the more important source of variation in the predicted incidence values. For example, there may be both uncertainty and variability in the ED05 values used to anchor the dose-response function for class 2 substances. Uncertainty could arise from the extrapolations required to calculate human equivalent values from experimental animal data, and variability within a population, where some people may be more susceptible to disease development because of genetic profiles, previously existing diseases, or environmental or occupational co-exposures. If the contributions of uncertainty and specific sources of variability could be distinguished, the results of sensitivity analyses variables might provide useful insight into the utility of specific policy decisions.

Gough (Gough 1997) identifies 'indeterminacy' as a type of uncertainty where causal links, networks, and processes cannot be predicted. It is possible that there are relationships important for predicting impacts of refinery emissions which have not been identified by the scientific community. However - it is not possible to test for or identify these during modelling. Acknowledging the limitations of HEIDI II and describing the assumptions inherent in its design and its intended use are attempts to frame the use of HEIDI II within a context of known relationships.

3.2.7 Valuation

Valuation of human health impacts is a question of how best to represent human morbidity and mortality for the purpose of the tool or study. Powell (Powell, Pearce et al. 1997) describes four main approaches to the valuation phase in LCIA: (i) distance-to-target techniques, in which the magnitude of deviation in performance from some environmental target or standard forms the basis of the weight; (ii) environmental control costs, in which the expense of controlling environmental damage is used to develop weights; (iii) environmental damage costs, in which explicit or implicit willingness to pay (WTP) measures (to avoid environmental impacts) are developed; and (iv) scoring approaches, in which weightings are derived by experts. Each approach is subject to limitations. For example, the distance-to-target and environmental control costs approach may be based on standards that are politically achievable rather than scientifically defensible, while WTP is an emerging technique that relies on currently available economic estimates of damage. Scoring approaches may not be transparent, and while they are likely to be based on a high degree of expert knowledge, they may not accurately reflect the interests of the society to which they will be applied.

DALYs, or disability-adjusted life years, are an example of a scoring approach and assign disability weights to aggregate the severity of different non-lethal disease stages. They incorporate the number of years lived with a disabling illness (YLD, years lived disabled) and the number of years lost to premature mortality (YLL, years of life lost) (Mathers, Stein et al. 2002). DALYs have been developed by both de Hollander (de Hollander, Melse et al. 1999) and the World Health Organization (Murray and Lopez 1996; Mathers, Stein et al. 2002) for a variety of health outcomes, and provide a practical, consistent metric for comparison of a wide range of illnesses of varying severity (Udo de Haes, Jolliet et al. 1999). As well, the metric is framed as a health loss, which may be intuitive for decision-makers.

DALYs are intended to account for the relative difference in quality and years of life lost from different types of impacts. They were incorporated into HEIDI II so that health endpoints of differing severity could be compared. Attempts to rank substances across classes using probabilistically generated DALYs resulted in collections of CDFs of very different shapes which overlapped extensively. It is difficult to extract a defensible prioritization order from such a comparison. A comparison of across-class ranking methods found that although PM (class 3) was frequently identified as a high priority substance, conclusions about class 1 and class 2 substances depended strongly on the method used to create the ranking.

DALYs may be sensitive to mild health impacts, weighting them too heavily. They compare health loss to a hypothetical profile (Hofstetter 2001), and may therefore imply an unrealistic comparison with perfect health. As well, although age-weighting is included in DALYs, its implementation still requires refinement (Hofstetter 2001), and in the operationalization of DALYs in HEIDI II specifically, the age structure of the population, the average duration of disease, and the valuation of death and disability was assumed to be similar to a Dutch population. This is likely a reasonable proxy for a Canadian population in order to simplify the analysis but does introduce an additional source of uncertainty. DALYs may not yet be sufficiently evolved to appropriately characterize the potential consequences of noncancer toxicological effects (Pennington, Crettaz et al. 2002), which would affect their utility in predicting impacts from class 2 substances in particular. Finally, DALYs may not account for cost of illness to individuals or to the community, which may be different for different types of outcomes and therefore be important for prioritization schemes.

3.3 Use of HEIDI II

HEIDI II was designed to be a transparent, publicly available ranking tool. It was developed with significant input from a variety of stakeholders, and was initially coded in a commonly used spreadsheet program. Code such as visual basic which prevented use of HEIDI II by several stakeholders due to agency-level security settings was avoided, and the final product was made available on a publicly accessible website (www.irr-neram.ca).

Currently, the probabilistic version of HEIDI II exists in Matlab code. The intent is to publish any relevant predictions or commentary resultant from development of this version of the model, but it can no longer be considered transparent or publicly available. The distributions used to represent each variable were selected by the researcher, sometimes in consultation with other academic personnel, but without input from a range of stakeholders. Matlab is not a program that is commonly used, limiting both the accessibility of the code and the results to interested parties with appropriate skills. Because some expertise is required to understand the code, run the program, and interpret the results, the model should be considered generally inaccessible.

The research carried out does suggest that the deterministic, excel-based version of HEIDI II may be as useful for prediction within-class rank order of refinery emissions as the probabilistic version. This suggests that the excel version should remain in the public domain. However, issues of clarity are likely to frustrate users of this version as well. Although HEIDI II is constructed in a software environment that is (almost) universally available, and is well-annotated and documents, the tool is not simple to understand and use and the technological report describing the assumptions and limitations of the model is dense. Proper application of HEIDI II requires a high level of literacy, scientific knowledge, and computer skill.

While the intent of HEIDI II was to develop a screening-level tool, the model provides predictions of annual case incidence. The current report uses these values of predicted incidence to investigate the model’s ability to function as well as its predictions for individual refineries and highlight substances that may be of concern – but simultaneously advises that these values are not reliable. This is likely to create confusion for anyone interested in understanding the results of HEIDI II. This report and the technical report that accompanies the original HEIDI II attempts to clarify the intent and limitations of the model, but cannot prevent its misuse or misinterpretation. In particular, it would not be surprising to find that incidence predicted by HEIDI II was cited by external sources such as community groups as if it was a valid prediction for a specific location.

Communication with all stakeholders is important for health risk, and for a tool that has been made publicly available as HEIDI II has, the public must be included as a stakeholder. The level of knowledge of interested members of the public should be explicitly considered when developing materials designed to help people use HEIDI II properly.

One difficulty of using HEIDI II in conjunction with the other information gathered by the NFPRER, in particular, the benchmarking data, is that not all the same emissions are addressed by each analysis. The benchmarking is intended to identify whether emissions from Canadian refineries are converging with emissions levels from refineries in the U.S. However, the benchmarking examined SOx, NOx, CO, VOC, PM_{10}, $PM_{2.5}$, benzene and ammonia. It does not include analysis of several emissions that were identified as being potentially important by HEIDI II; in particular, the metals (Ni and V), BTEX, PAH, HS, and sulphuric acid.

3.3.1 HEIDI II in a new political context?

The Canadian Government recently tabled a new Federal Clean Air Act (2006) which could change the way some of the pollutants included in HEIDI II are regulated. NOx, SOx, $PM_{2.5}$, ammonia and mercury are among the pollutants which would be recategorized under the proposed legislation. Currently, all of these (and many other substances included in HEIDI II) are classified as “CEPA Toxic”, which means that they are recognized as having harmful effects on the environment or present a danger to human life or health. For these substances, the federal government must provide at least one tool or instrument to prevent pollution from emissions of these substances. These tools can address any aspect of the substance’s lifecycle, and range from regulations, pollution prevention plans, environmental emergency plans, and environmental codes of practise to environmental release guidelines. In practise, National Ambient Air Quality Objectives (NAAQOs) were set as non-binding guidelines for several of these substances in the 1970s. While it is now recognized that these guidelines are no longer appropriate, Canada-Wide Standards (CWS) have been developed to replace the NAAQOs for only two substances: $PM_{2.5}$ and ozone. The CWS serve as numeric targets that jurisdictions (such as provinces) can choose to adopt as enforceable standards.

The new act defines new categories for air emissions: “air pollutants” and “greenhouse gases”, and would move several substances away from the CEPA Toxic list and into these categories. The proposed act appears to align treatment of these substances with the US approach, which sets enforceable ambient air standards for "criteria air contaminants" – defined as those which are present in the air as a result of emissions from multiple point and/or area sources. This could result in more strict regulation of these pollutants and more stringent requirements for pollution prevention planning by provinces. It is unclear what the final content of the act will be – or if it will even be accepted by the House of Commons before another election is called. The proposed act was referred to committee for possible revisions, as a result of wide criticism when it was first tabled.

3.4 Recommendations and Future Research

The NFPRER described a ten year plan for reviewing emissions levels, data needs, and impacts of refinery emissions. The NFPRER Steering committee proposed a that the health prioritization tool be reviewed in 2008 as part of the ten-year plan to gather feedback and improve the framework (CCME (Canadian Council of Ministers of the Environment) 2005). Feedback about HEIDI II will be gathered from the jurisdictions and stakeholders who may have used it – and a decision about whether to update the tool will be made based on stakeholder input. It is unclear whether the information collected will be made public but it would be useful for developers of future policy analysis tools for industrial emissions.

If HEIDI II was ever to be upgraded, an open source software development approach might be most beneficial. "Open source" means that the code for the software would be freely accessible to all users, such that anyone is able to copy it, modify it, and redistribute it back to the user community. This allows for a variety of approaches and agendas in development of a single software tool, and permits many people with adequate expertise and a vested interest in the product's ability to perform to work on developing the product simultaneously. The model could then be wrapped in a user-friendly GUI, allowing people who are unfamiliar with the technical details required to understand the code to use it and obtain results easily. They would still have access to criticism and commentary about the model, and information and opinion about its limitations and assumptions from the open source community involved in its development.

Future versions of HEIDI II should eliminate the Parkland and Oakville refineries, which were closed in 2001 and 2004, respectively. While their inclusion in the model does not affect model runtime or predictions for other jurisdictions, it does date the model, and add unnecessary complication and data.

If a viable methodology could be identified, future versions of HEIDI II should account for the impacts of emissions which contribute to smog formation, including O_3, VOCs, and NO_x. This must be done in a way that avoids double-counting.

As, well, the model should be continuously updated with new information about toxicity of each emission. Vanadium is an example of a substance which should be followed carefully as new evidence supporting or refuting its potential carcinogenicity becomes available.

4 Conclusions

Ultimately, science-based policy decisions all include a subjective element, and require inferences, extrapolations, and judgement (Sexton 1995). Regulators must decide what level of risk is protective, and how much uncertainty is acceptable. They often face significant pressure from corporations and the public and face difficult economic decisions. HEIDI II is one tool that may help identify emissions of concern from the petroleum refining sector.

References

(2006). An Act to amend the Canadian Environmental Protection Act, 1999, the Energy Efficiency Act and the Motor Vehicle Fuel Consumption Standards Act (Canada's Clean Air Act). Canada's Clean Air Act. First Reading.

Abt Associates (Nov. 2002). Particulate-Related Health Impacts of Emissions in 2001 From 41 Major US Power Plants. Prepared for the Environmental Integrity Project. Rockefeller Family Fund. Available from http://www.abtassociates.com/reports/Abt_41_power_plant_report_Nov19.pdf.

Agency for Toxic Substances and Disease Registry (ASTDR) (1998). Toxicological Profile for Sulfur Trioxide and Sulfuric Acid. Atlanta, GA, U.S. Department of Health and Human Services, Public Health Service.

Bailar, J. C. and A. J. Bailar (1999). "Common Themes at the Workshop on Uncertainty in the Risk Assessment of Environmental and Occupational Hazards." Annals New York Academy of Sciences **895**: 373-376.

Bailar, J. C. and A. J. Bailar (1999). "Risk Assessment - the Mother of All Uncertainties: Disciplinary Perspectives on Uncertainty in Risk Assessment." Annals New York Academy of Sciences **895**: 273-285.

Baird, S. J. S., A. Cohen, et al. (1996). "Noncancer risk assessment: a probabilistic alternative to current practice." Human and Ecological Risk Assessment **2**: 79-102.

Bare, J. (2004). traciUSCharFactorsjuly222004.xls. personal communication.

Bare, J. C., G. A. Norris, et al. (2003). "TRACI The Tool for the Reduction and Assessment of Chemical and other environmental impacts." Journal of Industrial Ecology **6**(3-4): 49-78.

Baukal, C. E., R. Hayes, et al. (2004). "Nitrogen Oxides Emissions Reduction Technologies in the Petrochemical and Refining Industries." Environmental Progress **23**(1): 19-28.

Bell, M., J. M. Samet, et al. (2004). "Time-series studies of particulate matter." Annual Reviews in Public Health **25**: 247-280.

Bilateral Air Quality Committee (2004). United States - Canada Air Quality Agreement: Progress Report 2004, International Joint Commission.

Brand, K., L. Rhomberg, et al. (1999). "Estimating noncancer uncertainty factors: are ratios NOAELs informative?" Risk Analysis **19**(2): 295-308.

Brand, K. P., G. M. Gray, et al. (1997). A Distributional Approach for Characterizing Cancer Potency. Boston, MA, School of Public Health, Harvard.

Brauer, M. and S. Vedal (1999). "Health Effects of Photochemical Smog: Seasonal and Acute Lung Function Change in Outdoor Workers." Journal of Environmental Medicine **1**: 163–170.

Bunce, N. J., L. Liu, et al. (1997). "Reaction of Naphthalene and Its Derivatives with Hydroxyl Radicals in the Gas Phase." Environmental Science & Technology **31**: 2252-2259.

Burke, T. A., J. Doull, et al. (1996). Human Health Impact Assessment In Life Cycle Assessment: Analysis By An Expert Panel, ILSI Health and Environmental Sciences Institute.

Burke, T. A., J. Doull, et al. (1996). Human Health Assessment and Life Cycle Assessment: Analysis by an Expert Panel. Washington, DC, International Life Sciences Institute.

Burnett, R. D., J. R. Brook, et al. (2000). "Association between particulate- and gas-phase components of urban air pollution and daily mortality in eight Canadian cities." Inhalation Toxicology **12(Supplement 4)**: 15-39.

Burnett, R. T., S. Cakmak, et al. (1998). "The effect of the urban ambient air pollution mix on daily mortality rates in 11 Canadian Cities." Canadian Journal of Public Health **89**(3): 152-156.

Burnett, R. T., M. Smith-Doiron, et al. (1999). "Effects of particulate and gaseous air pollution on cardiorespiratory hospitalizations." Archives of Environmental Health **54**(2): 130-139.

California Air Resources Board (2004). Health and Air Pollution, California Environmental Protection Agency. **2004.** Available from http://www.arb.ca.gov/research/health/health.htm.

California Air Resources Board (2005). Hot Spots Unit Risk and Cancer Potency Values, Office of Environmental Hazard Health Assessment. **2006**.

Calvert, J. G., R. Atkinson, et al. (2002). The Mechanisms of Atmospheric Oxidation of Aromatic Hydrocarbons. New York, Oxford University Press.

Canadian Council for Ministers of the Environment (2006). Canada-Wide Standards, Canadian Council for Ministers of the Environment.

CCME (Canadian Council of Ministers of the Environment) (2005). The National Framework for Petroleum Refinery Emission Reductions (NFPRER), CCME (Canadian Council of Ministers of the Environment) Retrieved February 14, 2005 from http://www.ccme.ca/initiatives/climate.html?category_id=69.

CCME (Canadian Council of Ministers of the Environment) (2005). The National Framework for Petroleum Refinery Emission Reductions (NFPRER). Winnipeg, MB, CCME (Canadian Council of Ministers of the Environment).

Chambers, A. (2004). Optical Measurement Technology for Fugitive Emissions from Upstream Oil and Gas Facilities. Edmonton, Alberta Research Council Inc.**:** 65.

Chambers, A. (2006). Measuring Fugitive Emissions of Hydrocarbons at Gas Processing Plants. 15th Annual International Emissions Inventory Conference - Reinventing Inventories - New Ideas in New Orleans, New Orleans, Louisiana, Alberta Research Council, Inc.

Charles, R. and O. Jolliet (2003). "Fate of pesticides in plant." Life Cycle Impact Assessment of Pesticides – When Active Substances are Spread into the Environment. 19th Discussion Forum on Life Cycle Assessment. Retrieved March 2007 from http://www.lcainfo.ch/DF/.

Cohen, A., H. Anderson, et al. (2004). Mortality Impacts of Urban Air Pollution. Comparative Quantification of Health Risks: Global and Regional Burden of Disease Attributable to Selected Major Risk Factors. Ezzati M, Lopez AD, Rodgers A and C. Murray. Geneva, World Health Organization.

Corporate Research Associates Inc. (1997). Tracking Survey of Canadian Attitudes Towards Natural Resources Issues, 1997 Final Report. Ottawa, Natural Resources Canada**:** 87.

Crouch, E. A. C. (1996). “Uncertainty distributions for cancer potency factors: Laboratory animal carcinogenicity bioassays and inter-species extrapolation.” Human and Ecological Risk Assessment **2**(1): 103-129.

Cullen, A. C. and H. C. Frey (1999). Probabilistic Techniques in Exposure Assessment. New York, Plenum Press.

Curran, K. (2004). Ambient Air Quality Data. personal communication with S. Gower. Ottawa.

Daniels, M. J., F. Dominici, et al. (2000). “Estimating Particulate Matter-Mortality Dose-Response Curves and Threshold Levels: An Analysis of Daily Time-Series for the 20 Largest US Cities.” American Journal of Epidemiology **152**: 397–406.

Dann, T. (1998). Ambient Air Measurements of Polycyclic Aromatic Hydrocarbons (PAH), Polychlorinated Dibenzo-p-Dioxins (PCDD) and Polychlorinated Dibenzofurans in Canada (1987-1997) Report Series Number AAQD 98-3. Ottawa, Analysis and Air Quality Division, Environmental Technology Centre, Environment Canada.

de Hollander, A. E., J. M. Melse, et al. (1999). “An aggregate public health indicator to represent the impact of multiple environmental exposures.” Epidemiology **10**: 606-617.

Decisioneering (2000). Crystal Ball. Denver, Optimization Technologies.

Dockery, D. W., A. Pope, et al. (1993). “An association between air pollution and mortality in six U.S. cities.” New England Journal of Medicine **329**: 1753-1759.

Dominici, F. and R. T. Burnett (2003). “Risk Models for Particulate Air Pollution.” Journal of Toxicology and Environmental Health, Part A **66**: 1883-1889.

Dutch Expert Committee on Occupational Standards (2003). Strong inorganic acid mists containing sulphuric acid: Evaluation of the carcinogenicity and genotoxicity. The Hague, Health Council of the Netherlands**:** 35.

Environment Canada (2003). National Air Pollution Surveillance (NAPS) Network Annual Data Summary for 2002. Ottawa, Environmental Technology Advancement Directorate, Environmental Protection Service, Environment Canada**:** 204.

Environment Canada (2005). 2004 NPRI National Databases - as of April 25, 2006 http://www.ec.gc.ca/pdb/npri/npri_dat_rep_e.cfm.

Environment Canada (2005). NPRI National Pollutant Release Inventory, The Green Lane. Accessed Feb 14, 2005 at http://www.ec.gc.ca/pdb/npri/npri_home_e.cfm. **2005**.

Environment Canada (2006). Case Study: Chevron Burnaby Refinery.

Environmental Health Directorate Health Protection Branch (1996). Health-Based Tolerable Daily Intakes/Concentrations and Tumorigenic Doses/Concentrations for Priority Substances. Ottawa, Health Canada**:** 1-15. Accessed at http://www.hc-sc.gc.ca/hecs-sesc/exsd/pdf/96ehd194.pdf.

Environmental Protection Agency (EPA) (2003). Hydrogen sulfide (CASRN 7783-06-4), IRIS (Intergrated Risk Information System).

Environmental Protection Agency (EPA) (2004). Final Regulatory Analysis: Control of Emissions from Nonroad Diesel Engines. Ann Arbour, MI, Office of Transportation andAir Quality**:** 17.

Environmental Protection Agency (EPA) (2005). Toluene (CASRN 108-88-3), IRIS (Integrated Risk Information System).

ESRI Inc. (1999-2002). ArcMap. Redlands, CA, ESRI.

European Centre for Environment and Health (2000). Quantification of the Health Effects of Exposure to Air Pollution Report of a WHO Working Group Bilthoven, Netherlands 20-22 November 2000, World Health Organization.

Evans, J. S., L. Rhomberg, et al. (2001). “Reproductive and developmental risks from ethylene oxide: a probabilistic risk characterization of regulatory thresholds.” Risk Analysis **21**: 697-718.

Evans, J. S., S. K. Wolff, et al. (2002). “Exposure efficiency: an idea whose time has come?” Chemosphere **49**: 1075–1091.

Farnsworth, P. (2005). Air Quality Policy – National Perspective, Transboundary Air Issues Branch (Environment Canada).

Gaylor, D. W. and R. L. Kodell (2000). “Percentiles of the Product of Uncertainty Factors for Establishing Probabilistic Reference Doses.” Risk Analysis **20**(2): 245-250.

Goedkoop, M. and R. Spriensma (1999). The Eco-indicator 99 A Damage Oriented Method for Life Cycle Impact Assessment. Amersfoort, Pre - product ecology consultants**:** 1-111. [Internet]. Retrieved July 2004 from www.pre.nl.

Gough, J. D. (1997). “Environmental Decisions Making and Risk Management for Groundwater Systems.” Risk **8**(155).

Granville, G. (2003). “Commentary: An Industry Perspective.” Journal of Toxicology and Environmental Health, Part A **66**: 1697-1699.

Hattis, D. and E. L. Anderson (1999). “What should be the implications of uncertainty, variability, and inherent "biases"/"conservatism" for risk management decision-making?” Risk Analysis **19**(1): 95-106.

Hattis, D., P. Banati, et al. (1999). “Human Interindividual Variability in Parameters Related to Health Risks.” Risk Analysis **19**(4): 711-726.

Hattis, D. and K. Barlow (1996). “Human interindividual variability in cancer risks - technical and management challenges.” Human and Ecological Risk Assessment **2**(1): 194-220.

Health Effects Institute (2000). Reanalysis of the Harvard Six Cities Study and the American Cancer Society Study of Particulate Air Pollution and Mortality: A Special Report of the Institute’s Particle Epidemiology Reanalysis Project. Cambridge MA, Health Effects Institute.

Hicks, J. (2005). Stack height for HEIDI II model. personal communication with S. Gower. Toronto.

Hoffman, F. O. and J. S. Hammonds (1994). “Propagation of uncertainty in risk assessments: the need to distinguish between uncertainty due to lack of knowledge and uncertainty due to variability.” Risk Analysis **14**(5): 707-712.

Hofstetter, P. (1998). Perspectives in Life Cycle Impact Assessment: A Structured Approach to Combine Models of the Technosphere, Ecosphere, and Valuesphere. Norwell, Kluwer Academic Publishers.

Hofzumahaus, A., U. Aschmutat, et al. (1998). “Intercomparison of Tropospheric OH Measurements by Different Laser Techniques during the POPCORN Campaign 1994.” Journal of Atmospheric Chemistry **31**(1-2): 227-246.

IARC (International Agency for Research on Cancer) (2006). IARC Monographs Vol 86 Cobalt in Hard Metals and Cobalt Sulfate, Gallium Arsenide, Indium Phosphide and Vanadium Pentoxide. Lyon, France`, IARC**:** 330.

International Agency for Research on Cancer (1997). Occupational Exposures to Mists and Vapours from Strong Inorganic Acids; and Other Industrial Chemicals, World Health Organization**:** 1-14.

Kalberlah, F., K. Schneider, et al. (2003). “Uncertainty in toxicological risk assessment for non-carcinogenic health effects.” Regulatory Toxicology and Pharmacology **37**: 92-104.

Kodell, R. L. and D. W. Gaylor (1999). “Combining uncertainty factors in deriving human exposure levels of noncarcinogenic toxicants.” Annals of New York Academy of Sciences **895**: 188-195.

Kunzli, N. (2002). “The public health relevance of air pollution abatement.” The European Respiratory Journal **20**(1): 198-209.

Leech, J. and K. Laporte (1996). “The Canadian Human Activity Pattern Survey: Report of Methods and Population Surveyed.” Chronic Disease in Canada **17**(3/4): 118-123.

Levy, J., A. M. Wilson, et al. (2003). “Estimation of primary and secondary particulate matter intake fractions for power plants in Georgia.” Environmental Science & Technology **37**: 5528-5536.

Levy, J. L., J. D. Spengler, et al. (2002). “Using CALPUFF to evaluate the impacts of power plant emissions in Illinois: model sensitivity and implications.” Atmospheric Environment **36**: 1063-1075.

Lewan, M. D. (1984). “Factors controlling the proportionality of vanadium to nickel in crude oils.” Geochimica et Cosmochimica Acta **48**(11): 2231-2238.

Limpert, E., W. A. Stahel, et al. (2001). “Log-normal Distributions across the Sciences: Keys and Clues.” BioScience **5**(5): 341-352.

Mantel, N., N. R. Bohidar, et al. (1975). “An improved Matel-Bryan procedure for "safety" testing of carcinogens.” Cancer Research **35**: 865-872.

Mantel, N. and W. R. Bryan (1961). “"Safety" testing of carcinogens.” Journal of the National Cancer Institute **27**(2): 455-470.

Mathers, C. D., C. Stein, et al. (2002). Global Burden of Disease 2000: Version 2 methods and results, World Health Organization**:** 108. Retrieved August 2004 from www.fic.nih.gov/dcpp/ppts/gbdpaper.pdf.

Mathworks (2002). Matlab, Mathworks.

McColl, S. (2003). conc_response~final.xls. S. Gower. Waterloo.

McColl, S. and S. Gower (2004). HEIDI II Priority Ranking Tool – User’s Guide (v 2.0). Waterloo, NERAM (Network for Environmental Risk Assessment and Management)**:** 1-30. Retrieved August 2004 from www.irr-neram.ca.

McColl, S., S. Gower, et al. (2004). Development of a Health Effects-Based priority Ranking System for Emissions Reductions from Oil Refineries in Canada. Prepared for the Health Prioritization Sub-group of the National Framework for Petroleum Refinery Emission Reductions (NFPRER), a multi-stakeholder initiative of the Canadian Council of Ministers of the Environment (CCME). Waterloo, NERAM (Network for Environmental Risk Assessment and Management) and IRR (Institute for Risk Research)**:** 105.

McColl, S., J. Hicks, et al. (2003). Assessment of Comparative Human Health Risk-based Prioritization Schemes for Petroleum Refinery Emission Reductions. Waterloo, NERAM (Network for Environmental Risk Assessment and Management)**:** 1-98. Retrieved May 2004 from www.irr-neram.ca.

McKay, M. D. (1988). Sensitivity and Uncertainty Analysis Using a Statistical Sample of Inputs. Uncertainty Analysis. Y. Ronen. Boca Raton, CRC Press**:** 145-186.

Melse, J. M., M.-L. Essink-Bot, et al. (2000). "A national burden of disease calculation: Dutch disability-adjusted life-years." American Journal of Public Health **90**: 1241-1247.

Microsoft (2000). Excel. Redmond, Microsoft Corporation.

Microsoft Office online (Excel 2003). Excel specifications and limits, Microsoft Corp., http://office.microsoft.com/en-us/assistance/HP051992911033.aspx.

Morgan, M. G. and M. Henrion (1990). Uncertainty: a Guide to Dealing with Uncertainty in Quantitative Risk and Policy Analysis. Cambridge, Cambridge University Press.

Murray, C. J. L. and A. D. Lopez (1996). The Global Burden of Disease. Boston, WHO, World Bank and Harvard School of Public Health.

National Institute of Standards and Technology (2005). Standard Reference Database 17, Version 7.0 (Web Version), Release 1.3 "A compilation of kinetics data on gas-phase reactions", National Institute of Standards and Technology.

National Research Council (2004). Air Quality Management in the United States. Washington, DC, The National Academies Press.

Office of Emergency and Remedial Response (2001). RAGS (Risk Assessment Guidance for Superfund) Volume III - Part A, Process for Conducting Probabilistic Risk Assessment. Washington, D.C., U.S. Environmental Protection Agency**:** A-1 to A-37.

Office of Environmental Health Hazard Assessment (2005). Safe Draining Water and Toxic Enforcement Act of 1986 (Proposition 65) Notice to Interested Parties Chemical Listed Effective February 11, 2005 as known to teh state of California to Cause Cancer, California Environmental Protection Agency.

Ontario Clean Air Alliance (2003). Dirty Coal, Dirty Power, Dirty Air.

Ontario Ministry of the Environment (2006). Fact Sheet: Proposed new and updated standards for 15 air pollutants, Government of Ontario.

Pennington, D. W., G. Norris, et al. (2000). "Environmental comparison metrics for life cycle impact assessment and process design." Environmental Progress **19**(2): 83-91.

Pope, A. (2000). "Invited Commentary: Particulate Matter-Mortality Exposure-Response Relations and Threshold." American Journal of Epidemiology **152**(5): 407-412.

Pope, C. A., M. J. Thun, et al. (1995). "Particulate air pollution as a predictor of mortality in a prospective study of U.S. adults." American Journal of Respiratory and Critical Care Medicine **151**(669-74).

Powell, J. C., D. W. Pearce, et al. (1997). "Approaches to valuation in LCA Impact Assessment." International Journal of Life Cycle Assessment **2**(1): 11-16.

Price, P. S., R. E. Keenan, et al. (1997). “An approach for modeling noncancer dose-responses with an emphasis on uncertainty.” Risk Analysis **17**(4): 427-437.

Prinn, R. G., J. Huang, et al. (2001). “Evidence for Substantial Variations of Atmospheric Hydroxyl Radicals in the Past Two Decades.” Science **292**: 1882-1888.

Prinn, R. G., R. F. Weiss, et al. (1995). “Atmospheric Trends and lifetime of CH3CCl3 and Atmospheric OH.” Science **269**(5221): 187-192.

Pruss, A., C. F. Corvalan, et al. (2001). “Methodologic considerations in estimating burden of disease from environmental risk factors at national and global levels.” International Journal of Occupational and Environmental Health **7**: 58-67.

Saltelli, A. (2002). “Sensitivity Analysis for Importance Assessment.” Risk Analysis **22**(3): 579-590.

Saltelli, A. (2004). Global Sensitivity Analysis: An Introduction. International Conference on Sensitivity Analysis, Santa Fe, New Mexico. Retrieved January 2005 from http://www.stat.lanl.gov/SAMO2004/abstracts/pdf_files/Abs_008%20A_Saltelli.pdf.

Saltelli, A., S. Tarantola, et al. (2004). Sensitivity Analysis in Practice A Guide to Assessing Scientific Models. Chichester, UK., Wiley.

Samoli, E., A. Analaits, et al. (2005). “Estimating the Exposure–Response Relationships between Particulate Matter and Mortality within the APHEA Multicity Project.” Environmental Health Perspectives **113**(1): 88–95.

Sathiakumar, N., E. Delzell, et al. (1997). “Epidemiologic evidence on the relationship between mists containing sulfuric acid and respiratory tract cancer.” Critical Reviews in Toxicology **27**(3): 233-251.

Schwartz, J., F. Laden, et al. (2002). “The Concentration–Response Relation between PM2.5 and Daily Deaths.” Environmental Health Perspectives **110**(10): 1025-1029.

Sexton, K. (1995). “Science and policy in regulatory decision making: getting the facts right about hazardous air pollutants.” Environmental Health Perspectives **103(Suppl 6)**: 213-222.

Slob, W. and M. Pieters (1998). “A Probabilistic Approach for Deriving Acceptable Human Intake Limits and Human Health Risks from Toxicological Studies: General Framework.” Risk Analysis **18**(6): 787-798.

Soskolne, C. L., G. S. Jhangri, et al. (1992). “Occupational exposure to sulfuric acid in southern Ontario, Canada, in association with laryngeal cancer.” Scandanavian Journal of Work and Health **18**: 225-232.

Statistics Canada (2002). Census of Canada 2001, Statistics Canada.

Stayner, L., A. J. Bailar, et al. (1999). “Sources of uncertainty in dose-response modeling of epidemiological data for cancer risk assessment.” Annals New York Academy of Sciences **895**: 212-222.

Strom, D. J. (2001). LOGNORM4 in Microsoft QuickBasic 4.5. Richland, Washington, Pacific Northwest National Laboratory.

Strom, D. J. and P. S. Stansbury (2000). “Determining parameters of lognormal distributions from minimal information.” American Industrial Hygiene Association Journal **61**(877-880).

Swartout, J. C., P. S. Price, et al. (1988). “A Probabilistic Framework for the Reference Dose (Probabilistic RfD).” Risk Analysis **18**(3): 271-281.

The Mathworks (2002). Learning Matlab 6.5. Natick, MA, The Mathworks.

Toxicology Excellence for Risk Assessment (TERA) & Concurrent Technologies Corporation (2004). ITER - International Toxicity Estimates for Risk Database. **2004.** Accessed at http://www.tera.org/iter/.

U.S. Environmental Protection Agency (2001). Appendix A: Sensitivity Analysis: How Do We Know What’s Important? Risk Assessment Guidance for Superfund: Volume III - Part A, Process for Conducting Probabilistic Risk Assessment. Washington, DC, Office of Emergency and Remedial Response**:** A1 -A37.

U.S. Environmental Protection Agency (2004). IRIS - Integrated Risk Information System, U.S. Environmental Protection Agency Office of Research and Development. Retrieved 2004 from http://www.epa.gov/iriswebp/iris/index.html.

Udo de Haes, H. A., O. Jolliet, et al. (1999). “Best available practice regarding impact categories and category indicators in life cycle impact assessment.” International Journal of Life Cycle Assessment **4**(3): 167-174.

Valko, M., C. J. Rhodes, et al. (2006). “Free radicals, metals and antioxidants in oxidative stress-induced cancer.” Chemico-Biological Interactions **160**: 1-40.

Vermeire, T., M. Pieters, et al. (2001a). Probabilistic Assessment Factors for Human Health Risk Assessment RIVM Report 601516 005; TNO Report V3489. Bilthoven, Netherlands, RIVM.

Vermeire, T., H. Stevenson, et al. (1999). “Assessment Factors for Human Health Risk Assessment: A Discussion Paper.” Critical Reviews in Toxicology **29**(5): 439-490.

Wang, C., R. G. Prinn, et al. (1997). A Global Interactive Chemistry and Climate Model. Boston, Massachusetts Institute of Technology Joint Program on the Science and Policy of Global Change. Retrieved August 2005 from http://web.mit.edu/afs/athena.mit.edu/org/g/globalchange/www/rpt24.html.**:** 1-34.

WHO (World Health Organization) (2000). Air Quality Guidelines for Europe, Second Edition. Copenhagen, WHO Regional Publications, European Series**:** 92-98.

World Health Organization (WHO) (2003). Report on a WHO Working Group. Health Aspects of Air Pollution with Particulate Matter, Ozone and Nitrogen Dioxide. Bonn, Germany. Retrieved from http://www.who.dk/document/e79097.pdf.

World Health Organization (WHO) (2004). Health Aspects of Air Pollution. Results from the WHO Project "Systematic Review of Health Aspects of Air Pollution in Europe). Copenhagen, DK, Regional Office for Europe of the World Health Organization**:** 24.

Zador, J., V. Wagner, et al. (2005). “Quantitative assessment of uncertainties for a model of tropospheric ethene oxidation using the European Photoreactor (EUPHORE).” Atmospheric Environment **39**: 2805-2817.

Appendix A: Common Probability Distributions

Adapted from (Morgan and Henrion 1990)

Distribution	Functional Representation (PDF)	Description
Normal	$f(x)=\frac{1}{(2\pi)^{1/2}\sigma}\exp\left(\frac{-(x-\mu)^2}{2\sigma^2}\right);$ $\infty \ge x \ge -\infty$	Arises in many applications (in part because of the Central Limit Theorem). Commonly used to represent uncertainty in unbiased measurement errors.
Lognormal	$f(x)=\frac{1}{(2\pi)^{1/2}\phi x}\exp\left(\frac{-(\ln x-\xi)^2}{2\phi^2}\right);$ $0 \le x \le \infty$	Arises when the logarithm of the random variable is normally distributed; used to represent physical quantities constrained to be non-negative and positively skewed
Exponential	$f(x)=\lambda\exp(-\lambda x);$ $0 \le x \le \infty$	Describes times between successive events, when events are purely random.
Poisson	$p(x)=\frac{\alpha^x\exp(-\alpha)}{x!};$ $x=1,2,3...$	Describes discrete, non-negative events.
Gamma	$f(x)=\frac{\lambda^k x^{k-1}\exp(-\lambda x)}{\Gamma(k)};$ $0 \le x \le \infty$	Similar to lognormal but less positively skewed and less "tail-heavy"
Weibull	$f(x)=\frac{k}{c}\left(x/c\right)^{k-1}\exp\left[-\left(x/c\right)^k\right];$ $0 \le x \le \infty$	Applies to non-negative physical quantities (i.e., failure time in reliability models)
Uniform	$f(x)=\frac{1}{b-a};$ $a \le x \le b$	For use when a range of possible values has been identified, but there is no knowledge about which is more probable
Triangular	$f(x)=\frac{b-\lvert x-a\rvert}{b^2};$ $a-b \le x \le a+b$	Values toward the middle of the distribution are more likely than those at each extreme; may also convey sense that knowledge about the distribution is imperfect
Beta	$f(x)=\frac{1}{B(c,d)}x^{c-1}(1-x)^{d-1};$ $0 \le x \le 1$	Flexible means of representing variability over a fixed range

Appendix B: Variables List and Description (HEIDI II deterministic)

Variable	**Source for Data**	**Data Description/Type**	**Variable Description/Type**	**Relationships to other variables**
Air Exposure Module				
Refinery Emissions	Environment Canada's 2001 NPRI (National Pollutant Release Inventory) database	Empirical	Continuous; "left-centred" – i.e. continuous down to a regulatory guideline value Average annual emissions for each substance included in the HEIDI II model for each of Canada's 20 refineries The estimate for each pollutant is a composite of point source (i.e. stack), area, and volume emissions from a variety of emission sources within a refinery location, or losses through spills evaporation and escape from containment	Forms the basis for determining the exposure concentration in each of the 20 quadrants around each refinery. It is adjusted using dispersion adjustment factors, photodegradation rates, and background concentrations
Dispersion model adjustment factors	Dispersion adjustment factors for each quadrant and zone were determined outside the HEIDI II model. These were based on a generic meteorological profile For the meteorological profile, 1996-2000 meteorological data for the southwestern Ontario region are used.	Default – although they were developed from application ISC3/AERMOD to generic meteorological profile for a vector of zones j at refineries i, values will be taken as "given" for the purpose of analyses carried out as a part of this project	Continuous; These are applied to the raw emissions data to predict concentration of each substance in each of the 20 quadrants/zones	For Refinery i, zone j (NPRI emissions)$_i$*Dispersion model adjustment factor$_{i,j}$ = Dispersed Concentration$_{i,j}$
Secondary PM concentrations	Primary PM concentrations, conversion factors		Continuous positive	Calculated based on emitted SOx and NOx at source, wind speed, reaction rate, assumption of ½-day of sunlight

Stack Change Factor	Provided by John Hicks	Default	Categorical Allows the dispersion in each of the 20 zones to be calculated for 15 metre and 5 metre stack heights relative to a 30 metre stack height.	For Refinery i, zone j, stack height k Concentration of substance$_{i,j,k}$ = Dispersed Concentration$_{i,j}$* Stack Change Factor$_{j,k}$
Stack Height (input)	N/A – selected by user	User-specified Choices are 5, 15, 30 metres	Interval Allows the user to choose an appropriate stack height for his/her modeling needs	Determines which Stack Change Factor is used
Photodegradation time (input)	N/A – selected by user	User-specified Choices are 8, 12, 16 hours	Interval Allows the user to choose an appropriate number of daylight hours appropriate for his/her modeling needs	Determines format of photodegradation equation for calculating degraded, dispersed concentration$_{i,j,k}$: For 0 hours: = dispersed concentration For 8 hours: $=(2/3)*\text{dispersed}_{i,j,k}+(1/3)*\text{dispersed}_{i,j,l}*(e^{-kt})$ For 12 hours: $=(1/2)*\text{dispersed}_{i,j,l}+(1/2)*\text{dispersed}_{i,j,l}*(e^{-kt})$ For 16 hours: $=(1/3)*\text{dispersed}_{i,j,l}+(2/3)*\text{dispersed}_{i,j,l}*(e^{-kt})$
Atmospheric OH rate constant (used to calculate atmospheric half-lives of chemicals)	SRC (Syracuse Research Centre) Database Value at 25 °C	Empirical	Continuous Substance-specific value which allows calculation of half-life of substances emitted to air	For each substance: Half life (hours) = $\frac{\ln(2)}{k_{OH}*[OH]*3600\,\text{sec}/hr}$
Atmospheric [OH] (concentration)	Assumed [OH] of 1.5e6 molecules/cm^3; follows conventions used by EPA	Empirical	Continuous Required in order to calculate half-life of substances emitted to air	Half life (hours) = $\frac{\ln(2)}{k_{OH}*[OH]*3600\,\text{sec}/hr}$

Background Concentrations	Based on empirical data collected by NAPS near each refinery **or** surrogate values estimated using NAPS data	Empirical	Continuous; positive Is required for calculations where dose-response relationship is not linear – the background level of a substance may alter the probability that a given emission will/will not have an impact	For Refinery i, zone j, stack height k Daylight hours l: Delivered Concentration$_{i,j,k,l}$ = Degraded dispersed concentration$_{i,j,k,l}$ + Background Concentration$_{i}$ Also in the Health Effects Module, Discounted incidence = incidence(delivered concentration) – incidence (background concentration)
Health Effects Module				
Toxicity/C-R data for air toxics (non-threshold)	Health Canada, USEPA, CalEPA, HEAST	Default	Continuous - linear Unit risk values – sometimes derived from Health Canada's TC01 values	For Refinery i, zone j, stack height k Daylight hours l, population subgroup m: Predicted Case Incidence$_{i,j,k,l,m}$ = Degraded Dispersed$_{i,j,k,l}$*Unit Risk*Population$_{i,j,m}$
Toxicity/C-R data for air toxics (threshold)	Health Canada, USEPA, CalEPA, HEAST	Default	Continuous – nonlinear Dose-response is characterized using a log(dose):probit approach anchored on the ED05 The special case of the log(dose):probit approach used is called the "Mantel Bryan approach". However, a slope of 1.5 is used for the curve as opposed to the more conventional value of 1 for slope.	For Refinery i, zone j, stack height k Daylight hours l, population subgroup m: Undiscounted case incidence = LOGNORMDIST(Delivered Concentration$_{i,j,k,l,}$ LN(ED05/1000) + (2.303*(1.6449/1.5)), (2.303/1.5))* Population$_{m}$) Discounted case incidence = Undiscounted case incidence - LOGNORMDIST(Background Concentration$_{i,}$ LN(ED05/1000) + (2.303*(1.6449/1.5)), (2.303/1.5))* Population$_{m}$)

Toxicity/C-R data for CACs (Criteria Air Contaminants)	American Cancer Society Study; Harvard Six Cities Study; HEI Reanalyses where appropriate	Default	Continuous - linear	For Refinery i, zone j, stack height k Daylight hours l, population subgroup m: Predicted Case Incidence$_{i,j,k,l,m}$ = Delivered conc. (no background included)$_{,j,k,l}$*Epi risk coefficient$_{m}$*Population$_{i,j,m}$
BTEX toxicity data	Weighted value calculated from individual toxicity values for Benzene, Toluene, Ethylbenzene and Xylene	Derived	Weighted by toxicity for sum of effects of individual components	For substance n of B, T, E, X Weighted ED$_{05}$ $\frac{\sum_{1}^{4}\left(\left(ED_n\right)*\left(Conc_n\right)\right)}{\sum_{1}^{n}\left(Conc_n\right)}$ Weighted BTEX Conc: $\sum_{1}^{n}\left(\frac{\left(\frac{Conc_n}{ED_{05n}}\right)}{\sum_{1}^{n}\left(\frac{1}{ED_{05n}}\right)}\right)$
PAH toxicity data	Used B[a]P as representative of PAH mixtures Potency estimates for the surrogate mixture have been developed by the MOE, the WHO, and in the Netherlands.	Default value used was 2.3 E-5 developed by the MOE (1997)	The surrogate model, or whole mixture model (WMM) estimates the potency of a PAH fraction of a mixture as a whole, assuming that its potency is proportional to the B(a)P content of the mixture. An assumption inherent in this approach is that as the concentration of B(a)P increases, so does the concentration of all other PAHs. As a result, the potency value used represents the potency of the mixture as a whole, not just of B(a)P	Potency of PAH fraction = [B[a]P](µg/m^3)*Surrogate Mix Potency (Lifetime Risk)

Population data	2001 Statistics Canada Census data (To determine population profiles in the 20 quadrant zones around each refinery, census data at the DA (dissemination area) level was imported into ArcMap GIS software	Empirical	Continuous Number of children, adults, and seniors living in each of 20 defined geographic zones surrounding each refinery	See 3 cells above, also used to determine extent of discounting for disease endpoints that may not apply to all age groups.
Age		Default separation into children, youth, seniors	Categorical (based on continuous data)	Population descriptor at zone level; may induce discounting for some endpoints
Sex		Default separation into Male/Female	Categorical	Population descriptor at zone level; may induce discounting for some endpoints
Fraction of population that is male/female	Default	Default value of 0.5	Default	Determines extent of discounting for some disease endpoints that may not apply to all sex groups
Age-sex discounting multiplier	N/A – discounting was done for reproductive disease endpoints that could not physiologically apply to one gender or to pre-pubertal adolescents.	Default	Categorical “Weighting” – note subjectivity of decision to discount in certain cases 1 if disease affects target group (male/female, child/adult/senior) 0 if disease does not affect target group	Applies a values of 0 to predicted incidence for age-gender subpopulations where it is impossible
Health Impacts Module				
DALYp values (simple)	ILSI	Derived Divide health endpoints into three categories: (i) irreversible/life-shortening, (ii) may be reversible, could be life-shortening, (iii) generally reversible, generally not life-threatening	Continuous DALYs per person - an aggregrate indicator which assumes an average duration of disease and/or years of life lost within a population	Predicted DALYs(simple) = predicted incidence*DALYp(simple)

DALYp values (complex)	WHO Global burden of disease approach	Derived	Continuous DALYs per person - an aggregrate indicator which assumes an average duration of disease and/or years of life lost within a population	Predicted DALYs(complex) = predicted incidence*DALYp(complex)

Appendix C: Variables List and Description

C1 User-Defined Parameters

<table>
<tr><td>Variable:
Refinery (input)</td><td>Value(s) used in HEIDI II:
Chevron Canada Limited - Burnaby Refinery
Consumer's Co-operative Refineries Ltd./NewGrade Energy Inc.
Husky Oil Operations Limited - Prince George Refinery
Imperial Oil - Dartmouth Refinery
Imperial Oil - Nanticoke Refinery
Imperial Oil - Sarnia Refinery Plan
Imperial Oil - Strathcona Refinery
Irving Oil Ltd - Irving Oil Ltd. - Refining
North Atlantic Refining - North Atlantic Refinery
Nova Chemicals (Ltd.) - Nova Chemicals (Canada) Ltd.
Parkland Refining Ltd. - Bowden Refinery
Petro-Canada - Edmonton Refinery
Petro-Canada - Mississauga Lubricant Center
Petro-Canada - Raffinerie de Montreal
Petro-Canada - Oakville Refinery
Produits Shell Canada - Raffinerie de Montreal-est
Shell Canada Products - Sarnia Manufacturing Centre
Shell Canada Products - Shell Scotford Refinery
Sunoco Inc. - Sarnia Refinery
Ultramar Ltee - Raffinerie St. Romuald
Hypothetical Worst Case Refinery</td></tr>
<tr><td colspan="2">Sensitivity Analysis: Comparison across refineries will indicate whether priorities for emissions reduction in the refining sector must be determined on a facility basis, or whether general recommendations can be made.</td></tr>
<tr><td colspan="2">Justifications/notes:
“Hypothetical worst-case Refinery” uses the maximum observed emission from any real refinery for each substance</td></tr>
<tr><td colspan="2">Possible Correlations:
N/A</td></tr>
</table>

<table>
<tr><td>Variable:
Stack Height (input)</td><td>Value(s) used in HEIDI II:
5 metres
15 metres
30 metres (default value)</td></tr>
<tr><td colspan="2">Sensitivity Analysis: HEIDI II assumes that all emissions from a given refinery originate from one stack; however in reality refineries may have several stacks of varying heights, and some emissions may be fugitive (i.e., at locations close to the ground). The default value used in HEIDI II was 30 metres. Sensitivity analysis with 5, 15, 30 metre stack heights will provide information on the validity of the assumption of one stack height to represent all emissions.</td></tr>
<tr><td colspan="2">Justifications/notes:
Stack is assumed to be located in the centre of the refinery property. Stack heights of 30 metres are probably most representative of a realistic situation; however 5 m was included to enable assessments for fugitive emissions.
Unclear from HEIDI II documentation whether the stack height is a physical stack height or an “effective” stack height.</td></tr>
<tr><td colspan="2">Possible Correlations:
N/A</td></tr>
</table>

<table>
<tr><td>Variable:
Photodegradation time (input)</td><td>Value(s) used in HEIDI II:
0-24 hours (default value = 12 hours)</td></tr>
<tr><td colspan="2">Sensitivity Analysis: Sensitivity analysis with values in range from 0-24 hours will provide some indication of whether the amount of sunlight – and therefore photodegradation could affect the relative importance of various emissions for health impact</td></tr>
<tr><td colspan="2">Justifications/notes:
The photodegradation time variable is intended to account for the average amount of sunlight per day at the refinery location. The difference in amount of photodegradation that occurs at varying distances away from the refinery is not accounted for. Scenarios of either 0 or 24 hours are unlikely to ever occur in the Canadian locations specified by the refineries being observed. Values from 8-12 hours of daylight are probably most representative of reality for the locations under consideration.</td></tr>
<tr><td colspan="2">Possible Correlations:
In the current setup, there are likely no correlations; however, if the model were revised to include a measure of ambient temperature (which would affect dispersion, formation of secondary PM, and reaction rates), this might correlate with photodegradation time. (All would be a function of general weather patterns).</td></tr>
</table>

C2 Parameters Built into HEIDI

Variable:	**Value(s) used in deterministic HEIDI II:**	**Parametric description:**
Refinery Emissions	2001 values extracted from NPRI (See Appendix D)	Average and stdev was calculated based on were annual emissions for 2001-2003 extracted from NPRI[26]. (See Appendix D) Although probability distributions were used for sensitivity analyses, point estimates (using average emissions) were used to generate model prediction

Potential sources of Uncertainty/Variability:

Emissions are averaged annually; NPRI values do not provide information about variability in emission rates over time throughout the year. Emissions may change over time if the amount or type of refining changes. Three years of data may be insufficient to accurately characterize the variability in annual emissions. The data is also uncertain: it is unclear to what extent emissions below reporting guidelines are actually reported. Emissions are calculated based on a Canadian Association of Petroleum Producers (CAPP)-sanctioned formula that has been show to be inaccurate and imprecise for other upstream oil and gas applications (Chambers 2004).

Level of Uncertainty: Risk

Level of Evidence: Strong

Sensitivity Analysis: Sensitivity analysis can be performed using to assess the relative importance of emissions as a primary model input, and also to investigate the impact of variability in annual emissions on predicted incidence related to each substance.

Justifications/notes:

Emissions must be ≥ 0

Emissions below the regulatory guideline probably exist. Therefore the distribution of actual rather than reported emissions may not be left-centred. Emissions below reporting guidelines may not be accounted for in HEIDI II. However, since many emissions are reported at levels below the guidelines, it is unlikely that this type of non-reporting occurs frequently. For similar reasons it does not make sense to truncate a distribution at the reporting guideline – this would exclude most of the data.

During the Monte Carlo simulation, average values for emissions across several reporting years were used, but the emissions variable was not described using a probability distribution. To check for trends in emissions, substance-specific emissions were plotted over time for each refinery. Only at the Shell Scotford refinery did there appear to be any overall trend (decrease in emissions of all reported substances). Reporting

---

[26] Provisional 2004 emissions values were also available from the NPRI but as they were not confirmed by Environment Canada at the time of analysis they were not included.

for sulphuric acid emissions may be unreliable: although sulphuric acid emissions are generally high (>100 tonnes/year), they are occasionally not reported or reported as zero, especially for the year 2001. Sulphuric acid is included in the NPRI substance lists for each 2001-2003 year, so the source of this discrepancy is unclear.

Possible Correlations:

Emissions of groups of substances are likely to be correlated with each other (i.e., increase and decrease in concert) – this may depend on the composition of the crude oil, including the specific impurities. Total emissions may be correlated to refinery, where some refineries emit higher amounts of all substances and others emit lower amounts. This will be mostly a function of the amount of refining that occurs at each facility and does not affect the analysis being performed here.

Variable:

Dispersion model adjustment factors for air toxics.

These are applied to annual average emissions values (of air toxics) to predict the concentration of any substances in each of 20 zones around the refinery based on meteorology

Value(s) used in deterministic HEIDI II:

Stack Height = 30 metres

	Direction (degrees)			
Distance (km)	45 (NE)	135 (SE)	225 (SW)	315 (NW)
1	0.33381	0.26981	0.10207	0.14900
2.5	0.10423	0.08344	0.03717	0.05575
5	0.04831	0.04508	0.02030	0.03128
10	0.02905	0.03307	0.01491	0.02331
25	0.01256	0.01622	0.00786	0.01286

Stack Height = 15 metres

Distance (km)	45 (NE)	135 (SE)	225 (SW)	315 (NW)
1	0.78760	0.76521	0.33394	0.48564
2.5	0.44230	0.54686	0.26287	0.39039
5	0.22338	0.29487	0.14990	0.22803
10	0.08624	0.11713	0.06077	0.09526
25	0.01938	0.02682	0.01405	0.02290

Stack Height = 5 metres

Distance (km)	45 (NE)	135 (SE)	225 (SW)	315 (NW)
1	3.51727	4.57842	2.37253	3.4416
2.5	0.78282	1.03784	0.5347	0.79119
5	0.24009	0.3209	0.16462	0.24931
10	0.07077	0.09482	0.04849	0.07548
25	0.01282	0.01696	0.00867	0.01398

Parametric description:

None – to be taken as “given”

Potential sources of Uncertainty/Variability: Physical air distribution patterns are not site-specific: a generic meteorological profile representing the southern Ontario region is used as the default scenario. The modeling also assumes that the refinery is located in flat terrain. Steady state emissions are assumed over 365 days.
Level of Uncertainty: Scientific uncertainty
Level of Evidence: Medium
Sensitivity Analysis: None
Justifications/notes: Determined by John Hicks using ISCLT3 technology. Creating distributions to represent these dispersion adjustment factors would be a complex process which would have to be carried out by someone familiar with the original derivation of the factors. Knowledge about these distributions may not add value to the probabilistic version of HEIDI in the policy context since the meteorology used for the model is not location specific, and cannot be controlled by policy in any case. Any parametric representations developed for these factors would be representative of the technological limitations of the dispersion estimation method.
Possible Correlations: Depends on selected stack height

Variable:	**Value(s) used in deterministic HEIDI II:**	**Parametric description:**
Secondary PM concentrations	Values are calculated based on tonnes of NO_2, SO_x, and primary PM released from each refinery. These values are for a base-case of a 30-metre stack. For other stack heights, the "PM stack change factors" must be applied (see below)	Average and stdev was calculated based on were annual emissions for 2001-2003 extracted from NPRI[1]. (See Appendix E) Although probability distributions were used for sensitivity analyses, point estimates (using average emissions) were used to generate model prediction.
Potential sources of Uncertainty/Variability: HEIDI II does not perform nonlinear simulation modeling of photooxidant formation and secondary PM formation. Photooxidants and secondary PM are estimated using algebraic transfer functions and extrapolations based on conversion factors available in the research and technical literature -- primarily from controlled chamber studies. Predicted secondary PM concentration values are based on reported emissions of NO_2, SO_2, and primary PM to the NPRI. These values represent annual averages, and uncertainties inherent in using this type of data (see comments regarding air toxics data) are relevant for calculated concentrations of secondary PM. Three years of data may be insufficient to accurately characterize the uncertainty in annual emissions		
Level of Uncertainty: Scientific uncertainty		
Level of Evidence: Medium		
Sensitivity Analysis: Sensitivity analysis can be performed using to assess the relative importance of emissions as a primary model input, and		

also to investigate the impact of variability in annual emissions on predicted incidence related to each substance.

Justifications/notes:

Because PM is not considered to photodegrade, the model variables k and OH are irrelevant to predicted incidence.

Possible Correlations:

Correlated to primary PM concentrations; may be related to amount of other emitted substances (i.e., total emissions at a refinery may change in concert depending on amount and type of refining occurring)

Variable:

PM Stack Change Factor

This is used to predict the concentration of PM reaching each of 20 zones around the refinery for different stack heights.

Value(s) used in deterministic HEIDI II:

	Stack change factor (30 m to 30 m)			
	Degrees from North			
Distance (km)	45.00	135.00	225.00	315.00
0.5	1	1	1	1
1	1	1	1	1
2.5	1	1	1	1
5	1	1	1	1
10	1	1	1	1
25	1	1	1	1
Distance (km)	Stack change factor (30 m to 15 m)			
0.5	2.37	2.01	2.46	2.26
1	2.36	2.83	3.27	3.26
2.5	4.25	6.59	7.11	8.38
5	4.65	6.56	7.50	7.35
10	2.97	3.55	4.00	4.13
25	1.46	1.69	2.00	1.77
Distance (km)	Stack change factor (30 m to 5 m)			
0.5	14.68	18.64	30.59	27.59
1	10.51	16.96	23.24	23.09
2.5	7.53	12.51	14.46	13.64
5	5.00	7.13	8.25	8.03
10	2.45	2.88	3.20	3.26
25	1.00	1.06	1.29	1.08

Parametric description:

None – to be taken as “given”

Potential sources of Uncertainty/Variability: Physical air distribution patterns are not site-specific: a generic meteorological profile representing the southern Ontario region is used as the default scenario. The modeling also assumes that the refinery is located in flat terrain. Steady state emissions are assumed over 365 days.
Level of Uncertainty: Scientific uncertainty
Level of Evidence: Medium
Sensitivity Analysis: None
Justifications/notes: Determined by John Hicks using ISCLT3 technology. Creating distributions to represent these dispersion adjustment factors would be a complex process which would have to be carried out by someone familiar with the original derivation of the factors. Knowledge about these distributions may not add value to the probabilistic version of HEIDI in the policy context since the meteorology used for the model is not location specific, and cannot be controlled by policy in any case. Any parametric representations developed for these factors would be representative of the technological limitations of the dispersion estimation method.
Possible Correlations: Depends on selected stack height

<table>
<tr>
<td>Variable:

kOH

(referred to also as k)

Atmospheric OH rate constant

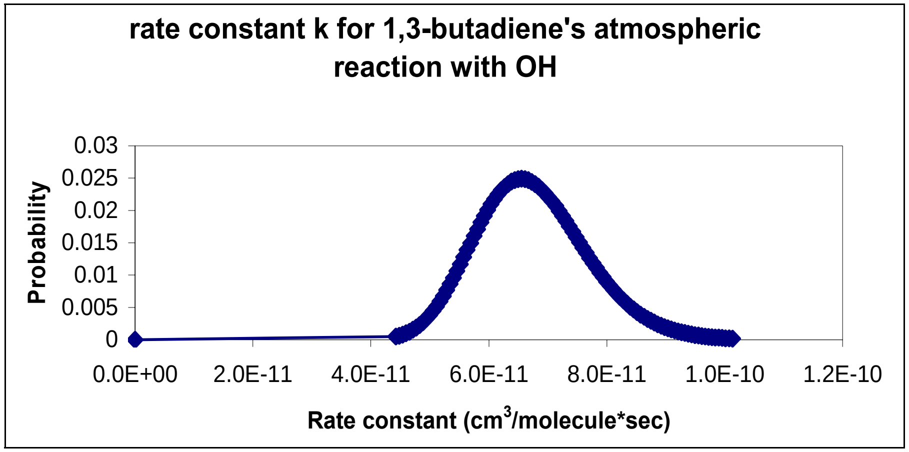
Used to calculate atmospheric half-lives of</td>
<td>Value(s) used in deterministic HEIDI II:
<table>
<tr><th>Substance</th><th>(cm3/molecule-sec)</th></tr>
<tr><td>1,3-Butadiene</td><td>6.66E-11</td></tr>
<tr><td>Benzene</td><td>1.23E-12</td></tr>
<tr><td>Ethylene</td><td>8.52E-12</td></tr>
<tr><td>Nickel</td><td>0.00E+00</td></tr>
<tr><td>PAHs (BaP surrogate class)</td><td>5.00E-11</td></tr>
<tr><td>Formaldehyde</td><td>9.37E-12</td></tr>
<tr><td>Acetaldehyde</td><td>1.58E-11</td></tr>
<tr><td>1,2,4-trimethylbenzene</td><td>3.25E-11</td></tr>
<tr><td>Ammonia</td><td>0.00E+00</td></tr>
<tr><td>Benzene (as BTEX potentiator)</td><td>1.23E-12</td></tr>
<tr><td>Cyclohexane</td><td>7.49E-12</td></tr>
<tr><td>Dicyclopentadiene</td><td>1.19E-10</td></tr>
<tr><td>Diethanolamine</td><td>9.27E-11</td></tr>
</table>
</td>
<td>Parametric description:

Distributions were derived using values extracted from the NIST (National Institute of Standards and Technology) database (National Institute of Standards and Technology 2005). NIST values for 298 K are used. (See Appendix F)

For xylene, which has three isomers, a conservative approach was used and the lowest value of k from among the three isomers was chosen.

Lognormal distributions were used.

Example:</td>
</tr>
</table>

chemicals	Ethylbenzene	7.10E-12	
	Hydrogen Sulphide	0.00E+00	
	Isoprene	*1.11E-10*	
	Mercury	0.00E+00	
	Methanol	9.44E-13	
	Methyl Ethyl Ketone (MEK)	1.15E-12	
	Methyl Isobutyl Ketone (MIBK)	1.41E-11	
	Methyl Tert-Butyl Ether (MTBE)	2.94E-12	
	Naphthalene	2.16E-11	
	n-Hexane	5.61E-12	
	Phenol	2.63E-11	
	Propylene	2.63E-11	
	Styrene	5.80E-11	
	Sulphuric Acid	2.80E-13	
	Toluene	5.96E-12	
	Vanadium	0.00E+00	
	Xylene	1.87E-11	
	Zinc	0.00E+00	

Potential sources of Uncertainty/Variability:
Degradation is assumed to be a first-order process. Rate constants included in the NIST are based on experimental or estimation methods; the level of knowledge may depend on the individual substance. k is temperature-dependent in most if not all cases; k values used here are for 298 K, which is inappropriate for much of Canada most of the time. The rate constant for BaP was used to represent the PAH mixture since PAH toxicity was described in terms of “BaP-equivalents”. It is unclear how appropriate this is.

Level of Uncertainty: Risk

Level of Evidence: Medium

Sensitivity Analysis: Performed to explore the implication of parametric uncertainty in k values. Atkinson’s values with associated error may be used to confirm the validity of values chosen for the sensitivity analysis.

Justifications/notes:
Depends on individual substance; must be ≥ 0.
Many values for k_{OH} are measured experimentally and are subject to experimental error and the limits of detection. Atkinson has developed values of k with associated uncertainty measures; these have been published in several places including the Journal of Physical and Chemical Reference Data (Atkinson, et al., 1999) for IUPAC (International Union of Pure and Applied Chemistry) and a book of which he is a co-author (Calvert, et al., 2002). Atkinson states that assignment of uncertainties is arbitrary and is “based mainly on our state of knowledge of a particular reaction

which is dependent upon factors such as the number of independent investigations carried out and the number of different techniques used. On the whole, our assessment of uncertainty limits tends toward the cautious side." (Atkinson, et al., 1999). kOH values are also available from other sources including NASA (Sander, et al., 2003), the NIST (National Institute of Standards and Technology, 2005) (National Institute of Standards and Technology (formerly National Bureau of Standards)), and the SRC database (Syracuse Research Corporation, 2005), which is where the original HEIDI II data was obtained.

For the substances that do not appear in the Atkinson's data or in the NIST (Benzo[a]pyrene, dicyclopentadiene, diethanolamine, sulphuric acid), the value from the SRC research database will be used in place of the arithmetic mean, and estimates for the other parameters will be derived using LOGNORM4 software (Strom 2001), based on the coefficients of variation from those substances for which adequate data is available. (The greyed-out parameters are those that were estimated using LOGNORM4).

Substance	**Arithmetic mean**	**variance**	**stdev**	**Cov**	**GEO mean**	**sigma**	**GSD**
1,3-Butadiene	6.73E-11	9.25E-23	9.62E-12	1.43E-01	6.68E-11	1.42E-01	1.15E+00
Benzene	1.17E-12	6.91E-26	2.63E-13	2.25E-01	1.14E-12	2.22E-01	1.25E+00
Ethylene	6.96E-12	4.94E-24	2.22E-12	3.19E-01	6.52E-12	3.12E-01	1.37E+00
Nickel	NO RXN	NO RXN	NO RXN	NO RXN	NO RXN	NO RXN	NO RXN
PAHs (BaP surrogate class)	5.00E-11	1.28E-22	1.13E-11	2.26E-01	4.88E-11	2.23E-01	1.25E+00
Formaldehyde	8.92E-12	2.82E-23	5.31E-12	5.96E-01	5.31E-12	5.51E-01	1.74E+00
Acetaldehyde	1.50E-11	3.13E-24	1.77E-12	1.18E-01	1.49E-11	1.18E-01	1.12E+00
1,2,4-Trimethylbenzene	3.45E-11	9.66E-24	3.11E-12	9.01E-02	3.44E-11	8.99E-02	1.09E+00
Ammonia	1.51E-13	7.58E-27	8.70E-14	5.78E-01	1.27E-13	5.37E-01	1.71E+00
Cyclohexane	7.05E-12	6.29E-25	7.93E-13	1.13E-01	7.00E-12	1.12E-01	1.12E+00
Dicyclopentadiene	1.19E-10	7.23E-22	2.69E-11	2.26E-01	1.16E-10	2.23E-01	1.25E+00
Diethanolamine	9.27E-11	4.29E-22	2.10E-11	2.26E-01	9.04E-11	2.23E-01	1.25E+00
Ethylbenzene	7.28E-12	3.92E-25	6.26E-13	8.61E-02	7.25E-12	8.59E-02	1.09E+00
Hydrogen Sulphide	4.64E-12	7.75E-25	8.81E-13	1.90E-01	4.56E-12	1.88E-01	1.21E+00
Isoprene	8.77E-11	2.23E-22	1.49E-11	1.70E-01	8.66E-11	1.69E-01	1.18E+00
Mercury	No RXN	No RXN	No RXN	No RXN	No RXN	No RXN	No RXN
Methanol	8.82E-13	8.79E-26	2.96E-13	3.36E-01	7.82E-13	3.27E-01	1.39E+00
Methyl Ethyl Ketone (MEK)	1.90E-12	1.15E-24	1.07E-12	5.64E-01	1.64E-12	5.26E-01	1.69E+00
Methyl Isobutyl Ketone (MIBK)	1.38E-11	7.43E-25	8.62E-13	6.23E-02	1.38E-11	6.22E-02	1.06E+00
Methyl Tert-Butyl Ether (MTBE)	2.93E-12	9.26E-26	3.04E-13	1.04E-01	2.92E-12	1.04E-01	1.11E+00

Naphthalene	2.34E-11	4.48E-24	2.12E-12	9.05E-02	2.33E-11	9.03E-02	1.09E+00
n-Hexane	5.50E-12	6.29E-25	7.93E-13	1.44E-01	5.43E-12	1.44E-01	1.15E+00
Phenol	2.96E-11	7.05E-24	2.66E-12	8.96E-02	2.96E-11	8.94E-02	1.09E+00
Propylene	2.20E-11	6.21E-23	7.88E-12	3.58E-01	2.00E-11	3.48E-01	1.42E+00
Styrene	6.27E-11	6.17E-22	2.48E-11	3.96E-01	5.96E-11	3.82E-01	1.46E+00
Sulphuric Acid	2.80E-13	4.01E-27	6.33E-14	2.26E-01	2.73E-13	2.23E-01	1.25E+00
Toluene	6.00E-12	5.57E-25	7.47E-13	1.24E-01	5.96E-12	1.24E-01	1.13E+00
Vanadium	No RXN	No RXN	No RXN	No RXN	No RXN	No RXN	No RXN
Xylene - use ortho-isomer as a conservative assumption since it has the slowest degradation	1.31E-11	9.95E-25	9.98E-13	7.65E-02	1.30E-11	7.63E-02	1.08E+00
Zinc	No RXN	No RXN	No RXN	No RXN	No RXN	No RXN	No RXN
Average CoV = 0.226; stdev of CoV = 0.17							

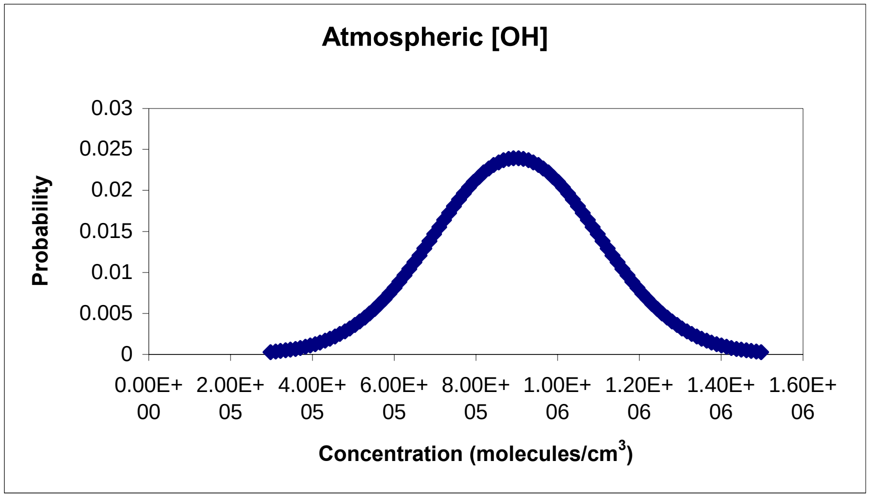
The distributions for k_{OH} are likely lognormal: NASA suggests that the probability distribution of k values may not follow the normal Gaussian form (Sander, et al., 2003), and lognormal distributions have previously been assumed for gas-phase rate constants (Zador, Wagner et al. 2005).

****Note that the reaction products are not accounted for in HEIDI at all – for example, reactions of aromatics with OH often produce ozone – a major contributor to formation of smog. The health effects that could result from exposure to these breakdown products are not accounted for in HEIDI II.

Possible Correlations:

None identified

Variable:	**Value(s) used in deterministic HEIDI II:**	**Parametric description:**
Atmospheric [OH] (concentration)	$1.50*10^6$ molecule/cm^3	[OH] = 8.98 ± $2.02*10^5$ molecules/cm^3; normal distribution



Potential sources of Uncertainty/Variability:
[OH] is highly variable locally over space and time and depends on level of biogenic emissions and levels of pollutants (Wang and Prinn, 1998) as well as solar intensity and prevailing concentration of ozone. Several estimations of the global levels of OH have been made, although even these are complicated by year-to-year variations of OH concentrations resulting from a complicated combination of meteorological variability and chemical concentration due to variable emissions and stratospheric O_3 (Koumoutsaris and Bey, 2004). The most commonly used value of $1.5*10^6$ molecules/cm^3 (which was the value used in HEIDI II) is adjusted to an average 12-hour period and therefore most applicable to spring and Fall.

Level of Uncertainty: Risk

Level of Evidence: Medium

Sensitivity Analysis: Values for sensitivity analysis (to assess impact of variability) include:
$5 *10^5$ (night; below detection limit) to max of $2\text{-}10*10^6$ (Hofzumahaus, Aschmutat et al. 1998)
$1.15 *10^6$ in Toronto (Bunce, Liu et al. 1997)
Global OH = $10.48*10^5$ (Koumoutsaris) and $9.7 \pm 0.6*10^5$ (Prinn)

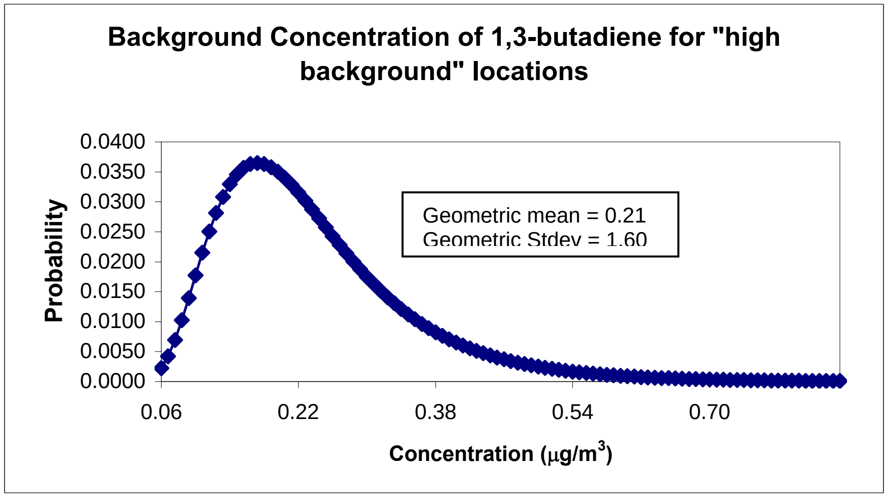
Justifications/notes:
Hofzmanhaus (Hofzumahaus, Aschmutat et al. 1998)suggests that OH radical concentrations can range from $5*10^5$ at night (below detection limit) to a maximum of $(2\text{-}10) *10^6$ at noon during the summer (at peak photolysis). In Toronto specifically, peak values in 1988 (measured at midday in July) ranged from $1* 10^6$ to $1.5*10^7$ molecule/cm^3 (Bunce, Liu et al. 1997). Some 1995 estimates of global [OH] include $10.4*10^5$ radical/cm^3 (Wang, Prinn et al. 1997), and $(9.7 \pm 0.6) *10^5$ radicals/cm^3 (Prinn, Weiss et al. 1995) (where the uncertainty does not include

uncertainty in the rate constants used to deduce the value). In 2001, Prinn et al provided normal distributions for OH concentrations globally ($9.43 \pm 1.30 * 10^5$ molecules/cm^3), and for northern and southern hemispheres: $8.98 \pm 2.02 * 10^5$ molecules/cm^3 and $9.93 \pm 2.02* 10^5$ molecules/cm^3, respectively (Prinn, Huang et al. 2001).
Prinn's (2001) value is for the northern hemisphere; it is slightly lower than values measured in Toronto in 1988. In general, [OH] is highly variable over space and time and depends on levels of biogenic emissions and levels of pollutants.

Possible Correlations:
It is difficult to know whether the level of background pollution would affect and therefore be correlated to atmospheric OH concentration. While the presence of CO and hydrocarbons tends to deplete the amount of OH in the atmosphere, presence of NO_x can boost OH formation. All three are typically present in any polluted urban atmosphere.

Variable:	**Value(s) used in deterministic HEIDI II:**	**Parametric description:**
Background Concentrations (In HEIDI II, the term "background" implies ambient levels due to all sources except refineries)	Most background data was collected by NAPS (National Ambient Pollution Survey) monitors at the nearest Environment Canada location.Data on VOCs was provided by Tom Dann, otherwise, NAPS data was extracted from NAPS 2002 Annual Report (Environment Canada 2003)or from the document "Ambient Air Measurements of Polycyclic Aromatic Hydrocarbons (PAH), Polychlorinated Dibenzo-p-Dioxins (TCDD) and Polychlorinated Dibenzofurans in Canada (1987-1997) (Dann 1998), or from data sent by Kristina Curran of Environment Canada (Curran 2004). For rural locations without monitoring data,	Sensitivity analysis (described below) determined that division into high/medium/low is appropriate. Mean and standard deviations were derived from the values used across refineries in locations deemed "high", "Medium", and "low" background. Lognormal distributions truncated at zero; geometric means and standard deviations will be used to describe the distributions (See Appendix H) Example distribution:

<table>
<tr><td></td><td>50% of lowest monitored value for each chemical was used. In special cases such as for MTBE, values were based on specific measurements or set to zero

(See Appendix G for details)</td><td>
</td></tr>
<tr><td colspan="3">**Potential sources of Uncertainty/Variability:**
Limited data – some site specific concentrations are based on 1 month’s worth of measurement data. Technical limitations of the equipment used to measure concentrations. Assumptions were made where data was lacking (i.e., the ideal location for a monitor is nearby and upwind. This was not always available, so the closest geographic monitor was selected.) Assumptions made where no data existed, i.e. for rural locations with no monitoring data, 50% of the lowest observed value at a monitor was used.</td></tr>
<tr><td colspan="3">**Level of Uncertainty:** Risk</td></tr>
<tr><td colspan="3">**Level of Evidence:** Weak</td></tr>
<tr><td colspan="3">**Sensitivity Analysis:**
HEIDI II used site-specific measures of background concentrations for each chemical; however, due to the nature of the data this may be an overparameterization, or the data used may be inappropriate. Background data for many of the urban sites was based on nearby monitors; however these may not have been upwind of the refineries. For example, many of the values used for “background” in Sarnia were from monitors in Windsor, and background levels used for the Scotford refinery were often actually measured in Edmonton. The most rural sites did not have site-specific monitoring data. As well, although data was generally provided on a monthly basis, the amount of available data was variable, and annual averages were occasionally calculated using as few as one month of the year, which is not truly representative of an annual average.

With these limitations in mind, it was felt more appropriate to create a limited number of background scenarios, with refineries assigned to the most relevant scenario. Selected scenarios are:</td></tr>
</table>

Low – background levels are calculated based on half of the lowest observed concentration at any of the monitors originally considered in the HEIDI II model. (In most cases refineries designated as “low” do not have any nearby monitoring data.)

Medium - for refineries located in smaller communities where industrial penetration is minimal, and would be calculated based on the average background levels observed across the designated communities.

High: for refineries located in the largest cities or in smaller cities with a strong industrial presence and would be calculated based on the average background levels observed across the designated communities

The population scenarios used were also considered when developing the background scenarios. For example, a large population combined with a rural background scenario would be inappropriate.

Classification of the Refineries:

Use weighted sum of background levels across substances to rank refineries; use population as secondary basis for classification divisions. This method also tends to group refineries geographically, so that refineries in the same location (urban centre) will be represented as having the same background levels

Rank based on Background	**Rank based on site-specific background levels (identical rank = same background levels)**	**Population**	**Rank based on Population**	**Classification**
Chevron -Burnaby	1	1694061	3	High
Petro-Canada - Oakville	2	1095580	5	High
Petro-Canada - Montreal	3	2560328	2	High
Shell - Montreal East	3	2612269	1	High
Imperial - Strathcona	5	929299	7	High
Petro-Canada - Edmonton	5	929431	6	High
Shell - Scotford	7	31231	18	High
Petro-Canada - Mississauga	8	1572665	4	Medium
Ultramar - St. Romuald	9	631211	8	Medium
Imperial - Sarnia	10	98730	13	Medium
NOVA - Corunna	10	102094	12	Medium
Shell - Sarnia	10	96725	15	Medium
Sunoco - Sarnia	10	96977	14	Medium
Imperial - Dartmouth	14	317113	9	Medium
Consumers' Co-operative - Regina	15	193214	10	Low
Irving - Saint John	16	109203	11	Low
Imperial - Nanticoke	17	47143	17	Low
North Atlantic Refining - Come by Chance	18	4710	20	Low
Parkland - Bowden	18	25933	19	Low
Husky - Prince George	20	81895	16	Low

Justifications/notes:

Values must be ≥ 0.

Bortnick and Stetzer (2002) detail the types of uncertainty inherent in ambient air toxics monitoring data, suggesting that a coefficient of variation of 10-15% is reasonable given monitoring capacities. The uncertainty in the estimates included in HEIDI II is much higher, reflecting the limited data on which the estimates were made. Distribution for background is likely lognormal (Limpert, Stahel et al. 2001).

Possible Correlations:

Background concentrations of individual substances may be correlated with each other, background concentrations may be correlated to total population.

Variable:

Toxicity/C-R data for air toxics (linear, non-threshold dose-response assumed)

Value(s) used in deterministic HEIDI II:

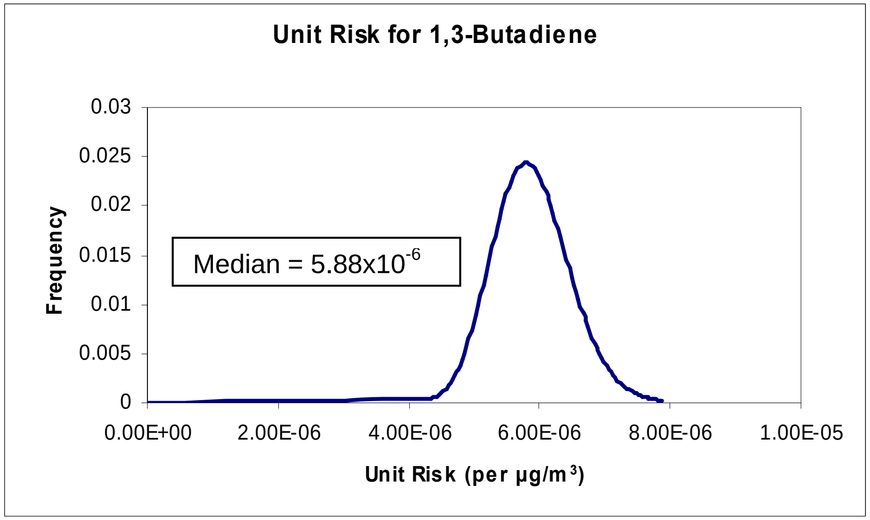
Substance	Unit Risk Value
1,3-Butadiene	5.88E-06
Benzene	3.50E-06
Ethylene Oxide (as ethylene metabolite)	2.27E-05
Nickel (and its compounds)	1.25E-03
PAHs	2.30E-02
Formaldehyde	5.30E-06
Acetaldehyde	5.80E-07

Parametric description:

(See Justifications/notes)

Substance	Inhalation unit risk (median)	Sigma	GSD	SD
1,3-Butadiene	5.88E-06	2.40	11	1.04E-04
Benzene	3.50E-06	2.40	11	6.19E-05
Ethylene (as oxide)	2.27E-05	2.40	11	4.01E-04
Nickel (and its compounds)	1.25E-03	2.40	11	2.21E-02
PAH (as benzo(a)pyrene)	2.30E-02	2.40	11	4.07E-01
Formaldehyde	5.30E-06	2.40	11	9.38E-05
Acetaldehyde	5.80E-07	2.40	11	1.03E-05

Example probability distribution:

<table>
<tr><td></td><td></td><td>
</td></tr>
<tr><td colspan="3">Potential sources of Uncertainty/Variability:
Using the unit risk value as a central value for toxicity when cancer potency actually represents the 95% upper confidence limit of the cancer potency value; extrapolating from animal data to human data, extrapolating from high to low dose, assumption that the dose-response shape is linear at low doses, and variability within a population - interindividual susceptibility to cancer is generally acknowledged based on genetic and environmental factors (such as concurrent exposures to other carcinogens). Assumption that the evidence for carcinogenicity is clear and that it is equally compelling for all substances included in HEIDI.</td></tr>
<tr><td colspan="3">Level of Uncertainty: Risk</td></tr>
<tr><td colspan="3">Level of Evidence: Medium</td></tr>
<tr><td colspan="3">Sensitivity Analysis: Required for individual chemicals: those for which values are controversial or difficult to identify. These include

PAH: values from WHO = 80–100×10-3 (μg/m^3)$^{-1}$; RIVM = 100×10-3 (μg/m^3)$^{-1}$; MOE = 23 ×10-3 (μg/m^3)$^{-1}$
Vanadium: values from WHO = 20 μg/m^3 , values from IIEQ = 100 μg/m^3 , 1-20 μg/m^3
Nickel: values from Health Canada = 1.25 ×10-3 (μg/m^3)$^{-1}$, EPA(nickel subsulfide) =4.8E^{-4} (μg/m^3)$^{-1}$, EPA (refinery dust) = 2.4E^{-3} (μg/m^3)$^{-1}$</td></tr>
<tr><td colspan="3">Justifications/notes:
The toxicity values used to characterize the dose-response relationship for nonthreshold air toxics were unit risk values (although occasionally, these were derived from TC$_{05}$ values).
Hattis (Hattis and Barlow 1996) uses Monte Carlo simulation to derive probabilistic estimates of risk from exposure to carcinogens</td></tr>
</table>

based on a previously derived uncertainty distribution for cancer potency factors and interindividual parameters which affect susceptibility. All inputs were specified as being lognormal. Outputs were tabulated as percentiles for various levels of susceptibility. Hattis' predicted distributions were anchored on a hypothetical $1/10^6$ cancer risk, the shape and spread of the distribution should equally apply to the levels of risk observed in HEIDI II. The Hattis distributions, however, would have to be adapted such that the mean centered on the unit risk values for the individual chemicals included in HEIDI II. This method only applies to genetically-acting metabolically activated carcinogens; also the experiments on which it is based were not limited to inhalation – so some aspects of metabolism which were modeled are not relevant.

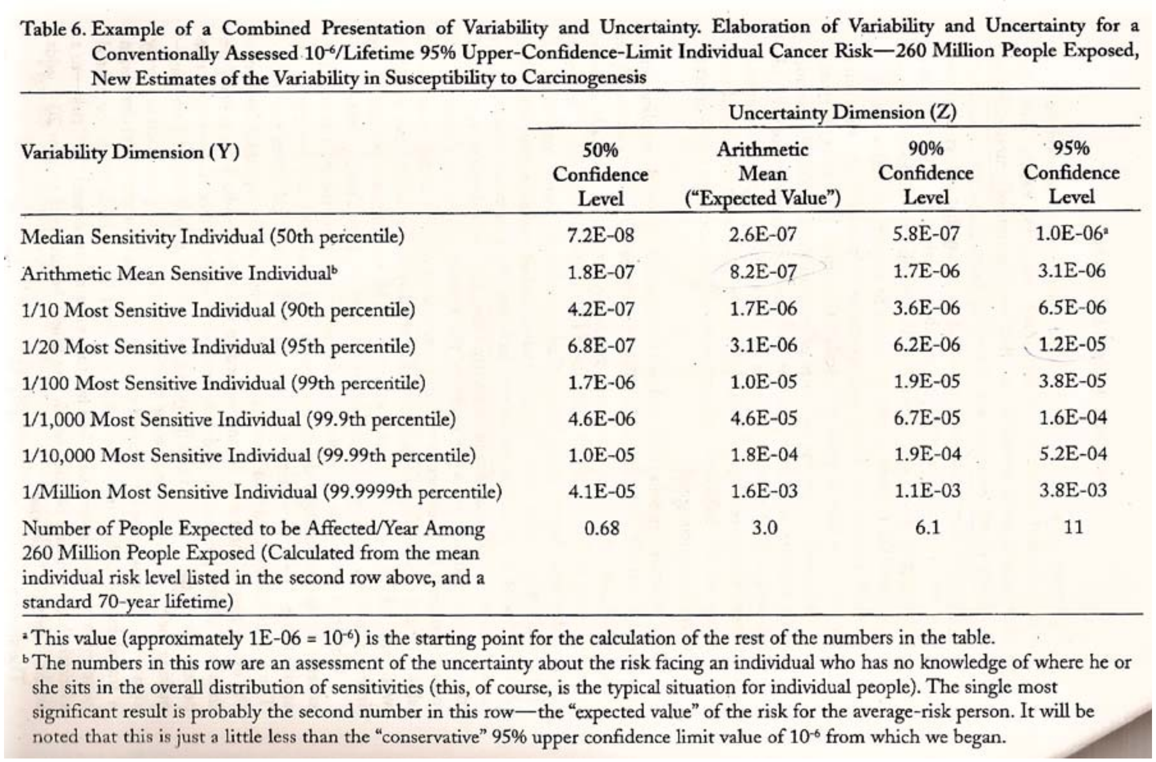


Table 6. Example of a Combined Presentation of Variability and Uncertainty. Elaboration of Variability and Uncertainty for a Conventionally Assessed 10^{-6}/Lifetime 95% Upper-Confidence-Limit Individual Cancer Risk—260 Million People Exposed, New Estimates of the Variability in Susceptibility to Carcinogenesis

	Uncertainty Dimension (Z)			
Variability Dimension (Y)	50% Confidence Level	Arithmetic Mean ("Expected Value")	90% Confidence Level	95% Confidence Level
Median Sensitivity Individual (50th percentile)	7.2E-08	2.6E-07	5.8E-07	1.0E-06[a]
Arithmetic Mean Sensitive Individual[b]	1.8E-07	8.2E-07	1.7E-06	3.1E-06
1/10 Most Sensitive Individual (90th percentile)	4.2E-07	1.7E-06	3.6E-06	6.5E-06
1/20 Most Sensitive Individual (95th percentile)	6.8E-07	3.1E-06	6.2E-06	1.2E-05
1/100 Most Sensitive Individual (99th percentile)	1.7E-06	1.0E-05	1.9E-05	3.8E-05
1/1,000 Most Sensitive Individual (99.9th percentile)	4.6E-06	4.6E-05	6.7E-05	1.6E-04
1/10,000 Most Sensitive Individual (99.99th percentile)	1.0E-05	1.8E-04	1.9E-04	5.2E-04
1/Million Most Sensitive Individual (99.9999th percentile)	4.1E-05	1.6E-03	1.1E-03	3.8E-03
Number of People Expected to be Affected/Year Among 260 Million People Exposed (Calculated from the mean individual risk level listed in the second row above, and a standard 70-year lifetime)	0.68	3.0	6.1	11

[a] This value (approximately 1E-06 = 10^{-6}) is the starting point for the calculation of the rest of the numbers in the table.

[b] The numbers in this row are an assessment of the uncertainty about the risk facing an individual who has no knowledge of where he or she sits in the overall distribution of sensitivities (this, of course, is the typical situation for individual people). The single most significant result is probably the second number in this row—the "expected value" of the risk for the average-risk person. It will be noted that this is just a little less than the "conservative" 95% upper confidence limit value of 10^{-6} from which we began.

Figure 41: Combined uncertainty and variability estimates for carcinogenesis in a population of 260 milion. From (Hattis and Barlow, 1996)

If we assume that the unit risk value applies to the median sensitivity individual and is situated at the median of the range of uncertainty, then a comparison between Hattis' "median individual" value and the 95% confidence level for a 95th percentile of sensitivity in individuals will provide a basis to calculate the level of spread in the distribution (assuming lognormality).
The freeware program "LOGNORM4" (Strom and Stansbury 2000) allows calculation of any parameters of a lognormal distribution given any two. Thus, based on the median and the 95th percentile value, the coefficient of variance can be determined. This, in turn, can be applied to the unit risks in HEIDI II (which can be considered chemical-specific median values) and used to calculate the characteristics of the chemical-specific distributions.

I.e., given: median = $2.6*10^{-7}$, and 95th percentile = 1.2e-5

LOGNORM calculates:

GSD	sigma	SD	CV	variance	skewness	kurtosis
10.27434	2.32965	5.90E-05	15.0508	3.48E-09	3454.562	2.70E+09

This value of GSD is close to a GSD of ~11 that was calculated by both Crouch (Crouch 1996) and Gaylor, and later and used by Brand (Brand, Gray et al. 1997) to account for interspecies scaling including variability across chemicals and experiments. Therefore, HEIDI II will adopt a constant GSD of 11 to apply to cancer potency/unit risk values in the model.

Applying this coefficient of variance to the chemical-specific unit risk values gives, using LOGNORM4:

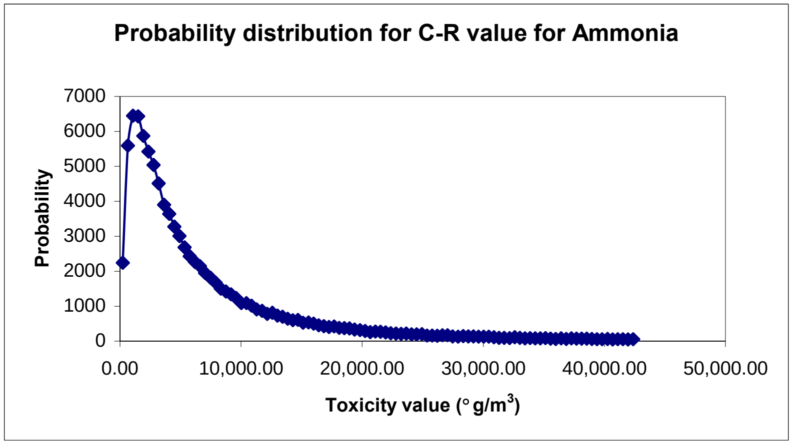
Substance	**Inhalation unit risk (assume equivalent to arithmetic mean)**	**Sigma**	**GSD**	**Median (used as proxy for geometric mean)**	**SD**
1,3-Butadiene	5.88E-06	2.40	11	3.32E-07	1.04E-04
Benzene	3.50E-06	2.40	11	1.97E-07	6.19E-05
Ethylene (as oxide)	2.27E-05	2.40	11	1.28E-06	4.01E-04
Nickel (and its compounds)	1.25E-03	2.40	11	7.05E-05	2.21E-02
PAH (as benzo(a)pyrene)	2.30E-02	2.40	11	1.30E-03	4.07E-01
Formaldehyde	5.30E-06	2.40	11	2.99E-07	9.38E-05
Acetaldehyde	5.80E-07	2.40	11	3.27E-08	1.03E-05

Possible Correlations:

None Identified

<table>
<tr><th>Variable:</th><th>Value(s) used in deterministic HEIDI II:</th><th>Parametric description:</th></tr>
<tr>
<td>Toxicity/C-R data for air toxics (“threshold” – modeled using Mantel-Bryan formulation anchored at ED05)

ED05</td>
<td>
<table>
<tr><th>Substance</th><th>Value</th><th>Type of value</th></tr>
<tr><td>1,2,4-Trimethylbenzene</td><td>22000</td><td>LOAEL (adj) ug/m3</td></tr>
<tr><td>Ammonia (Total)</td><td>2300</td><td>NOAEL (HEC) (ug/m3)</td></tr>
<tr><td>Benzene (as BTEX potentiator)</td><td colspan="2">Mixture value calculated; value depends on relative concentrations at specific site</td></tr>
<tr><td>BTEX</td><td colspan="2">Mixture value calculated; value depends on relative concentrations at specific site</td></tr>
<tr><td>Cyclohexane</td><td>1722000</td><td>LOAEL(HEC) ug/m3</td></tr>
<tr><td>Dicyclopentadiene</td><td>2000</td><td>LOAEL ug/m3</td></tr>
<tr><td>Diethanolamine (and its salts)</td><td>2700</td><td>LOAEL adj (ug/m3)</td></tr>
<tr><td>Ethylbenzene</td><td colspan="2">Mixture value calculated; value depends on relative concentrations at specific site</td></tr>
<tr><td>Hydrogen sulphide</td><td>640</td><td>NOAEL (HEC) ug/m3)</td></tr>
<tr><td>Isoprene</td><td>3748793</td><td>LOAEL</td></tr>
<tr><td>Mercury</td><td>9</td><td>LOAEL (HEC) ug/m3</td></tr>
<tr><td>Methanol</td><td>1910000</td><td>LOAEL (adj)</td></tr>
</table>
</td>
<td>ED05 values (or values used in place of ED05s where data was not available, as discussed below) were assigned a lognormal distribution and GSD of 7.5 if the value was based on animal data or GSD=3 if the value was based on epidemiologic data

Example:

ED05 = 2300; GSD = 3.</td>
</tr>
</table>

Methyl ethyl ketone	1517000	LEC (HEC) ug/m3
Methyl isobutyl ketone	1026000	NOAEL (HEC) (ug/m3)
Methyl tert-butyl ether	368,000	NOAEL (adj) ug/m3
Naphthalene	9300	LOAEL (HEC) ug/m3
n-Hexane	73000	LOAEL (HEC) ug/m3
Phenol (and its salts)	19245.39877	NOAEL (ug/m3)
Propylene	326000	LOAEL (adj) (ug/m3)
Styrene	46000	LOEL (adj) ug/m3
Sulphuric acid	380	LOAEL (ug/m3)
Toluene	Mixture value calculated; value depends on relative concentrations at specific site	
Vanadium (except when in an alloy) and its compounds	20	LOAEL ug/m3
Xylene (all isomers)	Mixture value calculated; value depends on relative concentrations at specific site	
Zinc (and its compounds)	350	RELx10 (ug/m3)

Potential sources of Uncertainty/Variability:
Extrapolating from animal data to human data, assumption that the dose-response shape invoked by the Mantel-Bryan formulation is appropriate at low doses for all chemicals, and variability within a population. In HEIDI II specifically, NOAELs and LOAELs are treated as being equivalent to ED05s. Assumption that the evidence for adverse health effects is clear and that it is equally compelling for all substances included in HEIDI. Variability within a population likely exists - interindividual susceptibility is probable and would result from genetic factors and/or environmental factors (such as concurrent exposures to other toxins).

Level of Uncertainty: Risk

Level of Evidence: Medium

Sensitivity Analysis: Vanadium: 20 $\mu g/m^3$ provisional LOAEL from WHO; limits of distribution could be 1 $\mu g/m^3$ (WHO value to which a 10-fold UF was applied); up to 50$\mu g/m^3$ which is the ACGIH limit value Note special case of BTEX; other substances for which sensitivity analysis might be necessary, i.e., V, Zn etc.

Justifications/notes:

Where the data is available, HEIDI II uses TC05 values to predict case incidence for endpoints associated with each chemical. In practice, however, the best available toxicity data for many substances is in the form of a NOAEL or benchmark dose. (As Hattis (Hattis and Anderson 1999) suggests, NOAELS are not incompatible with the concept of ED05 or TC05).

The preliminary testing of HEIDI II suggested that it will be important to characterize uncertainty and variability that exists in the toxicity data used. The uncertainties associated with the use of values such as NOAELs are widely recognized, and include experimental limitations arising from the selected spacing of doses and detection limits of instrumentation as well as issues such as interspecies extrapolation, intraspecies extrapolation, extrapolation from subchronic to chronic studies, and relevance for sensitive subpopulations (See, for example (Kalberlah, Schneider et al. 2003)). Typically, uncertainty/adjustment factors are applied to NOAELs to account for some of this lack of knowledge.

In general, it appears that lognormal distributions for the values will be a generally accepted format for the family of distributions (Hattis, Banati et al. 1999):

> *"Such a distribution would be expected if there are many factors, each contributing modestly to the individual variability in threshold doses, and if each factor tends to act multiplicatively to affect individual thresholds. This assumption of log-normality of population distributions of thresholds is by no means new—it is the basis for traditional probit analysis of toxicological data that predates Lehman and Fitzhugh"*
>
> (Hattis and Anderson 1999).

The "non-threshold-acting" substances in HEIDI II were assessed individually to determine which uncertainty factors were relevant to each one. If the EPA applied a particular type of uncertainty factor when developing and RfC, this was taken as an indicator that the associated type of uncertainty was relevant in determining a range of possible values for the threshold. However, it is noted that the central NOAEL/LOAEL/TC05 values used in HEIDI have already been adjusted to account for the animal to human extrapolation, and for subchronic to chronic extrapolations (but the uncertainty inherent in these extrapolations was not described).

Attempts were made to characterize the uncertainty in the adjustment factors by calculating ratios of values found in different experiments; i.e., collating values of NOAELs calculated for rats and mice and using the ratios between the results to describe the interspecies adjustment factor, or similar approaches to compare chronic and subchronic results, with the mean representing the "true" difference in NOAELs between the species and the spread of the values intended to represent heterogeneity in response across chemicals. While intuitively, this approach makes sense, there is evidence that use of the ratios can invoke systematic errors (Brand, Rhomberg et al. 1999). Other efforts have developed theoretical distributions which are designed to be consistent with the use of 10 as a conservative adjustment factor. Some results are presented below:

Type of Uncertainty	Estimated GSD	Method	Reference
Subchronic -> chronic Interspecies Interindividual	2.1 4.9 2.3	Database-derived (ratios comparison)	(Baird, Cohen et al. 1996)
Subchronic -> chronic Interspecies interindividual	2 2 2	Theoretical distributions developed to be consistent with default factor of 10	(Price, Keenan et al. 1997)
Subchronic -> chronic Interspecies Interindividual	2.3 1.6 1.3	Theoretical distributions developed to be consistent with default factor of 10	(Slob and Pieters 1998)
Subchronic -> chronic Interspecies interindividual	2 2 2	Theoretical distributions developed to be consistent with default factor of 10	(Swartout, Price et al. 1988)
interindividual	2.95	Estimated aggregate GSD for inhaled chronic systemic toxicant based on variability in pharmacokinetic parameters	(Hattis, Banati et al. 1999)
Subchronic -> chronic Interspecies interindividual	4.5 1.6 3.5	Database-derived (ratios comparison)	(Vermeire, Stevenson et al. 1999)
LOAEL ->NOAEL Subchronic -> chronic Interspecies interindividual	0.6 1.30 1.66 1.64	Compilation of previous ratios comparisons by various authors	(Kodell and Gaylor 1999)
LOAEL ->NOAEL Subchronic -> chronic Interspecies interindividual	0.6 1.72 1.64 1.66	Compilation of previous ratios comparisons by various authors	(Gaylor and Kodell 2000)
Interspecies Interindividual	3 3	historical data	(Evans, Rhomberg et al. 2001)
Combined	7.5	Regulatory agency (RIVM) review of evidence	(Vermeire, Pieters et al. 2001a)

In some sense, all available methods to characterize uncertainty in noncancer toxicological values are unsatisfactory. The uncertainty in the values used to derive the distributions suggests that the distributions may not be representative of reality. However, in the context of HEIDI II and the uncertainties present throughout the model, using a GSD of 7.5 chosen by a regulatory agency after reviewing the available data seems reasonable. This value encompasses both uncertainty and variability in the available data. However - not all of the toxicological values in HEIDI II are subject to the same uncertainties. While the data is not mature enough to differentiate between all types of uncertainty and assign a GSD to each, studies that are based on epidemiologic evidence are likely to be less uncertain. Hattis' value of GSD~3 will be used in those cases.

(Note:"y" (=yes) indicates that uncertainty factor applies)

Substance	Value	Type	Subchronic to chronic	Animal to Human	LOAEL/ NOAEL	Human variability	Other/ Notes	GSD	Median (≈ geometric mean)	SD	Sigma
1,2,4-Trimethylbenzene	22000	LOAEL (adj) ug/m3	y	y	y	y	No UFs have been applied; this is a LOAEL direct from a publication	7.5	2890	$1.7*10^5$	2.01
Ammonia	2300	NOAEL (HEC) (ug/m3)				y	y (database deficiencies)	3	1259	3521	1.10
Benzene	14700	TC05 (ug/m3)	y		y	y	y (database deficiencies)	7.5	1931	$1.1*10^5$	2.01
BTEX	Values is a combination of individual B, T, E, X values										
Cyclohexane	1722000	LOAEL(HEC) ug/m3		y		y	y (database deficiencies)	7.5	226179	$1.3*10^7$	2.01
Dicyclopentadiene	2000	LOAEL ug/m3	y	y	y	y	Assume since known to be 10 000 in total	7.5	263	15095	2.01
Diethanolamine (and its salts)	2700	LOAEL adj (ug/m3)	y	y	y	y		7.5	355	20378	2.01
Ethylbenzene	434000	NOAEL (HEC) ug/m3)		y		y	y (database deficiencies)	7.5	57004	$3.3*10^6$	2.01
Hydrogen	640	NOAEL	y	y		y		7.5	84	4830	2.01

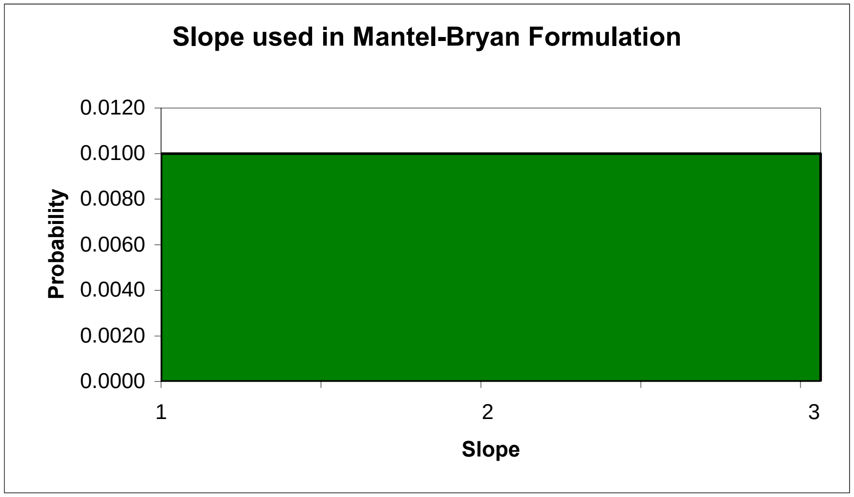
Sulphide		(HEC) ug/m3)									
Isoprene	3748793	LOAEL		y	y	y		7.5	492391	$2.8*10^7$	2.01
Mercury	9	LOAEL (HEC) ug/m3			y		y (database deficiencies)	7.5	1.2	68	2.01
Methanol	1910000	LOAEL (adj) ug/m3		y		y		7.5	250872	$1.4*10^7$	2.01
Methyl Ethyl Ketone (MEK)	1517000	LEC (HEC) ug/m3		y		y	y	7.5	199253	$1.1*10^7$	2.01
Methyl Isobutyl Ketone (MIBK)	1026000	NOAEL (HEC) (ug/m3)		y		y	y	7.5	134761	$7.7*10^6$	2.01
Methyl Tert-Butyl Ether (MTBE)	368000	NOAEL (adj) ug/m3	y	y	y	y		7.5	48335	$2.8*10^6$	2.01
Naphthalene	9300	LOAEL (HEC) ug/m3		y	y	y	y	7.5	1222	7.010^4	2.01
n-Hexane	73000	LOAEL (HEC) ug/m3			y	y	y	7.5	9588	$5.5*10^5$	2.01
Phenol	19245	NOAEL (ug/m3)	y	y		y		7.5	2528	$1.4*10^5$	2.01
Propylene	326000	LOAEL (adj) (ug/m3)		y	y	y		7.5	42819	$2.5*10^6$	2.01
Styrene	46000	LOEL (adj) ug/m3		y	y	y		7.5	6042	$3.5*10^5$	2.01
Sulphuric	380	LOAEL	y	y	y	y		7.5	50	2868	2.01

Acid		(ug/m3)									
Toluene	37500	adj NOEL ug/m3				y		3	20509	$5.7*10^4$	1.10
Vanadium	20	LOAEL ug/m3			y	y		7.5	3	151	2.01
Xylene	180000	LOEL (adj) ug/m3		y	y	y		7.5	23642	$1.4*10^6$	2.01
Zinc	350	RELx10 (ug/m3)				y		3	191	536	1.10

LOGNORM4 was used to derive various parameters of the lognormal distribution for each substance's ED05 (or value used to represent the ED05 as described above).

Possible Correlations:

None identified

Variable:	**Value(s) used in deterministic HEIDI II:**	**Parametric description:**
Toxicity/C-R data for air toxics ("threshold" – modeled using Mantel-Bryan formulation anchored at ED05) Dose-response slope	1.5 Based on Mantel Bryan method where slope represents change in probits (number of standard deviations) relative to log of the dose. 1 is a conservative estimate and a value of 1.5 appeared to represent the data well.	A rectangular distribution with the endpoints at values of 1 and 3. 

Potential sources of Uncertainty/Variability:
The Mantel-Bryan dose-probit method is just one way of carrying out low-dose extrapolations for systemic toxicants. A comparison of extrapolations using (i) a linearized unit risk approach (ii) the Mantel Bryan formulation with the default slope of 1, and (iii) a steep probit (Mantel Bryan-type) approach using a slope of 1.5 indicated that the concentration of a hypothetical contaminant with an ED05 of 500 µg/m^3 associated with a *de minimis* risk level of 10^{-5} would range from 0.1-5 µg/m^3 depending on the approach. The steep Mantel Bryan formulation predicted that the air concentration corresponding to a 10^{-5} risk is roughly equivalent to the ED05/100 (e.g the ED05=500 µg/3, and the 10^{-5} risk concentration=5 µg/m^3). Hence the LN(dose)-probit function with slope=1.5 produces the same tolerable concentration (TC) level as the ED05/100 (or NOAEL/100) formula for deriving the default TC values for threshold-acting agents (McColl 2003).
Alternative methods of extrapolating to low doses for “threshold-acting” toxins might predict different values or incidence.

Level of Uncertainty: Risk

Level of Evidence: Medium

Sensitivity Analysis: The Mantel-Bryant slope can be varied to determine its importance for the predictions of HEIDI II; this is essence tests various exposure-response functions within the probit family. Investigation of any interaction between the ED05 and the slope value can also be accomplished through response surface analysis.

Justifications/notes:
The preliminary testing of HEIDI II suggested that it will be important to characterize uncertainty and variability that exists in the toxicity data used.
Mantel and Bryan (Mantel and Bryan 1961; Mantel, Bohidar et al. 1975) note that with systemic poisons, rather steep dose-response slopes are observed (even up to 10-50 probits per tenfold dose). However, for therapeutic agents and virus assays, slopes tend to be lower; within the range of 2-3. For this reason they select 1 as an (arbitrary) conservative estimate. While it is possible to create a distribution for the dose-response slope that contains higher values the following points indicate that that this is unnecessary:

> In HEIDI, natural log rather than $\log_{10}$ is used, so all slopes should be adjusted by an order of 2.303, which leads to slopes of ~5-25
>
> a steeper dose-response will likely lead to lower predicted incidence in the low exposure region, and likely cause underflow of predicted cases to zero in any case.

Values ranging up to three were chosen for the uniform distribution because preliminary local sensitivity analyses indicated that responses disappeared to zero at values of 3 and so extending the distribution to 5 does not add any information

Possible Correlations:
None identified

Variable:

Toxicity/C-R data for CACs (Criteria Air Contaminants)

Value(s) used in deterministic HEIDI II:

The reference documentation for PM health effects endpoints and concentration-response function information was obtained from the report by Abt Associates (Abt Associates Nov. 2002)

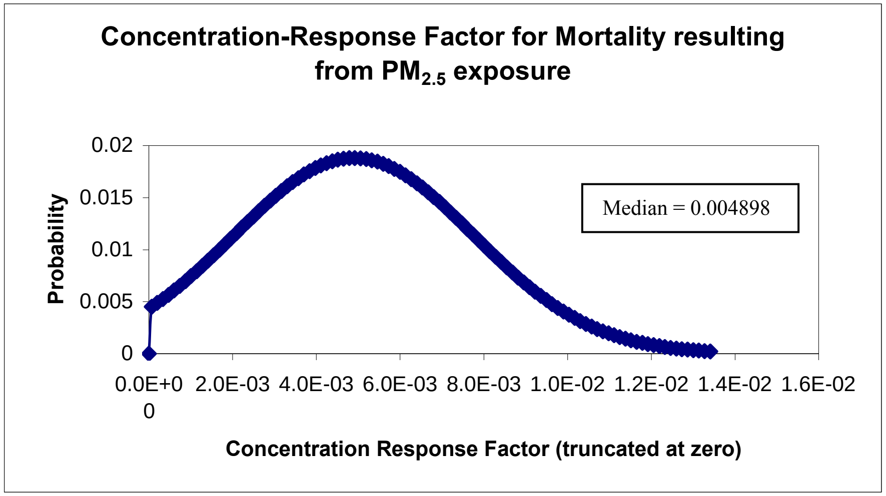
	child (0-18)	***adult (19-65)***	***elderly (65+)***
annual mortality risk coefficient by age-group	0	0.000044	0.000059
annual chronic bronchitis risk coefficient by age-group	0	0.000072	0.000096
annual asthma hospitalization risk coefficient by age-group	0.000004	0.000004	0
annual asthma ER visit risk coefficient by age-group	0.000006	0.000006	0

Parametric description:

Arithmetic Normal truncated below zero (formula for calculation provided below)

Outcome	**Concentration-response factor (β)**	**Standard error of β (using upper bound of reported RR)**	**Standard error of β (using lower bound of reported RR)**
Mortality	0.004897959	0.001457726	0.001249479
Chronic bronchitis	0.025454545	0.009276438	0.009276438
Asthma hospital admissions	0.0016498	0.001177394	0.000784929
Asthma ER visits	0.003865382	0.00200157	0.00133438

Example of concentration-response factor (which is used alongside death rate and population at risk to predicted incidence of mortality)

Potential sources of Uncertainty:

For the asthma outcomes, the RR is based on PM_{10}, but the formula is not adjusted to represent only $PM_{2.5}$, which it was for the case of chronic bronchitis. From the discussions and literature review it was not clear why the analysis was inconsistent.

Level of Uncertainty: Risk

Level of Evidence: Medium

Sensitivity Analysis:

Justifications/notes:

The epidemiological concentration-response (C-R) functions are linear non-threshold in form, so that the C-R function is based on a linear risk coefficent that incorporates a slope factor according to the following equation:

Incident Cases = Risk Coefficient * Conc $PM_{2.5}$ * at-risk population (both population prevalence and C-R slope factors are accounted for in the risk coefficient)

The C-R relationships used to predict incidence of mortality, chronic bronchitis, and asthma ER visits and hospital admissions were developed by Abt Associates (Abt Associates Nov. 2002) using widely accepted and used RR estimates. The approach also allows for calculation of the standard error associated with the mean RR, providing an estimate of the 5% and 95% confidence intervals. As applied in HEIDI I *(following Abt)…*:

$$\Delta Mortality = -\left[y_o * \left(\left(\frac{(1-RR)}{\Delta PM_{2.5}(ACS)} \right) * \Delta PM_{2.5} \right) \right] * pop$$

There appears to be limited available research describing an appropriate shape for the probability distribution for the relative risks. Comparing the mean with 5% and 95% values indicates some skewness (to the right) in the distribution. The EPA elicited distributions for PM C-R functions from experts in its “Final Regulatory Analysis: Control of Emissions from Nonroad Diesel Engines”, published in 2004 (Environmental Protection Agency (EPA) 2004). They found that most C-R functions were slightly skewed, although they did not generalize a specific distribution type that might be appropriate. Clearly, the distributions for relative risk must be bounded on the lower end, such that exposure to $PM_{2.5}$ should not predict a gain in health status.

Either a Weibull or a lognormal distribution may best represent the uncertainty in the PM C-R functions. Alternately, a normal distribution bounded at zero may be appropriate.

It has been suggested that epidemiologic data should only be used in risk assessment when certain conditions are met: a moderate to strong positive association exists, strong biases can be ruled out, confounding is well-controlled or limited, and exposures have been well-characterized (in) (Stayner, Bailar et al. 1999). Use of epidemiologic data should consider
Study design (i.e., sample size, follow-up timeframe, confounding)
Choice of data, choice of D-R model
Exposure estimates
Using exposure rather than dose (is exposure proportional to dose?)
Variations in susceptibility

Possible Correlations:
Non identified

Variable:	**Value(s) used in HEIDI II:**	**Parametric description:**
Population data	Population living in each of 20 zones surrounding each refinery was determined using data	None – it is most appropriate to perform sensitivity analysis with various patterns of population density relative to the refinery location

Potential sources of Uncertainty:
Movement of people into/out of areas
Changes in population since the 2001 census for other reasons – births, deaths, aging (which would affect the number of people in each age group)
Uncertainties introduced by ArcMAP – I.e., resolution is at average level of census dissemination areas. Where these are geographically large, there is no way of knowing where in the area people are living.

Level of Uncertainty: Risk

Level of Evidence: Strong

Sensitivity Analysis: To address variability, it was performed with a variety of patterns: homogeneous population density, dense close to refinery, dense at 20-25 km from refinery, dense in the four cardinal directions (N, S, E, and W) from refinery

Justifications/notes:
For policy analysis, it is most useful to know what patterns of population density surrounding refinery are associated with greatest impacts. Unless new developments are built or rezoning occurs, the patterns of population around a refinery are likely to remain relatively stable. Characterizing the uncertainty in the number of people living around each refinery is not likely to affect the prioritization of refinery emissions

Possible Correlations:
Correlation with background concentrations?

Variable:	**Value(s) used in HEIDI II:**	**Parametric description:**
Age	Child: 0-18 years Adult: 19-59 years Senior: 60+ years	N/A

Level of Uncertainty: N/A – assigned

Sensitivity Analysis: N/A

Justifications/notes:
Age distinctions are only used to predict incidence from exposure to CACs (primary and secondary $PM_{2.5}$)

Possible Correlations:
N/A

Variable:	**Value(s) used in HEIDI II:**	**Parametric description:**
	Male/Female	None

Gender		
Potential sources of Uncertainty: N/A – assigned		
Sensitivity Analysis: N/A		
Justifications/notes: Switching variable only		
Possible Correlations: N/A		

Variable: Fraction of population that is male/female	**Value(s) used in HEIDI II:** 0.5	**Parametric description:** None – to be taken as "given"
Sensitivity Analysis: None		
Justifications/notes: Approximate value for the population in Canada. Potential to affect predictions exists only for disease endpoints which apply to only one gender		
Possible Correlations: None identified		

Variable: Age-sex discounting multiplier	**Value(s) used in HEIDI II:** 0 if specific age-sex group is not a target; 1 if group is a target	**Parametric description:** None – to be taken as "given"
Sensitivity Analysis: None		
Justifications/notes: Potential to affect predictions exists only for disease endpoints which apply to only specific age groups		
Possible Correlations: None identified		

<table>
<tr>
<td>Variable:

DALYp values (simple)</td>
<td>Value(s) used in HEIDI II:

<table>
<tr><th>ILSI definition for selection of simple DALY (Burke, Doull et al. 1996)</th><th>Mode</th></tr>
<tr><td>Irreversible/Life-shortening effects (cancer, mutagenicity, teretogenic</td><td>6.7</td></tr>
</table>
</td>
<td>Parametric description:

None was used. DALY values were treated as point values due to a lack of information. Including distributions of DALYs could only have attempted to describe the uncertainty currently associated with these values, which is</td>
</tr>
</table>

	or reproductive effects)		deemed to be large. Data collected in an effort to identify potential distributions is retained below.
	May be irreversible/life-shortening effects (immunotoxicity, neurotoxicity, kidney damage, liver damage, heart disease, pulmonary disease)	0.67	
	Reversible/ not life-shortening effects (irritation, sensitization)	0.067	

Potential sources of Uncertainty:

These are derived values and allow for only three categories; imply valuation for aspects of life and illness which may be difficult to justify. Values used in HEIDI are aggregate values of DALYs per person, which assumed that the population in Canada can be represented by the populations in the reference study: in terms of age structure, average age at onset of illness, duration of illness and severity weights/valuation of disability or death.

Level of Uncertainty: Scientific Uncertainty

Level of Evidence: Weak

Sensitivity Analysis: None

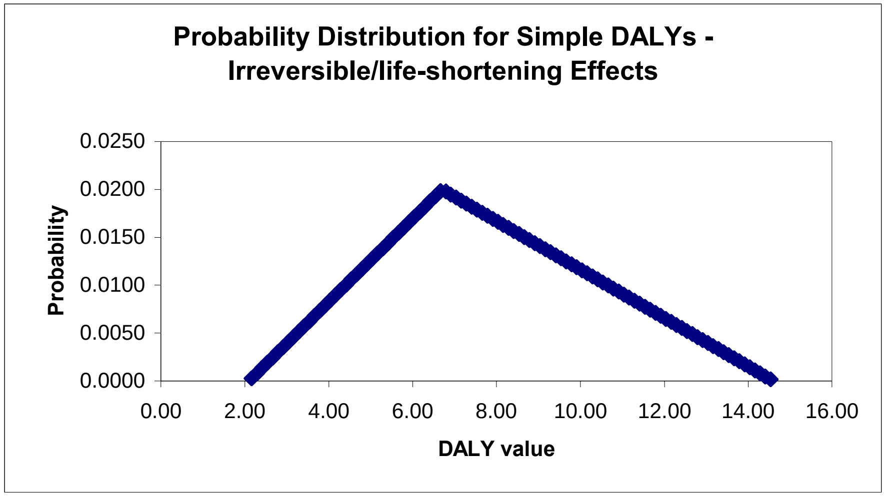
Justifications/notes:

A range of values has been calculated for various disease endpoints. For example, for cancer endpoints, Charles and Jolliet (Charles and Jolliet 2003) suggest that different cancers have more or less the same severity, calculate an average DALYp = 6.6 [yr lost/pers], and suggest this as a default. However, the various DALYp values calculated for different cancers range from 2.1 for prostate cancer to 14.6 for leukemia. These could be used to create a triangular distribution for the simple DALY framework, having a mode at 6.7, the simple DALYp value used in HEIDI II for cancer endpoints, and bounded at 2.1 at the low end and 14.6 at the high end. As the ILSI "simple DALYs" are simply divisions by ten of each other to account for varying degrees of uncertainty, it should be appropriate to adapt this triangular (or maybe even uniform) distribution in a similar manner.

ILSI definition for selection of simple DALY	Mode	Proposed endpoints for triangular distribution
Irreversible/Life-shortening effects (cancer, mutagenicity, teretogenic or reproductive effects)	6.7	Low: 2.1 High: 14.6
May be irreversible/life-shortening effects (immunotoxicity, neurotoxicity, kidney damage, liver	0.67	Low: 0.21

Reversible/ not life-shortening effects (irritation, sensitization)	0.067	Low: 0.021 High:0.146

Example:



Limitations: the endpoint/exposure list in de Hollander is by no means inclusive of all endpoints, so the coefficients of variance will reflect primarily DALYs calculated for exposures to particulates or inhaled carcinogens. Also, since an average CV will be used, the level of uncertainty will be over- or under- estimated in the case of many endpoints. Finally, the uncertainty estimate does not include any assessment of the broader uncertainty associated with this method, such as the "correctness" of the severity weights, the uncertainty imposed by social preferences and cultural contexts.

Possible Correlations:
Toxicity values

<table>
<tr>
<td>Variable:
DALYp values (complex)</td>
<td>Value(s) used in HEIDI II:
<table>
<tr><th>Substance</th><th>DALYp</th><th>Substance</th><th>DALYp</th></tr>
<tr><td>1,3-Butadiene</td><td>23.44</td><td>Methanol</td><td>35.00</td></tr>
<tr><td>Benzene</td><td>23.44</td><td>Methyl ethyl ketone</td><td>1.40</td></tr>
</table>
</td>
<td>Parametric description:
None was used. DALY values were treated as point values due to a lack of information. Including distributions of DALYs could only have attempted to</td>
</tr>
</table>

Ethylene (as oxide)	23.44	Methyl isobutyl ketone	1.40
Nickel (and its compounds)	14.75	Methyl tert-butyl ether	0.72
PAH (as benzo(a)pyrene)	14.75	Naphthalene	1.29
Formaldehyde	14.75	n-Hexane	0.72
Acetaldehyde	14.75	Phenol	0.97
1,2,4-Trimethylbenzene	0.01	Propylene	0.07
Ammonia (Total)	0.07	Styrene	1.40
Benzene (as BTEX component)	0.97	Sulphuric acid	0.07
BTEX	0.97	Toluene (as BTEX component)	0.97
Cyclohexane	1.40	Vanadium and its compounds	0.07
Dicyclopentadiene	0.95	Xylene (as BTEX component)	0.97
Diethanolamine (and its salts)	0.07	Zinc (and its compounds)	0.01
Ethylbenzene (as BTEX component)	0.97	PM death	10.9
Hydrogen sulphide	0.07	PM chronic bronchitis	0.47
Isoprene	0.95	PM asthma hospitalization	0.024
Mercury (and its compounds)	11.44	PM asthma ER visits	0.018

describe the uncertainty currently associated with these values, which is deemed to be large.

Data collected in an effort to identify potential distributions is retained below.

Potential sources of Uncertainty:

These are derived values; imply valuation for aspects of life and illness which may be difficult to justify. Values used in HEIDI are aggregate values of DALYs per person, which assumed that the population in Canada can be represented by the populations in the reference study: in terms of age structure, average age at onset of illness, duration of illness and severity weights/valuation of disability or death.

Level of Uncertainty: Scientific Uncertainty

Level of Evidence: Weak

Sensitivity Analysis:

Justifications/notes:

The complex DALYs used in HEIDI II originate from a variety of sources, including de Hollander (de Hollander, Melse et al. 1999), Melse (Melse, Essink-Bot et al. 2000), and the Global Burden of Disease (Murray and Lopez 1996). de Hollander's estimates are provided alongside 5th and 95th percentile values derived from Monte Carlo simulations. It is not specified whether the central estimate presented is the mode, median, or mean, however, and there is no information provided about the characteristics of the input distributions. A superficial examination of the point estimates alongside the 5th and 95th percentiles indicates that most of the distributions are skewed to the right, although the degree of skew appears to vary. Calculation of the coefficients of variation (assuming a normal distribution for the sake of investigation) reveal varying degrees of variation among the predicted DALYs for the various environmental factor/outcome combinations.

The input variables used to calculate these DALY values are: a set of functions which includes exposure and the associated relative risk to represent the population attributable fraction of the condition, annual incidence of response, and a severity factor discounting time spent with the condition, and the duration of the condition (or loss of life expectancy). It would be anticipated that both exposure and duration of the condition would be characterized by skewed distributions. Determining whether RR distributions are likely to be skewed is less intuitive, but even if both RR and the severity weighting factor had been assigned normal distributions, the output DALY distributions would likely be skewed to the right.

Therefore, the following was initially proposed to develop a distribution for the complex DALYp values: lognormal distributions centred at the DALYp value previously selected in HEIDI II. An average coefficient of variance will be derived using the DALY and 95th and DALY and 5th percentile values reported in de Hollander for exposures and endpoints that are also included in HEIDI II.

The proposed approach leads to the following parameters for the various complex DALYp values used (LOGNORM4 was used to calculate the coefficients of variation from the original de Hollander data under the assumption of lognormal distribution, and was also used to extract the following data):

DALYp	**CV**	**GSD**	**sigma**	**SD**	**variance**	**skewness**	**kurtosis**
0.01	0.92	2.19	0.78	0.01	0.00	3.54	28.40
0.02	0.92	2.19	0.78	0.02	0.00	3.54	28.40
0.02	0.92	2.19	0.78	0.02	0.00	3.54	28.40
0.07	0.92	2.19	0.78	0.06	0.00	3.54	28.40
0.47	0.92	2.19	0.78	0.43	0.19	3.54	28.40
0.72	0.92	2.19	0.78	0.66	0.44	3.54	28.40
0.95	0.92	2.19	0.78	0.87	0.76	3.54	28.40
0.97	0.92	2.19	0.78	0.89	0.80	3.54	28.40
1.29	0.92	2.19	0.78	1.19	1.41	3.54	28.40
1.40	0.92	2.19	0.78	1.29	1.66	3.54	28.40
10.90	0.92	2.19	0.78	10.02	100.49	3.54	28.40

11.44	0.92	2.19	0.78	10.52	110.69	3.54	28.40
14.75	0.92	2.19	0.78	13.57	184.01	3.54	28.40
23.44	0.92	2.19	0.78	21.56	464.70	3.54	28.40
35.00	0.92	2.19	0.78	32.19	1036.09	3.54	28.40

Possible Correlations:

Toxicity values

Appendix D – Annual Emissions Data Extracted from NPRI

	Facility Name														
Chemical Name	Chevron - Burnaby					Consumers' Co-operative - Regina					Husky - Prince George				
Linear non-threshold-acting	2001	2002	2003	mean	std dev	2001	2002	2003	mean	std dev	2001	2002	2003	mean	std dev
1,3-Butadiene															
Benzene	1.33	2.60	2.13	2.02	0.64	14.89	9.62	11.31	11.94	2.69	0.00	0.00	0.00	0.00	0.00
Ethylene	0.12	0.19	0.37	0.23	0.13	38.87	19.33	18.71	25.63	11.47	1.90	1.98	1.93	1.94	0.04
Nickel (and its compounds)		0.22	0.25	0.23	0.02	0.01	0.00	0.10	0.04	0.06					
Benzo(a)pyrene	0.00	0.00	0.00	0.00	0.00							0.00	0.00	0.00	0.00
Formaldehyde															
Acetaldehyde															
Sublinear threshold-acting															
1,2,4-Trimethylbenzene	0.42	0.80	0.82	0.68	0.22	9.78	15.13	16.58	13.83	3.58	0.00	0.00	0.00	0.00	0.00
Ammonia (Total)	0.00	0.00	0.00	0.00	0.00	8.78	8.78	8.78	8.78	0.00					
Benzene (as BTEX potentiator)	1.33	2.60	2.13	2.02	0.64	14.89	9.62	11.31	11.94	2.69	0.00	0.00	0.00	0.00	0.00
Cyclohexane	0.53	1.11	1.47	1.04	0.47	31.95	16.61	17.54	22.03	8.60	1.29	1.27	1.40	1.32	0.07
Dicyclopentadiene															
Diethanolamine (and its salts)	0.00	0.00	0.00	0.00	0.00										
Ethylbenzene	0.48	0.64	0.67	0.60	0.11	8.22	8.69	10.67	9.19	1.30	0.00	0.00	0.00	0.00	0.00
Hydrogen sulphide	2.33	3.54	1.59	2.49	0.98	26.09	26.23	29.81	27.38	2.11	1.80	1.87	1.87	1.85	0.04
Isoprene															
Mercury (and its compounds)		0.00		0.00											
Methanol	0.01	0.02		0.02	0.01										
Methyl ethyl ketone															
Methyl isobutyl ketone															
Methyl tert-butyl ether	9.95	10.25		10.10	0.22										
Naphthalene	0.07	0.12	0.12	0.11	0.03	0.92	2.58	2.94	2.15	1.08	0.00	0.00	0.00	0.00	0.00
n-Hexane	2.80	6.00	5.33	4.71	1.69		23.64	29.22	26.43	3.95	3.93	4.24	4.25	4.14	0.18
Phenol (and its salts)	0.01	0.02	0.02	0.02	0.00	0.03	0.03	0.04	0.03	0.00					
Propylene	1.93	1.68	2.27	1.96	0.30	10.27	11.34	11.69	11.10	0.74	2.00	1.98	1.94	1.97	0.03
Styrene															
Sulphuric acid	0.00	6.22	6.49	4.24	3.67	0.21			0.21	#DIV/0!					
Toluene	2.41	5.55	3.37	3.77	1.61	31.46	34.24	36.53	34.08	2.54	1.12	1.16	1.10	1.13	0.03
Vanadium (except when in an alloy) ar		0.76	1.01	0.89	0.17	0.02	0.00	0.00	0.01	0.01					
Xylene (all isomers)	0.98	1.71	1.35	1.35	0.36	27.14	48.84	63.02	46.33	18.07	0.00	0.00	2.20	0.73	1.27
Zinc (and its compounds)	0.00	0.00	0.00	0.00	0.00										
SOx		1165.85	1149.98				2736.80	2640.51				1439.30	1197.97		
NOx		646.99	556.17				1157.61	1271.38				65.70	50.70		
primary PM2.5		18.70	21.98				0.00	0.00				0.85	1.73		

Chemical Name	Imperial - Dartmouth					Imperial - Nanticoke					Imperial - Sarnia				
Linear non-threshold-acting	2001	2002	2003	mean	std dev	2001	2002	2003	mean	std dev	2001	2002	2003	mean	std dev
1,3-Butadiene											0.068	0.06	0.015	0.05	0.03
Benzene	5.64	5.47	3.80	4.97	1.02	3.81	5.11	4.09	4.34	0.68	10.76	11.04	9.70	10.50	0.71
Ethylene	2.29	2.61	2.15	2.35	0.24	1.68	1.59	1.76	1.68	0.09	3.42	2.55	3.12	3.03	0.44
Nickel (and its compounds)											30.33	26.57	28.28	28.39	1.88
Benzo(a)pyrene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.15	0.00	0.00	0.05	0.09
Formaldehyde															
Acetaldehyde															
Sublinear threshold-acting															
1,2,4-Trimethylbenzene	2.44	2.29	1.72	2.15	0.38	1.75	2.47	1.62	1.94	0.46	4.39	3.71	2.67	3.59	0.87
Ammonia (Total)	9.86	2.87	11.79	8.17	4.70	3.79	20.74	1.19	8.57	10.62	0.39	7.31	5.07	4.26	3.53
Benzene (as BTEX potentiator)	5.64	5.47	3.80	4.97	1.02	3.81	5.11	4.09	4.34	0.68	10.76	11.04	9.70	10.50	0.71
Cyclohexane	5.04	5.60	3.97	4.87	0.83	2.85	3.10	2.52	2.82	0.29	12.15	10.77	7.62	10.18	2.32
Dicyclopentadiene											0.00	0.00	0.00	0.00	0.00
Diethanolamine (and its salts)	0.58	0.56	0.25	0.46	0.19	0.51	0.51	1.06	0.69	0.32					
Ethylbenzene	2.10	1.80	1.69	1.86	0.21	1.44	1.98	1.34	1.59	0.34	4.36	3.89	3.36	3.87	0.50
Hydrogen sulphide	2.94	4.03	3.36	3.44	0.55	8.55	28.18	11.47	16.07	10.59	10.42	3.62	6.70	6.91	3.41
Isoprene															
Mercury (and its compounds)	0.002	0.002	0.002	0.002	0.000	0.004	0.004	0.004	0.004	0.000	0.003	0.003	0.003	0.003	0.000
Methanol	1.17	1.04	1.92	1.38	0.47	0.82	0.76	0.71	0.77	0.06	30.61	9.47	4.99	15.02	13.68
Methyl ethyl ketone											50.60	44.90	57.74	51.08	6.43
Methyl isobutyl ketone											72.49	65.00	64.98	67.49	4.33
Methyl tert-butyl ether															
Naphthalene	0.60	0.80	0.74	0.71	0.10	0.37	0.48	0.33	0.39	0.08	0.85	0.85	0.54	0.75	0.18
n-Hexane	16.67	16.94	12.73	15.44	2.35	7.62	8.96	7.25	7.95	0.90	38.89	34.06	25.29	32.75	6.90
Phenol (and its salts)	0.36	0.28	0.29	0.31	0.04	0.15	0.06	0.06	0.09	0.06	1.71	1.67	3.68	2.36	1.15
Propylene	3.47	3.44	3.91	3.61	0.27	15.85	14.49	24.48	18.27	5.42	31.64	92.44	42.17	55.42	32.49
Styrene															
Sulphuric acid		125.11	107.69	116.40	12.32	103.81	103.64	105.39	104.28	0.96	421.29	421.29	164.43	335.67	148.29
Toluene	11.03	9.41	8.76	9.73	1.17	6.26	9.82	7.29	7.79	1.83	19.07	17.87	14.38	17.11	2.44
Vanadium (except when in an alloy) and its compounds											61.55	67.18	70.52	66.42	4.53
Xylene (all isomers)	11.16	10.04	10.07	10.42	0.64	6.54	9.62	6.74	7.63	1.73	19.20	15.98	13.04	16.07	3.08
Zinc (and its compounds)											9.11	8.71	0.43	6.08	4.90
SOx		4778.90	5967.94				3955.87	5819.97				24735.27	20704.35		
NOx		3525.55	3593.31				2001.38	2096.78				2752.17	2628.46		
primary PM2.5		294.92	282.18				160.16	157.08				402.09	443.79		

Chemical Name	Imperial - Strathcona					Irving - Saint John					North Atlantic Refining - Come by Chance				
Linear non-threshold-acting	2001	2002	2003	mean	std dev	2001	2002	2003	mean	std dev	2001	2002	2003	mean	std dev
1,3-Butadiene						0.05	0	0	0.02	0.03					
Benzene	3.70	3.70	3.53	3.64	0.10	1.26	0.00	23.44	8.23	13.19	16.38	11.71	7.00	11.70	4.69
Ethylene	6.14	6.57	7.09	6.60	0.47	16.94	14.67	0.00	10.54	9.20					
Nickel (and its compounds)						0.33	0.20	0.21	0.25	0.07	13.80	13.99	14.53	14.11	0.38
Benzo(a)pyrene	0.00	0.00	0.00	0.00	0.00						0.00	0.00	0.00	0.00	0.00
Formaldehyde															
Acetaldehyde															
Sublinear threshold-acting															
1,2,4-Trimethylbenzene	2.96	2.98	2.64	2.86	0.20	0.68	0.00	2.26	0.98	1.16	9.12	4.87	4.74	6.24	2.49
Ammonia (Total)	0.02	4.02	0.07	1.37	2.29	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Benzene (as BTEX potentiator)	3.70	3.70	3.53	3.64	0.10	1.26	0.00	23.44	8.23	13.19	16.38	11.71	7.00	11.70	4.69
Cyclohexane	1.52	2.27	1.33	1.71	0.50	2.41	1.66	14.60	6.22	7.26	15.40	9.88	6.08	10.45	4.68
Dicyclopentadiene															
Diethanolamine (and its salts)						0.00		0.00	0.00	0.00	2.02	1.32	9.33	4.22	4.44
Ethylbenzene	1.92	2.30	2.38	2.20	0.24	0.84	0.00	16.13	5.66	9.08	4.12	3.79	2.95	3.62	0.61
Hydrogen sulphide	3.65	3.88	3.25	3.60	0.32	0.17	0.00	6.04	2.07	3.44		4.18	4.68	4.43	0.35
Isoprene															
Mercury (and its compounds)	0.006	0.005	0.006	0.005	0.000		0.000	0.000	0.000	0.000					
Methanol	0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00					
Methyl ethyl ketone	22.07	18.96	29.74	23.59	5.55										
Methyl isobutyl ketone	17.04	14.04	23.40	18.16	4.78										
Methyl tert-butyl ether						9.21		6.94	8.08	1.61	93.29	65.29	99.84	86.14	18.35
Naphthalene	1.22	1.23	1.42	1.29	0.11	0.08	0.00	0.00	0.03	0.05					
n-Hexane	9.20	13.60	11.18	11.33	2.21	3.24	3.64	35.40	14.09	18.46	11.70	15.08	30.43	19.07	9.98
Phenol (and its salts)	0.29	0.16	0.10	0.18	0.09	0.00	0.00	0.00	0.00	0.00	0.13	0.13	0.00	0.09	0.08
Propylene	7.92	8.11	7.49	7.84	0.32	34.90	32.44	5.71	24.35	16.19					
Styrene						0.02	0.00		0.01	0.01					
Sulphuric acid	138.04	138.04	174.66	150.25	21.14	0.00	0.00	0.00	0.00	0.00					
Toluene	10.44	10.99	11.07	10.83	0.34	3.57	3.24	42.87	16.56	22.79	31.26	29.17	19.39	26.60	6.34
Vanadium (except when in an alloy) and its compounds						0.51	0.17	0.56	0.41	0.21	40.00	37.30	39.78	39.03	1.50
Xylene (all isomers)	13.22	13.32	12.99	13.17	0.17	3.74	2.63	19.09	8.49	9.20	21.04	19.65	18.78	19.82	1.14
Zinc (and its compounds)	8.16	9.20	0.37	5.91	4.83	0.00	0.00	0.00	0.00	0.00	0.50	0.50	0.47	0.49	0.02
SOx		4824.00	5330.21				4452.00	7474.36				14658.00	14136.00		
NOx		1845.33	1989.38				4211.00	4424.46				1260.00	1346.25		
primary PM2.5		221.21	227.08				194.80	237.31				173.00	184.57		

Chemical Name	NOVA - Corunna					Parkland - Bowden					Petro-Canada - Edmonton				
Linear non-threshold-acting	2001	2002	2003	mean	std dev	2001	2002	2003	mean	std dev	2001	2002	2003	mean	std dev
1,3-Butadiene	11.33	17.63	11.16	13.37	3.69										
Benzene	46.84	56.43	11.98	38.41	23.39	4.15	NO DATA	NO DATA	4.15		2.48	0.48	2.06	1.67	1.06
Ethylene	80.01	50.98	23.72	51.57	28.15						2.55	0.00	0.00	0.85	1.47
Nickel (and its compounds)											0.03	0.00	0.00	0.01	0.02
Benzo(a)pyrene	0.00			0.00							0.00	0.00	0.00	0.00	0.00
Formaldehyde															
Acetaldehyde															
Sublinear threshold-acting															
1,2,4-Trimethylbenzene	1.51	3.78	1.35	2.21	1.36	1.89			1.89		1.07	0.00	5.77	2.28	3.07
Ammonia (Total)		0.00	0.00	0.00	0.00						0.00	0.00	0.00	0.00	0.00
Benzene (as BTEX potentiator)	46.84	56.43	11.98	38.41	23.39	4.15			4.15		2.48	0.48		1.48	1.42
Cyclohexane	3.26	2.70	2.66	2.87	0.34	2.53			2.53		3.21	0.00	1.85	1.69	1.61
Dicyclopentadiene	4.97	17.12	0.16	7.42	8.74										
Diethanolamine (and its salts)											0.51	0.00	0.00	0.17	0.29
Ethylbenzene	5.05	5.89	1.19	4.04	2.51	0.81			0.81		1.16	0.68	3.84	1.89	1.70
Hydrogen sulphide	0.11	0.10	0.07	0.09	0.02						2.53	1.39	2.11	2.01	0.57
Isoprene	1.87	6.59	1.81	3.42	2.74										
Mercury (and its compounds)	0.001	0.001	0.005	0.002	0.002						0.001	0.004	0.004	0.003	0.002
Methanol															
Methyl ethyl ketone															
Methyl isobutyl ketone															
Methyl tert-butyl ether															
Naphthalene	1.44	3.73	0.73	1.97	1.57										
n-Hexane	7.72	5.85	23.30	12.29	9.58	12.08			12.08		9.09	13.41	17.14	13.21	4.03
Phenol (and its salts)			13.31	13.31							0.00	0.00	0.00	0.00	0.00
Propylene	46.48	28.45	30.88	35.27	9.79						2.53	1.34	0.00	1.29	1.27
Styrene	2.46	3.84	0.29	2.20	1.79										
Sulphuric acid		257.26	266.74	262.00	6.70						0.00	127.62	175.31	100.98	90.64
Toluene	22.84	24.79	6.97	18.20	9.78	7.71			7.71		5.67	2.65	19.72	9.35	9.11
Vanadium (except when in an alloy) and its compounds											0.01	0.00	0.00	0.00	0.01
Xylene (all isomers)	9.37	8.94	5.42	7.91	2.17	4.41			4.41		4.09	0.75	17.83	7.56	9.05
Zinc (and its compounds)											0.00	1.79	0.00	0.60	1.03
SOx		5730.62	5990.80									1907.85	1788.01		
NOx		2458.16	2890.20									1661.41	1547.90		
primary PM2.5		244.84	219.80									220.71	86.20		

Chemical Name	Petro-Canada - Mississauga					Petro-Canada - Montreal					Petro-Canada - Oakville				
Linear non-threshold-acting	2001	2002	2003	mean	std dev	2001	2002	2003	mean	std dev	2001	2002	2003	mean	std dev
1,3-Butadiene						0.005	0	0	0.002	0.003	0.093	0	0	0.031	0.054
Benzene	3.42	3.43	3.38	3.41	0.02	18.03	8.74	10.55	12.44	4.92	1.06	2.14	2.17	1.79	0.63
Ethylene						1.25	0.00	0.00	0.42	0.72	6.17	6.13		6.15	0.03
Nickel (and its compounds)		0.00	0.00	0.00	0.00	1.47	1.32	1.15	1.32	0.16	0.34	0.00	0.40	0.25	0.21
Benzo(a)pyrene						0.00	0.00	0.00	0.00	0.00	0.00	3.45	0.00	1.15	1.99
Formaldehyde															
Acetaldehyde															
Sublinear threshold-acting															
1,2,4-Trimethylbenzene	3.16	2.34	2.36	2.62	0.47	2.19	1.31	1.47	1.66	0.47	0.58	0.00	0.00	0.19	0.33
Ammonia (Total)						0.00	0.00	0.00	0.00	0.00	0.06	0.06	0.00	0.04	0.03
Benzene (as BTEX potentiator)	3.42	3.43	3.38	3.41	0.02	18.03	8.74	10.55	12.44	4.92	1.06	2.14	2.17	1.79	0.63
Cyclohexane	0.38	0.00	0.58	0.32	0.29	2.01	1.66	1.72	1.80	0.19	1.57	1.24	1.30	1.37	0.18
Dicyclopentadiene															
Diethanolamine (and its salts)	0.00	0.00	0.67	0.22	0.39	0.00	0.00	0.00	0.00	0.00	0.45	0.00	0.00	0.15	0.26
Ethylbenzene	0.92	3.47	0.85	1.75	1.49	3.14	1.54	1.54	2.07	0.92	0.50	0.00	0.00	0.17	0.29
Hydrogen sulphide	0.16	0.15	0.13	0.15	0.01	4.90	3.61	3.77	4.09	0.70	2.19	1.99	1.95	2.04	0.13
Isoprene															
Mercury (and its compounds)						0.003	0.005	0.004	0.004	0.001	0.001	0.002	0.002	0.002	0.001
Methanol						2.36	0.00	0.00	0.79	1.36					
Methyl ethyl ketone	16.96	22.85	7.96	15.92	7.50										
Methyl isobutyl ketone															
Methyl tert-butyl ether															
Naphthalene	2.33	1.75	1.72	1.93	0.35	0.41	0.00	0.00	0.14	0.24	0.34	0.00	0.00	0.11	0.19
n-Hexane	5.41	5.03	4.92	5.12	0.26	9.22	7.46	7.85	8.18	0.92	6.31	5.47	5.60	5.79	0.45
Phenol (and its salts)						0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Propylene		7.76	3.33	5.54	3.13	14.49	8.73	13.41	12.21	3.06	39.29	36.87	43.92	40.03	3.58
Styrene															
Sulphuric acid	0.00	58.30	49.77	36.02	31.49	0.06	159.43	135.19	98.23	85.88	0.63	261.98	231.20	164.60	142.84
Toluene	18.45	23.99	11.00	17.81	6.52	21.88	12.09	12.24	15.40	5.61	2.92	3.43	3.45	3.27	0.30
Vanadium (except when in an alloy) and its compounds						4.82	3.44	2.68	3.65	1.09	1.03	0.00	0.79	0.61	0.54
Xylene (all isomers)	5.21	14.59	4.19	7.99	5.73	15.70	2.80	2.60	7.03	7.50	1.92	1.72	1.79	1.81	0.10
Zinc (and its compounds)						0.00	6.23	0.42	2.22	3.48					
SOx		1293.19	1096.12				3393.90	4027.30				5984.20	5580.78		
NOx		747.01	436.73				1311.80	1413.20				625.89	605.89		
primary PM2.5		77.82	47.10				151.90	173.00				138.67	189.16		

Chemical Name	Shell - Montreal East					Shell - Sarnia					Shell - Scotford				
Linear non-threshold-acting	2001	2002	2003	mean	std dev	2001	2002	2003	mean	std dev	2001	2002	2003	mean	std dev
1,3-Butadiene															
Benzene	7.89	3.62	4.01	5.17	2.36	32.67	12.85	11.19	18.90	11.95	11.17	6.66	3.63	7.15	3.79
Ethylene	4.81	4.07	5.31	4.73	0.62	9.17	5.86	5.02	6.68	2.20					
Nickel (and its compounds)		0.00		0.00	#DIV/0!	6.97	6.61	6.63	6.74	0.20	0.00	0.01	0.00	0.00	0.00
Benzo(a)pyrene	0.01	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.21	0.07	0.12
Formaldehyde															
Acetaldehyde															
Sublinear threshold-acting															
1,2,4-Trimethylbenzene	2.68	1.43	1.76	1.96	0.65	3.66	1.85	1.63	2.38	1.11	2.68	2.95	2.24	2.62	0.36
Ammonia (Total)	1.58	3.39	1.60	2.19	1.04	0.02	0.05	0.03	0.03	0.02	0.02	0.00	0.00	0.01	0.01
Benzene (as BTEX potentiator)	7.89	3.62	4.01	5.17	2.36	32.67	12.85	11.19	18.90	11.95	11.17	6.66	3.63	7.15	3.79
Cyclohexane	2.24	1.16	2.03	1.81	0.57	7.37	5.58	4.90	5.95	1.27	0.18	0.12	0.18	0.16	0.03
Dicyclopentadiene															
Diethanolamine (and its salts)	1.59	1.41	1.59	1.53	0.10	4.62	4.50	4.62	4.58	0.07					
Ethylbenzene	3.92	2.98	2.85	3.25	0.58	9.87	6.36	6.32	7.52	2.04	3.08	1.94	1.15	2.06	0.97
Hydrogen sulphide	2.86	1.21	1.29	1.79	0.93	3.16	3.86	3.26	3.43	0.38	2.57	0.97	0.97	1.51	0.92
Isoprene															
Mercury (and its compounds)	0.003	0.003	0.003	0.003	0.000	0.004	0.002	0.002	0.002	0.001	0.000	0.001	0.005	0.002	0.003
Methanol						2.10	0.16	0.15	0.80	1.12					
Methyl ethyl ketone	16.73	6.44	7.29	10.15	5.71										
Methyl isobutyl ketone	6.81	2.34	2.73	3.96	2.48										
Methyl tert-butyl ether															
Naphthalene	0.91	0.49	0.58	0.66	0.22	0.69	0.30	0.32	0.44	0.22	0.44	0.32	0.25	0.33	0.10
n-Hexane	15.15	8.98	9.36	11.16	3.46	9.05	9.49	6.08	8.21	1.85	8.49	5.98	5.69	6.72	1.54
Phenol (and its salts)	0.02	0.06	0.01	0.03	0.03	0.00	0.00	0.00	0.00	0.00					
Propylene	16.72	5.40	6.70	9.61	6.19	24.31	8.81	7.03	13.39	9.50			2.57	2.57	#DIV/0!
Styrene															
Sulphuric acid		111.40	110.20	110.80	0.85		263.88	278.74	271.31	10.51	0.00	0.00	0.00	0.00	0.00
Toluene	50.42	18.05	22.31	30.26	17.59	54.95	37.21	35.41	42.53	10.80	22.07	13.54	7.24	14.28	7.45
Vanadium (except when in an alloy) and its compounds						14.70	13.93	14.10	14.24	0.40					
Xylene (all isomers)	26.02	9.21	12.77	16.00	8.86	29.27	14.47	13.20	18.98	8.93	17.80	12.78	7.98	12.85	4.91
Zinc (and its compounds)											0.00	0.00	0.00	0.00	0.00
SOx		5273.00	5401.00				12527.89	12212.98				368.00	91.30		
NOx		1869.00	1820.00				1853.69	1750.09				865.80	844.00		
primary PM2.5		178.12	174.17				379.00	403.17				11.70	10.72		

Chemical Name	Sunoco - Sarnia					Ultramar - St. Romuald					Grand Total				
Linear non-threshold-acting	2001	2002	2003	mean	std dev	2001	2002	2003	mean	std dev	2001	2002	2003	mean	std dev
1,3-Butadiene											11.554	17.69	11.175	13.473	3.65694
Benzene	22.28	11.84	11.32	15.15	6.19	4.15	4.15	3.19	3.83	0.55	211.64	159.57	128.48	166.56	42.02
Ethylene						12.35	3.52	1.64	5.83	5.72	188.57	120.05	70.81	126.48	59.14
Nickel (and its compounds)											53.29	48.92	51.55	51.25	2.20
Benzo(a)pyrene	0.01	0.00		0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.19	3.47	0.24	1.30	1.88
Formaldehyde		15.37	11.98	13.67	2.39							15.37	11.98	13.67	2.39
Acetaldehyde												0.00	0.00	0.00	0.00
												0.00	0.00	0.00	0.00
Sublinear threshold-acting												0.00	0.00	0.00	0.00
1,2,4-Trimethylbenzene	3.65	3.64	3.48	3.59	0.09	0.30	0.21	0.23	0.25	0.05	54.66	49.76	53.33	52.58	2.53
Ammonia (Total)	0.00	0.00	0.00	0.00	0.00	1.18	0.36	0.36	0.63	0.47	25.68	47.56	28.89	34.04	11.82
Benzene (as BTEX potentiator)	22.28	11.84	11.32	15.15	6.19	4.15	4.15	3.19	3.83	0.55	211.64	159.57	126.41	165.88	42.96
Cyclohexane	3.87	2.98	3.21	3.35	0.46	3.80	4.19	3.98	3.99	0.19	102.89	71.90	78.94	84.57	16.25
Dicyclopentadiene											4.97	17.12	0.16	7.42	8.74
Diethanolamine (and its salts)						0.00	0.00	0.00	0.00	0.00	10.36	8.31	17.51	12.06	4.83
Ethylbenzene	22.23	15.16	13.77	17.05	4.53	0.52	0.46	0.46	0.48	0.03	74.43	61.56	71.15	69.04	6.69
Hydrogen sulphide	0.84	2.27	1.58	1.56	0.71	15.17	5.35	5.62	8.71	5.60	92.67	96.43	89.51	92.87	3.46
Isoprene											1.87	6.59	1.81	3.42	2.74
Mercury (and its compounds)						0.000	0.000	0.000	0.000	0.000	0.03	0.03	0.04	0.03	0.01
Methanol	0.20	0.20	0.21	0.20	0.00						37.28	11.66	7.98	18.97	15.96
Methyl ethyl ketone											106.36	93.16	102.73	100.75	6.82
Methyl isobutyl ketone											96.34	81.38	91.11	89.61	7.59
Methyl tert-butyl ether											112.45	75.54	106.78	98.25	19.87
Naphthalene	0.53	0.47	0.46	0.48	0.04	0.05	0.05	0.05	0.05	0.00	11.25	13.15	10.20	11.53	1.49
n-Hexane	11.22	10.32	9.66	10.40	0.78	17.47	15.03	12.67	15.06	2.40	203.74	213.18	263.35	226.76	32.04
Phenol (and its salts)						0.00	0.00	0.00	0.00	0.00	2.70	2.40	17.51	7.54	8.63
Propylene		14.25	16.33	15.29	1.47	20.72	5.59	4.17	10.16	9.17	248.90	283.11	228.00	253.34	27.83
Styrene											2.48	3.84	0.29	2.20	1.79
Sulphuric acid	0.00	171.81	183.07	118.29	102.60	0.00	56.94	57.39	38.11	33.00	2.80	2262.90	2046.27	1437.32	1247.05
Toluene	48.72	51.62	28.58	42.97	12.55	4.22	4.51	4.20	4.31	0.17	375.40	313.31	295.86	328.19	41.80
Vanadium (except when in an alloy) and its compounds											107.95	122.78	129.44	120.06	11.00
Xylene (all isomers)	92.72	67.10	46.19	68.67	23.30	2.77	2.55	2.60	2.64	0.12	311.49	256.70	261.83	276.67	30.26
Zinc (and its compounds)											17.77	26.43	1.70	15.30	12.55
SOx		2404.10	2599.96				3499.93	3783.34							
NOx		939.85	964.58				1789.29	1846.59							
primary PM2.5		104.29	105.03				193.37	129.61							

Appendix E – Secondary PM Concentrations

Refinery and PM type	1 km							
	NE		SE		SW		NW	
	mean	stdev	mean	stdev	mean	stdev	mean	stdev
Chevron - Burnaby								
PM2.5 from SOx (NH4SO4)	0.21	0.00	0.17	0.00	0.06	0.00	0.09	0.00
PM2.5 from NOx (NH4NO3)	0.08	0.02	0.06	0.02	0.02	0.01	0.04	0.01
primary PM2.5	0.72	0.87	0.58	0.71	0.22	0.27	0.32	0.39
Consumer's Co-operative Refineries Ltd./NewGrade Energy Inc.								
PM2.5 from SOx (NH4SO4)	0.59	0.19	0.48	0.16	0.18	0.06	0.27	0.09
PM2.5 from NOx (NH4NO3)	0.17	0.02	0.14	0.02	0.05	0.01	0.08	0.01
primary PM2.5	0.53	0.92	0.43	0.74	0.16	0.28	0.24	0.41
Husky Oil Operations Limited - Prince George Refinery								
PM2.5 from SOx (NH4SO4)	No data![27]	No data	No data	No data	No data	No data	No data	No data
PM2.5 from NOx (NH4NO3)	No data	No data	No data	No data	No data	No data	No data	No data
primary PM2.5	No data	No data	No data	No data	No data	No data	No data	No data
Imperial Oil - Dartmouth Refinery								
PM2.5 from SOx (NH4SO4)	0.97	0.11	0.79	0.09	0.30	0.03	0.44	0.05
PM2.5 from NOx (NH4NO3)	0.52	0.02	0.42	0.02	0.16	0.01	0.24	0.01
primary PM2.5	3.49	0.76	2.82	0.61	1.07	0.23	1.57	0.34
Imperial Oil - Nanticoke Refinery								
PM2.5 from SOx (NH4SO4)	1.00	0.27	0.81	0.22	0.31	0.08	0.45	0.12
PM2.5 from NOx (NH4NO3)	0.31	0.01	0.25	0.01	0.09	0.00	0.14	0.00
primary PM2.5	2.01	0.58	1.63	0.47	0.61	0.18	0.90	0.26
Imperial Oil - Sarnia Refinery Plan								
PM2.5 from SOx (NH4SO4)	4.13	0.38	3.34	0.31	1.26	0.12	1.86	0.17
PM2.5 from NOx (NH4NO3)	0.41	0.01	0.33	0.01	0.12	0.00	0.18	0.00
primary PM2.5	5.86	2.40	4.73	1.94	1.79	0.73	2.63	1.08
Imperial Oil - Strathcona Refinery								
PM2.5 from SOx (NH4SO4)	0.89	0.05	0.72	0.04	0.27	0.02	0.40	0.02
PM2.5 from NOx (NH4NO3)	0.27	0.03	0.22	0.03	0.08	0.01	0.12	0.01
primary PM2.5	3.76	2.40	3.04	1.94	1.15	0.73	1.69	1.08
Irving - Saint John								
PM2.5 from SOx (NH4SO4)	1.04	0.27	0.84	0.22	0.32	0.08	0.47	0.12
PM2.5 from NOx (NH4NO3)	0.66	0.02	0.53	0.02	0.20	0.01	0.30	0.01
primary PM2.5	3.09	1.41	2.50	1.14	0.94	0.43	1.39	0.63
North Atlantic Refining - North Atlantic Refinery								
PM2.5 from SOx (NH4SO4)	2.75	0.31	2.22	0.25	0.84	0.09	1.24	0.14
PM2.5 from NOx (NH4NO3)	0.21	0.03	0.17	0.02	0.06	0.01	0.10	0.01
primary PM2.5	4.20	3.99	3.39	3.22	1.28	1.22	1.88	1.79
Nova Chemicals (Ltd.) - Nova Chemicals (Canada) Ltd.								
PM2.5 from SOx (NH4SO4)	No data	No data	No data	No data	No data	No data	No data	No data
PM2.5 from NOx (NH4NO3)	No data	No data	No data	No data	No data	No data	No data	No data
primary PM2.5	No data	No data	No data	No data	No data	No data	No data	No data
Parkland – Bowden								
PM2.5 from SOx (NH4SO4)	No data	No data	No data	No data	No data	No data	No data	No data
PM2.5 from NOx (NH4NO3)	No data	No data	No data	No data	No data	No data	No data	No data

---

[27] Where "no data" is displayed, PM emissions records were not available for all three years

primary PM2.5	No data	No data	No data	No data	No data	No data	No data	No data

Refinery and PM type	1 km							
	NE		SE		SW		NW	
	mean	stdev	mean	stdev	mean	stdev	mean	stdev
Petro-Canada - Edmonton Refinery								
PM2.5 from SOx (NH4SO4)	0.40	0.13	0.33	0.10	0.12	0.04	0.18	0.06
PM2.5 from NOx (NH4NO3)	0.23	0.03	0.18	0.02	0.07	0.01	0.10	0.01
primary PM2.5	1.80	0.77	1.46	0.63	0.55	0.24	0.81	0.35
Petro-Canada - Mississauga Lubricant Center								
PM2.5 from SOx (NH4SO4)	0.24	0.05	0.19	0.04	0.07	0.01	0.11	0.02
PM2.5 from NOx (NH4NO3)	0.09	0.02	0.08	0.02	0.03	0.01	0.04	0.01
primary PM2.5	0.86	0.38	0.70	0.31	0.26	0.12	0.39	0.17
Petro-Canada - Raffinerie de Montreal								
PM2.5 from SOx (NH4SO4)	0.68	0.07	0.55	0.05	0.21	0.02	0.31	0.03
PM2.5 from NOx (NH4NO3)	0.21	0.01	0.17	0.01	0.06	0.00	0.09	0.01
primary PM2.5	2.00	0.51	1.62	0.41	0.61	0.15	0.90	0.23
Petro-Canada - Oakville Refinery								
PM2.5 from SOx (NH4SO4)	1.04	0.04	0.84	0.03	0.32	0.01	0.47	0.02
PM2.5 from NOx (NH4NO3)	0.10	0.01	0.08	0.00	0.03	0.00	0.04	0.00
primary PM2.5	2.81	1.87	2.27	1.51	0.86	0.57	1.26	0.84
Produits Shell Canada - Raffinerie de Montreal-est								
PM2.5 from SOx (NH4SO4)	1.01	0.10	0.82	0.08	0.31	0.03	0.46	0.05
PM2.5 from NOx (NH4NO3)	0.28	0.01	0.23	0.01	0.09	0.00	0.13	0.01
primary PM2.5	2.75	1.53	2.22	1.24	0.84	0.47	1.23	0.69
Shell Canada Products - Sarnia Manufacturing Centre								
PM2.5 from SOx (NH4SO4)	2.22	0.03	1.79	0.03	0.68	0.01	1.00	0.01
PM2.5 from NOx (NH4NO3)	0.24	0.05	0.20	0.04	0.07	0.02	0.11	0.02
primary PM2.5	5.76	2.81	4.66	2.27	1.76	0.86	2.59	1.26
Shell Canada Products - Shell Scotford Refinery								
PM2.5 from SOx (NH4SO4)	0.04	0.02	0.03	0.02	0.01	0.01	0.02	0.01
PM2.5 from NOx (NH4NO3)	0.12	0.01	0.10	0.01	0.04	0.00	0.05	0.01
primary PM2.5	0.26	0.25	0.21	0.20	0.08	0.08	0.12	0.11
Sunoco Inc. - Sarnia Refinery								
PM2.5 from SOx (NH4SO4)	0.43	0.04	0.34	0.03	0.13	0.01	0.19	0.02
PM2.5 from NOx (NH4NO3)	0.14	0.00	0.11	0.00	0.04	0.00	0.06	0.00
primary PM2.5	1.72	1.06	1.39	0.86	0.53	0.32	0.77	0.48
Ultramar Ltee - Raffinerie St. Romuald								
PM2.5 from SOx (NH4SO4)	0.66	0.03	0.54	0.03	0.20	0.01	0.30	0.02
PM2.5 from NOx (NH4NO3)	0.24	0.06	0.20	0.05	0.07	0.02	0.11	0.03
primary PM2.5	1.62	0.37	1.31	0.30	0.49	0.11	0.73	0.17
Hypothetical Worst Case Refinery (Imperial Sarnia for PM)								
PM2.5 from SOx (NH4SO4)	4.13	0.38	3.34	0.31	1.26	0.12	1.86	0.17
PM2.5 from NOx (NH4NO3)	0.41	0.01	0.33	0.01	0.12	0.00	0.18	0.00
primary PM2.5	5.86	2.40	4.73	1.94	1.79	0.73	2.63	1.08

Refinery and PM type	**2.5 km**							
	NE		**SE**		**SW**		**NW**	
	mean	**stdev**	**mean**	**stdev**	**mean**	**stdev**	**mean**	**stdev**
Chevron - Burnaby								
PM2.5 from SOx (NH4SO4)	0.16	0.00	0.13	0.00	0.06	0.00	0.09	0.00
PM2.5 from NOx (NH4NO3)	0.06	0.02	0.05	0.01	0.02	0.01	0.03	0.01
primary PM2.5	0.22	0.27	0.18	0.22	0.08	0.10	0.12	0.15
Consumer's Co-operative Refineries Ltd./NewGrade Energy Inc.								
PM2.5 from SOx (NH4SO4)	0.46	0.15	0.37	0.12	0.16	0.05	0.25	0.08
PM2.5 from NOx (NH4NO3)	0.13	0.02	0.11	0.01	0.05	0.01	0.07	0.01
primary PM2.5	0.16	0.29	0.13	0.23	0.06	0.10	0.09	0.15
Husky Oil Operations Limited - Prince George Refinery								
PM2.5 from SOx (NH4SO4)	No data	No data	No data	No data	No data	No data	No data	No data
PM2.5 from NOx (NH4NO3)	No data	No data	No data	No data	No data	No data	No data	No data
primary PM2.5	No data	No data	No data	No data	No data	No data	No data	No data
Imperial Oil - Dartmouth Refinery								
PM2.5 from SOx (NH4SO4)	0.76	0.08	0.60	0.07	0.27	0.03	0.41	0.05
PM2.5 from NOx (NH4NO3)	0.41	0.02	0.32	0.01	0.14	0.01	0.22	0.01
primary PM2.5	1.09	0.24	0.87	0.19	0.39	0.08	0.59	0.13
Imperial Oil - Nanticoke Refinery								
PM2.5 from SOx (NH4SO4)	0.78	0.21	0.62	0.17	0.28	0.08	0.42	0.11
PM2.5 from NOx (NH4NO3)	0.24	0.01	0.19	0.00	0.09	0.00	0.13	0.00
primary PM2.5	0.63	0.18	0.50	0.14	0.22	0.06	0.34	0.10
Imperial Oil - Sarnia Refinery Plan								
PM2.5 from SOx (NH4SO4)	3.21	0.30	2.56	0.24	1.14	0.11	1.73	0.16
PM2.5 from NOx (NH4NO3)	0.32	0.01	0.25	0.01	0.11	0.00	0.17	0.00
primary PM2.5	1.82	0.75	1.46	0.60	0.65	0.27	0.98	0.40
Imperial Oil - Strathcona Refinery								
PM2.5 from SOx (NH4SO4)	0.69	0.04	0.55	0.03	0.25	0.01	0.37	0.02
PM2.5 from NOx (NH4NO3)	0.21	0.03	0.17	0.02	0.07	0.01	0.11	0.01
primary PM2.5	1.17	0.75	0.93	0.60	0.42	0.27	0.63	0.40
Irving - Saint John								
PM2.5 from SOx (NH4SO4)	0.80	0.21	0.64	0.17	0.29	0.08	0.43	0.11
PM2.5 from NOx (NH4NO3)	0.51	0.02	0.41	0.01	0.18	0.01	0.27	0.01
primary PM2.5	0.96	0.44	0.77	0.35	0.34	0.16	0.52	0.24
North Atlantic Refining - North Atlantic Refinery								
PM2.5 from SOx (NH4SO4)	2.13	0.24	1.70	0.19	0.76	0.09	1.15	0.13
PM2.5 from NOx (NH4NO3)	0.16	0.02	0.13	0.02	0.06	0.01	0.09	0.01
primary PM2.5	1.31	1.24	1.04	0.99	0.46	0.44	0.70	0.67
Nova Chemicals (Ltd.) - Nova Chemicals (Canada) Ltd.								
PM2.5 from SOx (NH4SO4)	No data	No data	No data	No data	No data	No data	No data	No data
PM2.5 from NOx (NH4NO3)	No data	No data	No data	No data	No data	No data	No data	No data
primary PM2.5	No data	No data	No data	No data	No data	No data	No data	No data
Parkland - Bowden								
PM2.5 from SOx (NH4SO4)	No data	No data	No data	No data	No data	No data	No data	No data
PM2.5 from NOx (NH4NO3)	No data	No data	No data	No data	No data	No data	No data	No data
primary PM2.5	No data	No data	No data	No data	No data	No data	No data	No data

Refinery and PM type	2.5 km							
	NE		SE		SW		NW	
	mean	stdev	mean	stdev	mean	stdev	mean	stdev
Petro-Canada - Edmonton Refinery								
PM2.5 from SOx (NH4SO4)	0.31	0.10	0.25	0.08	0.11	0.03	0.17	0.05
PM2.5 from NOx (NH4NO3)	0.18	0.02	0.14	0.02	0.06	0.01	0.10	0.01
primary PM2.5	0.56	0.24	0.45	0.19	0.20	0.09	0.30	0.13
Petro-Canada - Mississauga Lubricant Center								
PM2.5 from SOx (NH4SO4)	0.19	0.04	0.15	0.03	0.07	0.01	0.10	0.02
PM2.5 from NOx (NH4NO3)	0.07	0.02	0.06	0.02	0.03	0.01	0.04	0.01
primary PM2.5	0.27	0.12	0.21	0.09	0.10	0.04	0.14	0.06
Petro-Canada - Raffinerie de Montreal								
PM2.5 from SOx (NH4SO4)	0.53	0.05	0.42	0.04	0.19	0.02	0.29	0.03
PM2.5 from NOx (NH4NO3)	0.16	0.01	0.13	0.01	0.06	0.00	0.09	0.00
primary PM2.5	0.62	0.16	0.50	0.13	0.22	0.06	0.34	0.08
Petro-Canada - Oakville Refinery								
PM2.5 from SOx (NH4SO4)	0.81	0.03	0.64	0.02	0.29	0.01	0.43	0.02
PM2.5 from NOx (NH4NO3)	0.07	0.00	0.06	0.00	0.03	0.00	0.04	0.00
primary PM2.5	0.87	0.58	0.70	0.47	0.31	0.21	0.47	0.31
Produits Shell Canada - Raffinerie de Montreal-est								
PM2.5 from SOx (NH4SO4)	0.79	0.08	0.63	0.06	0.28	0.03	0.42	0.04
PM2.5 from NOx (NH4NO3)	0.22	0.01	0.18	0.01	0.08	0.00	0.12	0.00
primary PM2.5	0.86	0.48	0.68	0.38	0.30	0.17	0.46	0.26
Shell Canada Products - Sarnia Manufacturing Centre								
PM2.5 from SOx (NH4SO4)	1.72	0.02	1.38	0.02	0.61	0.01	0.93	0.01
PM2.5 from NOx (NH4NO3)	0.19	0.04	0.15	0.03	0.07	0.01	0.10	0.02
primary PM2.5	1.79	0.87	1.43	0.70	0.64	0.31	0.97	0.47
Shell Canada Products - Shell Scotford Refinery								
PM2.5 from SOx (NH4SO4)	0.03	0.02	0.03	0.02	0.01	0.01	0.02	0.01
PM2.5 from NOx (NH4NO3)	0.09	0.01	0.08	0.01	0.03	0.00	0.05	0.00
primary PM2.5	0.08	0.08	0.07	0.06	0.03	0.03	0.04	0.04
Sunoco Inc. - Sarnia Refinery								
PM2.5 from SOx (NH4SO4)	0.33	0.03	0.26	0.03	0.12	0.01	0.18	0.02
PM2.5 from NOx (NH4NO3)	0.11	0.00	0.09	0.00	0.04	0.00	0.06	0.00
primary PM2.5	0.54	0.33	0.43	0.26	0.19	0.12	0.29	0.18
Ultramar Ltee - Raffinerie St. Romuald								
PM2.5 from SOx (NH4SO4)	0.52	0.03	0.41	0.02	0.18	0.01	0.28	0.01
PM2.5 from NOx (NH4NO3)	0.19	0.04	0.15	0.04	0.07	0.02	0.10	0.02
primary PM2.5	0.50	0.12	0.40	0.09	0.18	0.04	0.27	0.06
Hypothetical Worst Case Refinery (Imperial Sarnia for PM)								
PM2.5 from SOx (NH4SO4)	3.21	0.30	2.56	0.24	1.14	0.11	1.73	0.16
PM2.5 from NOx (NH4NO3)	0.32	0.01	0.25	0.01	0.11	0.00	0.17	0.00
primary PM2.5	1.82	0.75	1.46	0.60	0.65	0.27	0.98	0.40

Refinery and PM type	5 km							
	NE		SE		SW		NW	
	mean	stdev	mean	stdev	mean	stdev	mean	stdev
Chevron - Burnaby								
PM2.5 from SOx (NH4SO4)	0.15	0.00	0.14	0.00	0.06	0.00	0.09	0.00
PM2.5 from NOx (NH4NO3)	0.05	0.02	0.05	0.01	0.02	0.01	0.04	0.01
primary PM2.5	0.10	0.13	0.10	0.12	0.04	0.05	0.07	0.08
Consumer's Co-operative Refineries Ltd./NewGrade Energy Inc.								
PM2.5 from SOx (NH4SO4)	0.41	0.14	0.39	0.13	0.17	0.06	0.27	0.09
PM2.5 from NOx (NH4NO3)	0.12	0.01	0.11	0.01	0.05	0.01	0.08	0.01
primary PM2.5	0.08	0.13	0.07	0.12	0.03	0.05	0.05	0.09
Husky Oil Operations Limited - Prince George Refinery								
PM2.5 from SOx (NH4SO4)	No data	No data	No data	No data	No data	No data	No data	No data
PM2.5 from NOx (NH4NO3)	No data	No data	No data	No data	No data	No data	No data	No data
primary PM2.5	No data	No data	No data	No data	No data	No data	No data	No data
Imperial Oil - Dartmouth Refinery								
PM2.5 from SOx (NH4SO4)	0.68	0.08	0.64	0.07	0.28	0.03	0.44	0.05
PM2.5 from NOx (NH4NO3)	0.37	0.02	0.34	0.01	0.15	0.01	0.24	0.01
primary PM2.5	0.50	0.11	0.47	0.10	0.21	0.05	0.32	0.07
Imperial Oil - Nanticoke Refinery								
PM2.5 from SOx (NH4SO4)	0.70	0.19	0.66	0.18	0.29	0.08	0.45	0.12
PM2.5 from NOx (NH4NO3)	0.22	0.01	0.20	0.00	0.09	0.00	0.14	0.00
primary PM2.5	0.29	0.08	0.27	0.08	0.12	0.03	0.19	0.05
Imperial Oil - Sarnia Refinery Plan								
PM2.5 from SOx (NH4SO4)	2.89	0.27	2.71	0.25	1.20	0.11	1.87	0.17
PM2.5 from NOx (NH4NO3)	0.28	0.01	0.27	0.01	0.12	0.00	0.18	0.00
primary PM2.5	0.84	0.34	0.79	0.32	0.35	0.14	0.54	0.22
Imperial Oil - Strathcona Refinery								
PM2.5 from SOx (NH4SO4)	0.62	0.04	0.58	0.04	0.26	0.02	0.40	0.02
PM2.5 from NOx (NH4NO3)	0.19	0.02	0.18	0.02	0.08	0.01	0.12	0.01
primary PM2.5	0.54	0.35	0.51	0.32	0.23	0.14	0.35	0.22
Irving - Saint John								
PM2.5 from SOx (NH4SO4)	0.73	0.19	0.68	0.18	0.30	0.08	0.47	0.12
PM2.5 from NOx (NH4NO3)	0.46	0.01	0.43	0.01	0.19	0.01	0.30	0.01
primary PM2.5	0.44	0.20	0.42	0.19	0.18	0.08	0.29	0.13
North Atlantic Refining - North Atlantic Refinery								
PM2.5 from SOx (NH4SO4)	1.92	0.22	1.80	0.20	0.80	0.09	1.24	0.14
PM2.5 from NOx (NH4NO3)	0.15	0.02	0.14	0.02	0.06	0.01	0.10	0.01
primary PM2.5	0.60	0.57	0.57	0.54	0.25	0.24	0.39	0.37
Nova Chemicals (Ltd.) - Nova Chemicals (Canada) Ltd.								
PM2.5 from SOx (NH4SO4)	No data	No data	No data	No data	No data	No data	No data	No data
PM2.5 from NOx (NH4NO3)	No data	No data	No data	No data	No data	No data	No data	No data
primary PM2.5	No data	No data	No data	No data	No data	No data	No data	No data
Parkland - Bowden								
PM2.5 from SOx (NH4SO4)	No data	No data	No data	No data	No data	No data	No data	No data
PM2.5 from NOx (NH4NO3)	No data	No data	No data	No data	No data	No data	No data	No data
primary PM2.5	No data	No data	No data	No data	No data	No data	No data	No data

Refinery and PM type	5 km							
	NE		SE		SW		NW	
	mean	stdev	mean	stdev	mean	stdev	mean	stdev
Petro-Canada - Edmonton Refinery								
PM2.5 from SOx (NH4SO4)	0.28	0.09	0.26	0.08	0.12	0.04	0.18	0.06
PM2.5 from NOx (NH4NO3)	0.16	0.02	0.15	0.02	0.07	0.01	0.10	0.01
primary PM2.5	0.26	0.11	0.24	0.10	0.11	0.05	0.17	0.07
Petro-Canada - Mississauga Lubricant Center								
PM2.5 from SOx (NH4SO4)	0.17	0.03	0.16	0.03	0.07	0.01	0.11	0.02
PM2.5 from NOx (NH4NO3)	0.07	0.02	0.06	0.02	0.03	0.01	0.04	0.01
primary PM2.5	0.12	0.05	0.12	0.05	0.05	0.02	0.08	0.04
Petro-Canada - Raffinerie de Montreal								
PM2.5 from SOx (NH4SO4)	0.48	0.05	0.45	0.04	0.20	0.02	0.31	0.03
PM2.5 from NOx (NH4NO3)	0.15	0.01	0.14	0.01	0.06	0.00	0.09	0.01
primary PM2.5	0.29	0.07	0.27	0.07	0.12	0.03	0.19	0.05
Petro-Canada - Oakville Refinery								
PM2.5 from SOx (NH4SO4)	0.73	0.03	0.68	0.02	0.30	0.01	0.47	0.02
PM2.5 from NOx (NH4NO3)	0.07	0.00	0.06	0.00	0.03	0.00	0.04	0.00
primary PM2.5	0.40	0.27	0.38	0.25	0.17	0.11	0.26	0.17
Produits Shell Canada - Raffinerie de Montreal-est								
PM2.5 from SOx (NH4SO4)	0.71	0.07	0.66	0.07	0.30	0.03	0.46	0.05
PM2.5 from NOx (NH4NO3)	0.20	0.01	0.19	0.01	0.08	0.00	0.13	0.01
primary PM2.5	0.39	0.22	0.37	0.21	0.16	0.09	0.26	0.14
Shell Canada Products - Sarnia Manufacturing Centre								
PM2.5 from SOx (NH4SO4)	1.55	0.02	1.46	0.02	0.65	0.01	1.00	0.01
PM2.5 from NOx (NH4NO3)	0.17	0.04	0.16	0.03	0.07	0.01	0.11	0.02
primary PM2.5	0.83	0.40	0.78	0.38	0.35	0.17	0.53	0.26
Shell Canada Products - Shell Scotford Refinery								
PM2.5 from SOx (NH4SO4)	0.03	0.02	0.03	0.02	0.01	0.01	0.02	0.01
PM2.5 from NOx (NH4NO3)	0.07	0.02	0.07	0.01	0.03	0.01	0.05	0.01
primary PM2.5	0.06	0.05	0.05	0.04	0.02	0.02	0.04	0.03
Sunoco Inc. - Sarnia Refinery								
PM2.5 from SOx (NH4SO4)	0.30	0.03	0.28	0.03	0.12	0.01	0.19	0.02
PM2.5 from NOx (NH4NO3)	0.10	0.00	0.09	0.00	0.04	0.00	0.06	0.00
primary PM2.5	0.25	0.15	0.23	0.14	0.10	0.06	0.16	0.10
Ultramar Ltee - Raffinerie St. Romuald								
PM2.5 from SOx (NH4SO4)	0.46	0.02	0.44	0.02	0.19	0.01	0.30	0.02
PM2.5 from NOx (NH4NO3)	0.17	0.04	0.16	0.04	0.07	0.02	0.11	0.03
primary PM2.5	0.23	0.05	0.22	0.05	0.10	0.02	0.15	0.03
Hypothetical Worst Case Refinery (Imperial Sarnia for PM)								
PM2.5 from SOx (NH4SO4)	2.89	0.27	2.71	0.25	1.20	0.11	1.87	0.17
PM2.5 from NOx (NH4NO3)	0.28	0.01	0.27	0.01	0.12	0.00	0.18	0.00
primary PM2.5	0.84	0.34	0.79	0.32	0.35	0.14	0.54	0.22

Refinery and PM type	**10 km**							
	NE		**SE**		**SW**		**NW**	
	mean	**stdev**	**mean**	**stdev**	**mean**	**stdev**	**mean**	**stdev**
Chevron - Burnaby								
PM2.5 from SOx (NH4SO4)	0.17	0.00	0.19	0.00	0.09	0.00	0.13	0.00
PM2.5 from NOx (NH4NO3)	0.06	0.02	0.07	0.02	0.03	0.01	0.05	0.01
primary PM2.5	0.06	0.08	0.07	0.09	0.03	0.04	0.05	0.06
Consumer's Co-operative Refineries Ltd./NewGrade Energy Inc.								
PM2.5 from SOx (NH4SO4)	0.48	0.16	0.55	0.18	0.25	0.08	0.38	0.12
PM2.5 from NOx (NH4NO3)	0.14	0.02	0.16	0.02	0.07	0.01	0.11	0.01
primary PM2.5	0.05	0.08	0.05	0.09	0.02	0.04	0.04	0.06
Husky Oil Operations Limited - Prince George Refinery								
PM2.5 from SOx (NH4SO4)	No data	No data	No data	No data	No data	No data	No data	No data
PM2.5 from NOx (NH4NO3)	No data	No data	No data	No data	No data	No data	No data	No data
primary PM2.5	No data	No data	No data	No data	No data	No data	No data	No data
Imperial Oil - Dartmouth Refinery								
PM2.5 from SOx (NH4SO4)	0.79	0.09	0.90	0.10	0.41	0.05	0.63	0.07
PM2.5 from NOx (NH4NO3)	0.43	0.02	0.49	0.02	0.22	0.01	0.34	0.01
primary PM2.5	0.30	0.07	0.35	0.07	0.16	0.03	0.24	0.05
Imperial Oil - Nanticoke Refinery								
PM2.5 from SOx (NH4SO4)	0.81	0.22	0.93	0.25	0.42	0.12	0.64	0.18
PM2.5 from NOx (NH4NO3)	0.25	0.01	0.29	0.01	0.13	0.00	0.20	0.00
primary PM2.5	0.17	0.05	0.20	0.06	0.09	0.03	0.14	0.04
Imperial Oil - Sarnia Refinery Plan								
PM2.5 from SOx (NH4SO4)	3.36	0.31	3.83	0.35	1.74	0.16	2.67	0.25
PM2.5 from NOx (NH4NO3)	0.33	0.01	0.38	0.01	0.17	0.00	0.26	0.01
primary PM2.5	0.51	0.21	0.58	0.24	0.26	0.11	0.40	0.16
Imperial Oil - Strathcona Refinery								
PM2.5 from SOx (NH4SO4)	0.73	0.04	0.83	0.05	0.38	0.02	0.58	0.03
PM2.5 from NOx (NH4NO3)	0.22	0.03	0.25	0.03	0.11	0.01	0.17	0.02
primary PM2.5	0.33	0.21	0.37	0.24	0.17	0.11	0.26	0.17
Irving - Saint John								
PM2.5 from SOx (NH4SO4)	0.84	0.22	0.96	0.25	0.44	0.12	0.67	0.18
PM2.5 from NOx (NH4NO3)	0.54	0.02	0.61	0.02	0.28	0.01	0.42	0.01
primary PM2.5	0.27	0.12	0.31	0.14	0.14	0.06	0.21	0.10
North Atlantic Refining - North Atlantic Refinery								
PM2.5 from SOx (NH4SO4)	2.24	0.25	2.55	0.29	1.16	0.13	1.78	0.20
PM2.5 from NOx (NH4NO3)	0.17	0.02	0.20	0.03	0.09	0.01	0.14	0.02
primary PM2.5	0.36	0.35	0.41	0.39	0.19	0.18	0.29	0.27
Nova Chemicals (Ltd.) - Nova Chemicals (Canada) Ltd.								
PM2.5 from SOx (NH4SO4)	No data	No data	No data	No data	No data	No data	No data	No data
PM2.5 from NOx (NH4NO3)	No data	No data	No data	No data	No data	No data	No data	No data
primary PM2.5	No data	No data	No data	No data	No data	No data	No data	No data
Parkland - Bowden								
PM2.5 from SOx (NH4SO4)	No data	No data	No data	No data	No data	No data	No data	No data
PM2.5 from NOx (NH4NO3)	No data	No data	No data	No data	No data	No data	No data	No data
primary PM2.5	No data	No data	No data	No data	No data	No data	No data	No data

Refinery and PM type	**10 km**							
	NE		**SE**		**SW**		**NW**	
	mean	**stdev**	**mean**	**stdev**	**mean**	**stdev**	**mean**	**stdev**
Petro-Canada - Edmonton Refinery								
PM2.5 from SOx (NH4SO4)	0.33	0.10	0.37	0.12	0.17	0.05	0.26	0.08
PM2.5 from NOx (NH4NO3)	0.19	0.02	0.21	0.02	0.10	0.01	0.15	0.02
primary PM2.5	0.16	0.07	0.18	0.08	0.08	0.03	0.12	0.05
Petro-Canada - Mississauga Lubricant Center								
PM2.5 from SOx (NH4SO4)	0.20	0.04	0.22	0.04	0.10	0.02	0.15	0.03
PM2.5 from NOx (NH4NO3)	0.08	0.02	0.09	0.02	0.04	0.01	0.06	0.02
primary PM2.5	0.07	0.03	0.09	0.04	0.04	0.02	0.06	0.03
Petro-Canada - Raffinerie de Montreal								
PM2.5 from SOx (NH4SO4)	0.55	0.05	0.63	0.06	0.29	0.03	0.44	0.04
PM2.5 from NOx (NH4NO3)	0.17	0.01	0.19	0.01	0.09	0.00	0.14	0.01
primary PM2.5	0.17	0.04	0.20	0.05	0.09	0.02	0.14	0.03
Petro-Canada - Oakville Refinery								
PM2.5 from SOx (NH4SO4)	0.84	0.03	0.96	0.03	0.44	0.02	0.67	0.02
PM2.5 from NOx (NH4NO3)	0.08	0.00	0.09	0.01	0.04	0.00	0.06	0.00
primary PM2.5	0.24	0.16	0.28	0.19	0.13	0.08	0.19	0.13
Produits Shell Canada - Raffinerie de Montreal-est								
PM2.5 from SOx (NH4SO4)	0.82	0.08	0.94	0.10	0.43	0.04	0.65	0.07
PM2.5 from NOx (NH4NO3)	0.23	0.01	0.26	0.01	0.12	0.00	0.18	0.01
primary PM2.5	0.24	0.13	0.27	0.15	0.12	0.07	0.19	0.11
Shell Canada Products - Sarnia Manufacturing Centre								
PM2.5 from SOx (NH4SO4)	1.81	0.03	2.06	0.03	0.93	0.01	1.43	0.02
PM2.5 from NOx (NH4NO3)	0.20	0.04	0.22	0.05	0.10	0.02	0.16	0.03
primary PM2.5	0.50	0.24	0.57	0.28	0.26	0.13	0.40	0.19
Shell Canada Products - Shell Scotford Refinery								
PM2.5 from SOx (NH4SO4)	0.03	0.02	0.04	0.02	0.02	0.01	0.03	0.02
PM2.5 from NOx (NH4NO3)	0.10	0.01	0.11	0.01	0.05	0.00	0.08	0.01
primary PM2.5	0.02	0.02	0.03	0.02	0.01	0.01	0.02	0.02
Sunoco Inc. - Sarnia Refinery								
PM2.5 from SOx (NH4SO4)	0.35	0.03	0.39	0.04	0.18	0.02	0.27	0.03
PM2.5 from NOx (NH4NO3)	0.11	0.00	0.13	0.00	0.06	0.00	0.09	0.00
primary PM2.5	0.15	0.09	0.17	0.10	0.08	0.05	0.12	0.07
Ultramar Ltee - Raffinerie St. Romuald								
PM2.5 from SOx (NH4SO4)	0.54	0.03	0.61	0.03	0.28	0.01	0.43	0.02
PM2.5 from NOx (NH4NO3)	0.20	0.05	0.22	0.05	0.10	0.02	0.16	0.04
primary PM2.5	0.14	0.03	0.16	0.04	0.07	0.02	0.11	0.03
Hypothetical Worst Case Refinery (Imperial Sarnia for PM)								
PM2.5 from SOx (NH4SO4)	3.36	0.31	3.83	0.35	1.74	0.16	2.67	0.25
PM2.5 from NOx (NH4NO3)	0.33	0.01	0.38	0.01	0.17	0.00	0.26	0.01
primary PM2.5	0.51	0.21	0.58	0.24	0.26	0.11	0.40	0.16

Refinery and PM type	**25 km**							
	NE		**SE**		**SW**		**NW**	
	mean	**stdev**	**mean**	**stdev**	**mean**	**stdev**	**mean**	**stdev**
Chevron - Burnaby								
PM2.5 from SOx (NH4SO4)	0.16	0.00	0.21	0.00	0.09	0.00	0.16	0.00
PM2.5 from NOx (NH4NO3)	0.06	0.02	0.08	0.02	0.03	0.01	0.06	0.02
primary PM2.5	0.03	0.03	0.03	0.04	0.02	0.02	0.03	0.03
Consumer's Co-operative Refineries Ltd./NewGrade Energy Inc.								
PM2.5 from SOx (NH4SO4)	0.44	0.14	0.59	0.19	0.26	0.08	0.44	0.14
PM2.5 from NOx (NH4NO3)	0.13	0.02	0.17	0.02	0.08	0.01	0.13	0.02
primary PM2.5	0.02	0.03	0.03	0.04	0.01	0.02	0.02	0.03
Husky Oil Operations Limited - Prince George Refinery								
PM2.5 from SOx (NH4SO4)	No data	No data	No data	No data	No data	No data	No data	No data
PM2.5 from NOx (NH4NO3)	No data	No data	No data	No data	No data	No data	No data	No data
primary PM2.5	No data	No data	No data	No data	No data	No data	No data	No data
Imperial Oil - Dartmouth Refinery								
PM2.5 from SOx (NH4SO4)	0.73	0.08	0.97	0.11	0.42	0.05	0.73	0.08
PM2.5 from NOx (NH4NO3)	0.39	0.02	0.52	0.02	0.23	0.01	0.39	0.02
primary PM2.5	0.13	0.03	0.17	0.04	0.07	0.02	0.13	0.03
Imperial Oil - Nanticoke Refinery								
PM2.5 from SOx (NH4SO4)	0.75	0.21	1.00	0.27	0.44	0.12	0.75	0.21
PM2.5 from NOx (NH4NO3)	0.23	0.01	0.31	0.01	0.14	0.00	0.23	0.01
primary PM2.5	0.07	0.02	0.10	0.03	0.04	0.01	0.07	0.02
Imperial Oil - Sarnia Refinery Plan								
PM2.5 from SOx (NH4SO4)	3.09	0.29	4.12	0.38	1.80	0.17	3.09	0.29
PM2.5 from NOx (NH4NO3)	0.30	0.01	0.41	0.01	0.18	0.00	0.30	0.01
primary PM2.5	0.21	0.09	0.28	0.11	0.12	0.05	0.21	0.09
Imperial Oil - Strathcona Refinery								
PM2.5 from SOx (NH4SO4)	0.67	0.04	0.89	0.05	0.39	0.02	0.67	0.04
PM2.5 from NOx (NH4NO3)	0.20	0.02	0.27	0.03	0.12	0.01	0.20	0.02
primary PM2.5	0.14	0.09	0.18	0.12	0.08	0.05	0.14	0.09
Irving - Saint John								
PM2.5 from SOx (NH4SO4)	0.78	0.21	1.03	0.27	0.45	0.12	0.78	0.21
PM2.5 from NOx (NH4NO3)	0.49	0.02	0.66	0.02	0.29	0.01	0.49	0.02
primary PM2.5	0.11	0.05	0.15	0.07	0.06	0.03	0.11	0.05
North Atlantic Refining - North Atlantic Refinery								
PM2.5 from SOx (NH4SO4)	2.06	0.23	2.74	0.31	1.20	0.14	2.06	0.23
PM2.5 from NOx (NH4NO3)	0.16	0.02	0.21	0.03	0.09	0.01	0.16	0.02
primary PM2.5	0.15	0.14	0.20	0.19	0.09	0.08	0.15	0.14
Nova Chemicals (Ltd.) - Nova Chemicals (Canada) Ltd.								
PM2.5 from SOx (NH4SO4)	No data	No data	No data	No data	No data	No data	No data	No data
PM2.5 from NOx (NH4NO3)	No data	No data	No data	No data	No data	No data	No data	No data
primary PM2.5	No data	No data	No data	No data	No data	No data	No data	No data
Parkland - Bowden								
PM2.5 from SOx (NH4SO4)	No data	No data	No data	No data	No data	No data	No data	No data
PM2.5 from NOx (NH4NO3)	No data	No data	No data	No data	No data	No data	No data	No data
primary PM2.5	No data	No data	No data	No data	No data	No data	No data	No data

Refinery and PM type	**25 km**							
	NE		**SE**		**SW**		**NW**	
	mean	**stdev**	**mean**	**stdev**	**mean**	**stdev**	**mean**	**stdev**
Petro-Canada - Edmonton Refinery								
PM2.5 from SOx (NH4SO4)	0.30	0.09	0.40	0.13	0.18	0.05	0.30	0.09
PM2.5 from NOx (NH4NO3)	0.17	0.02	0.23	0.03	0.10	0.01	0.17	0.02
primary PM2.5	0.06	0.03	0.09	0.04	0.04	0.02	0.06	0.03
Petro-Canada - Mississauga Lubricant Center								
PM2.5 from SOx (NH4SO4)	0.18	0.04	0.24	0.05	0.10	0.02	0.18	0.04
PM2.5 from NOx (NH4NO3)	0.07	0.02	0.09	0.02	0.04	0.01	0.07	0.02
primary PM2.5	0.03	0.01	0.04	0.02	0.02	0.01	0.03	0.01
Petro-Canada - Raffinerie de Montreal								
PM2.5 from SOx (NH4SO4)	0.51	0.05	0.68	0.07	0.30	0.03	0.51	0.05
PM2.5 from NOx (NH4NO3)	0.16	0.01	0.21	0.01	0.09	0.01	0.16	0.01
primary PM2.5	0.07	0.02	0.10	0.02	0.04	0.01	0.07	0.02
Petro-Canada - Oakville Refinery								
PM2.5 from SOx (NH4SO4)	0.78	0.03	1.03	0.04	0.45	0.02	0.78	0.03
PM2.5 from NOx (NH4NO3)	0.07	0.00	0.10	0.01	0.04	0.00	0.07	0.00
primary PM2.5	0.10	0.07	0.13	0.09	0.06	0.04	0.10	0.07
Produits Shell Canada - Raffinerie de Montreal-est								
PM2.5 from SOx (NH4SO4)	0.76	0.08	1.01	0.10	0.44	0.05	0.76	0.08
PM2.5 from NOx (NH4NO3)	0.21	0.01	0.28	0.01	0.12	0.00	0.21	0.01
primary PM2.5	0.10	0.05	0.13	0.07	0.06	0.03	0.10	0.05
Shell Canada Products - Sarnia Manufacturing Centre								
PM2.5 from SOx (NH4SO4)	1.66	0.02	2.21	0.03	0.97	0.01	1.66	0.02
PM2.5 from NOx (NH4NO3)	0.18	0.04	0.24	0.05	0.11	0.02	0.18	0.04
primary PM2.5	0.21	0.10	0.28	0.13	0.12	0.06	0.21	0.10
Shell Canada Products - Shell Scotford Refinery								
PM2.5 from SOx (NH4SO4)	0.03	0.02	0.04	0.02	0.02	0.01	0.03	0.02
PM2.5 from NOx (NH4NO3)	0.09	0.01	0.12	0.01	0.05	0.01	0.09	0.01
primary PM2.5	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Sunoco Inc. - Sarnia Refinery								
PM2.5 from SOx (NH4SO4)	0.32	0.03	0.42	0.04	0.19	0.02	0.32	0.03
PM2.5 from NOx (NH4NO3)	0.11	0.00	0.14	0.00	0.06	0.00	0.11	0.00
primary PM2.5	0.06	0.04	0.08	0.05	0.04	0.02	0.06	0.04
Ultramar Ltee - Raffinerie St. Romuald								
PM2.5 from SOx (NH4SO4)	0.50	0.03	0.66	0.03	0.29	0.01	0.50	0.03
PM2.5 from NOx (NH4NO3)	0.18	0.04	0.24	0.06	0.11	0.02	0.18	0.04
primary PM2.5	0.06	0.01	0.08	0.02	0.03	0.01	0.06	0.01
Hypothetical Worst Case Refinery (Imperial Sarnia for PM)								
PM2.5 from SOx (NH4SO4)	3.09	0.29	4.12	0.38	1.80	0.17	3.09	0.29
PM2.5 from NOx (NH4NO3)	0.30	0.01	0.41	0.01	0.18	0.00	0.30	0.01
primary PM2.5	0.21	0.09	0.28	0.11	0.12	0.05	0.21	0.09

Appendix F – NIST data for calculation of Atmospheric OH values

Substance	**NIST: values for ~289 K extracted; 2nd order rxn**		**Atkinson (book) (Calvert, Atkinson et al. 2002) [For Sensitivity Analysis]**
1,3-Butadiene	5.8x10^{-11} 6.66x10^{-11} 7.72x10^{-11}		
Benzene	1.25x10^{-12} 1.0x10^{-12} 1.2x10^{-12} 1.26x10^{-12} 1.53x10^{-12} 1.0x10^{-12} 8.8x10^{-13} 8.8x10^{-13}	8.8x10^{-13} 8.8x10^{-13} 1.2x10^{-12} 1.59x10^{-12} 1.24x10^{-12} <3.82x10^{-12} 1.59x10^{-12}	1.22*10^{-12} ± 20%
Ethylene	9.4x10^{-12} 6.59x10^{-12} 7.31x10^{-12} 7.31x10^{-12} 8.5x10^{-12} 8.5x10^{-12} 8.49x10^{-12} 8.0x10^{-12} 8.0x10^{-12} 9.96x10^{-12} 5.33x10^{-12}	3.64x10^{-12} 8.63x10^{-12} 4.0x10^{-12} 2.31x10^{-12} 5.33x10^{-12} 9.4x10^{-12} 3.01x10^{-12} 3.01x10^{-12} 1.66x10^{-12} 1.79x10^{-12}	
Nickel (and its comps)	NO RXN		
PAHs (BaP surrogate class)	No match Likely to associate with particles estimated half-life for reaction with photochemically produced hydroxyl radicals is 21.49 hr http://speclab.com/compound/c50328.htm		9.0*10^{-11} estimated… "very approximate"
Formaldehyde	2.01x10^{-13} 7.75x10^{-12} 8.14x10^{-12}	8.4x10^{-12} 1.5x10^{-11} 1.4x10^{-11}	
Acetaldehyde	1.45x10^{-11} <2.01x10^{-11} 1.44x10^{-11} 1.62x10^{-11}	1.69x10^{-11} 1.2x10^{-11} 1.6x10^{-11}	
1,2,4-Trimethylbenzene	3.25x10^{-11} 3.32x10^{-11} 4.0x10^{-11}	3.35x10^{-11} 3.32x10^{-11}	3.25*10^{-11} ± 25%
Ammonia	1.6x10^{-13} 1.2x10^{-13} 1.5x10^{-13}	4.1x10^{-14} 2.82x10^{-13}	
Cyclohexane	6.97x10^{-12}	5.25x10^{-12}	

	$6.71x10^{-12}$ $7.21x10^{-12}$ $7.61x10^{-12}$ $7.21x10^{-12}$ $7.36x10^{-12}$ $8.6x10^{-12}$	$6.19x10^{-12}$ $7.47x10^{-12}$ $6.79x10^{-12}$ $7.52x10^{-12}$ $6.71x10^{-12}$	
Dicyclopentadiene	No match Boiling point ~ 400 K		
Diethanolamine (and its salts)	No match Boiling point ~ 520 K		
Ethylbenzene	$7.51x10^{-12}$ $6.07x10^{-12}$ $7.51x10^{-12}$ $6.84x10^{-12}$	$7.52x10^{-12}$ $7.52x10^{-12}$ $7.97x10^{-12}$	$7.00*10^{-12}$ ± 25%
Hydrogen Sulphide	$4.7x10^{-12}$ $5.2x10^{-12}$ $5.2x10^{-12}$	$5.0x10^{-12}$ $3.11x10^{-12}$	
Isoprene	$6.79x10^{-11}$ $1.01x10^{-10}$ $1.0x10^{-10}$ $1.01x10^{-10}$	$9.6x10^{-11}$ $7.41x10^{-11}$ $7.41x10^{-11}$	
Mercury	NO RXN		
Methanol	$8.8x10^{-13}$ $1.06x10^{-12}$ $1.4x10^{-13}$ $9.0x10^{-13}$ $1.2x10^{-12}$	$1.0x10^{-12}$ $9.47x10^{-13}$ $9.0x10^{-13}$ $9.1x10^{-13}$	
Methyl Ethyl Ketone (MEK)	$9.71x10^{-13}$ $1.0x10^{-12}$ $8.8x10^{-13}$	$2.61x10^{-12}$ $2.61x10^{-12}$ $3.32x10^{-12}$	
Methyl Isobutyl Ketone (MIBK)	$1.4x10^{-11}$ $1.4x10^{-11}$ $1.41x10^{-11}$ $1.45x10^{-11}$	$1.3x10^{-11}$ $1.24x10^{-11}$ $1.49x10^{-11}$	
Methyl Tert-Butyl Ether (MTBE)	$2.97x10^{-12}$ $2.99x10^{-12}$	$3.24x10^{-12}$ $2.51x10^{-12}$	
Naphthalene	$2.31x10^{-11}$ $2.01x10^{-11}$ $2.59x10^{-11}$	$2.36x10^{-11}$ $2.42x10^{-11}$	$2.3x10^{-11}$ ± 25%
n-Hexane	$5.2x10^{-12}$ $5.53x10^{-12}$ $6.19x10^{-12}$ $6.09x10^{-12}$ $5.81x10^{-12}$ $5.6x10^{-12}$	$5.58x10^{-12}$ $5.21x10^{-12}$ $5.71x10^{-12}$ $6.31x10^{-12}$ $5.48x10^{-12}$ $3.24x10^{-12}$	
Phenol	$>3.01x10^{-11}$ $2.81x10^{-11}$	$2.81x10^{-11}$ $3.27x10^{-11}$	$2.7 *10^{-11}$ ± 25%
Propylene	$1.3x10^{-11}$ $3.01x10^{-11}$ $2.61x10^{-11}$ $2.19x10^{-11}$ $2.52x10^{-11}$ $3.01x10^{-11}$ $2.92x10^{-11}$ $2.71x10^{-11}$	$2.44x10^{-11}$ $2.47x10^{-11}$ $2.61x10^{-11}$ $2.47x10^{-11}$ $2.91x10^{-11}$ $5.0x10^{-12}$ $3.6x10^{-11}$ $1.45x10^{-11}$	

	2.52x10^{-11} 2.41x10^{-11} 2.41x10^{-11} 2.46x10^{-11} 2.56x10^{-11}	1.34x10^{-11} 1.45x10^{-11} 4.98x10^{-12} 1.1x10^{-11} 1.69x10^{-11}		
Styrene	1.06x10^{-10} 4.3x10^{-11} 5.86x10^{-11}	5.3x10^{-11} 5.3x10^{-11}		5.8x10^{-11} ± 20%
Sulphuric Acid	No match found			
Toluene	5.7x10^{-12} 5.7x10^{-12} 5.5x10^{-12} 6.48x10^{-12} 5.99x10^{-12} 5.35x10^{-12} 6.38x10^{-12} 7.21x10^{-12}	7.21x10^{-12} 5.99x10^{-12} 6.39x10^{-12} 6.11x10^{-12} 5.78x10^{-12} 4.15x10^{-12} 6.11x10^{-12}		5.63*10^{-12} ± 20%
Vanadium	NO RXN			
Xylene	o-xylene: 1.14x10^{-11} 1.22x10^{-11} 1.3x10^{-11} 1.24x10^{-11} 1.32x10^{-11} 1.33x10^{-11} 1.33x10^{-11} 1.27x10^{-11} 1.43x10^{-11} 1.27x10^{-11} 1.53x10^{-11} 1.28x10^{-11}	m-xylene: 2.13x10^{-11} 2.14x10^{-11} 2.14x10^{-11} 2.34x10^{-11} 2.18x10^{-11} 2.04x10^{-11} 2.32x10^{-11} 2.18x10^{-11} 2.46x10^{-11} 2.29x10^{-11} 2.09x10^{-11} 2.31x10^{-11} 2.27x10^{-11} 2.34x10^{-11} 2.16x10^{-11} 1.86x10^{-11} 1.86x10^{-11} 1.81x10^{-11} 2.32x10^{-12} 2.41x10^{-11} 2.03x10^{-11} 1.83x10^{-11} 2.36x10^{-11} 2.32x10^{-11}	p-xylene: 1.3x10^{-11} 1.3x10^{-11} 1.36x10^{-11} 1.36x10^{-11} 1.3x10^{-11} 1.53x10^{-11} 1.01x10^{-11} 8.8x10^{-12} 1.22x10^{-11} 1.23x10^{-11}	13.6 *10^{-12} ±25%–orth 23.1 *10^{-12} ±15%–met 14.3 *10^{-12} ±25%–para For xylene – use the most conservative estimate – which will imply choosing one of the isomers and using that one (i.e. the one with the slowest degradation).
Zinc (and its compounds)	NO RXN			
PM2.5 from SOx	CACs considered by alternate method			
PM2.5 from NOx	CACs considered by alternate method			
primary PM2.5	CACs considered by alternate method			

Appendix G – Background Concentrations Used in HEIDI II

Substance	Chevron - Burnaby	Consumers' Co-operative - Regina	Husky - Prince George	Imperial - Dartmouth	Imperial - Nanticoke
1,3-Butadiene	5.00E-01	3.00E-01	*5.00E-02*	3.00E-01	1.00E-01
Benzene	2.70E+00	1.20E+00	*4.00E-01*	1.50E+00	2.30E+00
Ethylene (as 5% Ethylene Oxide)	3.10E+00	2.70E+00	*4.50E-01*	2.90E+00	1.70E+00
Nickel (Elements totals bound to PM)	2.47E-03	2.03E-03	*7.11E-04*	4.90E-03	1.95E-03
PAHs (BaP surrogate class) BaP	9.00E-05	2.00E-05	*1.00E-05*	4.00E-05	4.00E-05
Formaldehyde	1.60E+00	*2.64E+00*	*8.00E-01*	*2.64E+00*	2.70E+00
Acetaldehyde	1.90E+00	*1.70E+00*	*6.50E-01*	*1.70E+00*	1.30E+00
1,2,4-trimethylbenzene	5.00E-01	4.00E-01	*5.00E-02*	6.00E-01	1.00E-01
Ammonia	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Benzene (as BTEX potentiator)	2.70E+00	1.20E+00	*4.00E-01*	1.50E+00	2.30E+00
BTEX	Special Case – derived using a combination of B, T, E, X				
Cyclohexane	6.40E+00	2.00E-01	*5.00E-02*	3.00E-01	1.00E-01
Dicyclopentadiene	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Diethanolamine (and its salts)	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Ethylbenzene	2.30E+00	6.00E-01	*1.00E-01*	7.00E-01	3.00E-01
Hydrogen Sulphide	6.97E-04	6.97E-04	*2.79E-04*	6.97E-04	6.97E-04
Isoprene	4.00E-01	3.00E-01	*5.00E-02*	3.00E-01	1.00E-01
Mercury (Elements totals bound to PM)	1.70E-03	3.45E-03	*6.67E-04*	3.94E-03	2.63E-03
Methanol	*1.43E+01*	*1.43E+01*	*3.57E+00*	*1.43E+01*	*1.43E+01*
Methyl Ethyl Ketone (MEK)	1.10E+00	*1.49E+00*	*2.50E-01*	*1.49E+00*	8.00E-01
Methyl Isobutyl Ketone (MIBK)	2.00E-01	*2.42E-01*	*5.00E-02*	*2.42E-01*	1.00E-01
Methyl Tert-Butyl Ether (MTBE)	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Naphthalene	9.00E-01	8.00E-01	*1.00E-01*	7.00E-01	5.00E-01
n-Hexane	8.00E+00	8.00E-01	*2.00E-01*	9.00E-01	7.00E-01
Phenol	4.05E+00	4.05E+00	*2.03E+00*	4.05E+00	4.05E+00
Propylene	3.40E+00	1.10E+00	*3.00E-01*	1.20E+00	1.30E+00
Styrene	2.00E-01	1.00E-01	*0.00E+00*	1.00E-01	1.00E-01
Sulphuric Acid	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Toluene	1.53E+01	3.60E+00	*7.00E-01*	3.80E+00	1.40E+00
Vanadium (Elements totals bound to PM)	9.71E-03	7.46E-03	*2.62E-03*	2.93E-02	6.65E-03
Xylene	1.07E+01	2.70E+00	*4.00E-01*	3.20E+00	9.00E-01
Zinc (Elements totals bound to PM)	1.37E-02	2.89E-02	*2.38E-03*	4.76E-03	2.29E-02
or PM2.5 (DC)p	8.00E+00	8.00E+00	*9.00E+00*	8.00E+00	1.10E+01
(from precursors)					
Ammonia	0	0	*0*	0	0
Nox (NO2, ppb)	11	13	11	17	8
SOx (SO2, ppb)	3	1	3	13	3

Substance	**Imperial - Sarnia**	**Imperial - Strathcona**	**Irving - Saint John**	**North Atlantic Refining - Come by Chance**	**NOVA - Corunna**
1,3-Butadiene	2.00E-01	2.00E-01	1.00E-01	*5.00E-02*	2.00E-01
Benzene	1.20E+00	1.70E+00	8.00E-01	*4.00E-01*	1.20E+00
Ethylene (as 5% Ethylene Oxide)	4.40E+00	3.70E+00	9.00E-01	*4.50E-01*	4.40E+00
Nickel (Elements totals bound to PM)	1.62E-03	1.64E-03	2.16E-03	*7.11E-04*	1.62E-03
PAHs (BaP surrogate class) BaP	2.60E-04	3.00E-05	1.50E-04	*1.00E-05*	2.60E-04
Formaldehyde	2.90E+00	*2.64E+00*	1.60E+00	*8.00E-01*	2.90E+00
Acetaldehyde	1.80E+00	*1.70E+00*	1.50E+00	*6.50E-01*	1.80E+00
1,2,4-trimethylbenzene	3.00E-01	9.00E-01	2.00E-01	*5.00E-02*	3.00E-01
Ammonia	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Benzene (as BTEX potentiator)	1.20E+00	1.70E+00	8.00E-01	*4.00E-01*	1.20E+00
BTEX	Special Case – derived using a combination of B, T, E, X				
Cyclohexane	1.10E+00	1.40E+00	4.00E-01	*5.00E-02*	1.10E+00
Dicyclopentadiene	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Diethanolamine (and its salts)	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Ethylbenzene	5.00E-01	8.00E-01	2.00E-01	*1.00E-01*	5.00E-01
Hydrogen Sulphide	6.97E-04	6.97E-04	6.97E-04	*2.79E-04*	6.97E-04
Isoprene	3.00E-01	9.00E-01	2.00E-01	*5.00E-02*	3.00E-01
Mercury (Elements totals bound to PM)	1.91E-03	1.33E-03	3.44E-03	*6.67E-04*	1.91E-03
Methanol	*1.43E+01*	*1.43E+01*	*1.43E+01*	*7.14E+00*	*1.43E+01*
Methyl Ethyl Ketone (MEK)	2.40E+00	*1.49E+00*	5.00E-01	*2.50E-01*	2.40E+00
Methyl Isobutyl Ketone (MIBK)	4.00E-01	*2.42E-01*	1.00E-01	*5.00E-02*	4.00E-01
Methyl Tert-Butyl Ether (MTBE)	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Naphthalene	6.00E-01	6.00E-01	7.00E-01	*1.00E-01*	6.00E-01
n-Hexane	2.40E+00	5.30E+00	4.00E-01	*2.00E-01*	2.40E+00
Phenol	4.05E+00	4.05E+00	4.05E+00	*2.03E+00*	4.05E+00
Propylene	1.50E+00	1.10E+00	8.40E+00	*3.00E-01*	1.50E+00
Styrene	1.00E-01	6.00E-01	0.00E+00	*0.00E+00*	1.00E-01
Sulphuric Acid	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Toluene	3.30E+00	3.40E+00	1.50E+00	*7.00E-01*	3.30E+00
Vanadium (Elements totals bound to PM)	5.23E-03	6.56E-03	6.60E-03	*2.62E-03*	5.23E-03
Xylene	1.60E+00	3.50E+00	8.00E-01	*4.00E-01*	1.60E+00
Zinc (Elements totals bound to PM)	7.59E-02	1.76E-02	3.22E-02	*2.38E-03*	7.59E-02
or PM2.5 (DC)p	1.10E+01	8.00E+00	6.00E+00	*2.50E+00*	1.10E+01
(from precursors)					
Ammonia	0	0	0	*0*	0
Nox (NO2, ppb)	17	24	5	*1.54E+01*	17
SOx (SO2, ppb)	10	2	4	*5.02E+00*	10

Substance	**Parkland - Bowden**	**Petro-Canada - Edmonton**	**Petro-Canada - Mississauga**	**Petro-Canada - Montreal**	**Petro-Canada - Oakville**
1,3-Butadiene	*5.00E-02*	2.00E-01	1.00E-01	2.00E-01	1.00E-01
Benzene	*4.00E-01*	1.70E+00	1.10E+00	3.00E+00	1.40E+00
Ethylene (as 5% Ethylene Oxide)	*4.50E-01*	3.70E+00	1.40E+00	3.70E+00	1.40E+00
Nickel (Elements totals bound to PM)	*7.11E-04*	1.64E-03	1.42E-03	3.97E-03	1.42E-03
PAHs (BaP surrogate class) BaP	*1.00E-05*	3.00E-05	1.90E-04	5.70E-04	1.90E-04
Formaldehyde	*8.00E-01*	*2.64E+00*	3.50E+00	2.80E+00	3.50E+00
Acetaldehyde	*6.50E-01*	*1.70E+00*	1.50E+00	2.00E+00	1.50E+00
1,2,4-trimethylbenzene	*5.00E-02*	9.00E-01	5.00E-01	5.00E-01	5.00E-01
Ammonia	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Benzene (as BTEX potentiator)	*4.00E-01*	1.70E+00	1.10E+00	3.00E+00	1.40E+00
BTEX	Special Case – derived using a combination of B, T, E, X				
Cyclohexane	*5.00E-02*	1.40E+00	6.00E-01	7.00E-01	6.00E-01
Dicyclopentadiene	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Diethanolamine (and its salts)	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Ethylbenzene	*1.00E-01*	8.00E-01	1.00E+00	1.20E+00	7.00E-01
Hydrogen Sulphide	*2.79E-04*	6.97E-04	6.97E-04	6.97E-04	6.97E-04
Isoprene	*5.00E-02*	9.00E-01	2.00E-01	2.00E-01	5.00E-01
Mercury (Elements totals bound to PM)	*6.67E-04*	1.33E-03	1.81E-03	1.82E-03	1.81E-03
Methanol	*7.14E+00*	*1.43E+01*	*1.43E+01*	*1.43E+01*	*1.43E+01*
Methyl Ethyl Ketone (MEK)	*2.50E-01*	*1.49E+00*	1.50E+00	1.20E+00	1.50E+00
Methyl Isobutyl Ketone (MIBK)	*5.00E-02*	*2.42E-01*	2.00E-01	2.00E-01	2.00E-01
Methyl Tert-Butyl Ether (MTBE)	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Naphthalene	*1.00E-01*	6.00E-01	2.00E-01	7.00E-01	7.00E-01
n-Hexane	*2.00E-01*	5.30E+00	9.00E-01	1.90E+00	3.30E+00
Phenol	*2.03E+00*	4.05E+00	4.05E+00	4.05E+00	4.05E+00
Propylene	*3.00E-01*	1.10E+00	6.00E-01	1.60E+00	1.01E+01
Styrene	*0.00E+00*	6.00E-01	3.00E-01	4.00E-01	1.00E-01
Sulphuric Acid	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Toluene	*7.00E-01*	3.40E+00	6.60E+00	5.90E+00	6.50E+00
Vanadium (Elements totals bound to PM)	*2.62E-03*	6.56E-03	5.47E-03	1.17E-02	5.47E-03
Xylene	*4.00E-01*	3.50E+00	3.90E+00	4.40E+00	3.00E+00
Zinc (Elements totals bound to PM)	*2.38E-03*	1.76E-02	3.30E-02	3.24E-02	3.30E-02
or PM2.5 (DC)p	*5.00E+00*	8.00E+00	9.00E+00	1.00E+01	9.00E+00
(from precursors)					
Ammonia	0	0	0	0	0
Nox (NO2, ppb)	14	24	26	14	16
SOx (SO2, ppb)	1	2	4	6	4

Substance	**Shell - Sarnia**	**Shell - Scotford**	**Shell - Montreal East**	**Sunoco - Sarnia**	**Ultramar - St. Romuald**
1,3-Butadiene	2.00E-01	2.00E-01	2.00E-01	2.00E-01	*3.00E-01*
Benzene	1.20E+00	1.70E+00	3.00E+00	1.20E+00	*1.31E+00*
Ethylene (as 5% Ethylene Oxide)	4.40E+00	3.70E+00	3.70E+00	4.40E+00	*9.00E-01*
Nickel (Elements totals bound to PM)	1.62E-03	1.64E-03	3.97E-03	1.62E-03	2.19E-02
PAHs (BaP surrogate class) BaP	2.60E-04	3.80E-04	5.70E-04	2.60E-04	*1.50E-04*
Formaldehyde	2.90E+00	*2.64E+00*	2.80E+00	2.90E+00	*1.60E+00*
Acetaldehyde	1.80E+00	*1.70E+00*	2.00E+00	1.80E+00	*1.50E+00*
1,2,4-trimethylbenzene	3.00E-01	9.00E-01	5.00E-01	3.00E-01	*2.00E-01*
Ammonia	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Benzene (as BTEX potentiator)	1.20E+00	1.70E+00	3.00E+00	1.20E+00	*8.00E-01*
BTEX	Special Case – derived using a combination of B, T, E, X				
Cyclohexane	1.10E+00	1.40E+00	7.00E-01	1.10E+00	*4.00E-01*
Dicyclopentadiene	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Diethanolamine (and its salts)	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Ethylbenzene	5.00E-01	8.00E-01	1.20E+00	5.00E-01	*2.00E-01*
Hydrogen Sulphide	6.97E-04	5.58E-04	6.97E-04	6.97E-04	6.97E-04
Isoprene	3.00E-01	9.00E-01	2.00E-01	3.00E-01	*2.00E-01*
Mercury (Elements totals bound to PM)	1.91E-03	1.33E-03	1.82E-03	1.91E-03	2.19E-03
Methanol	*1.43E+01*	*1.43E+01*	*1.43E+01*	*1.43E+01*	*1.43E+01*
Methyl Ethyl Ketone (MEK)	2.40E+00	*1.49E+00*	1.20E+00	2.40E+00	*5.00E-01*
Methyl Isobutyl Ketone (MIBK)	4.00E-01	*2.42E-01*	2.00E-01	4.00E-01	*1.00E-01*
Methyl Tert-Butyl Ether (MTBE)	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Naphthalene	6.00E-01	6.00E-01	7.00E-01	6.00E-01	*7.00E-01*
n-Hexane	2.40E+00	5.30E+00	1.90E+00	2.40E+00	*4.00E-01*
Phenol	4.05E+00	4.05E+00	4.05E+00	4.05E+00	4.05E+00
Propylene	1.50E+00	1.10E+00	1.60E+00	1.50E+00	*8.40E+00*
Styrene	1.00E-01	6.00E-01	4.00E-01	1.00E-01	*0.00E+00*
Sulphuric Acid	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*	*0.00E+00*
Toluene	3.30E+00	3.40E+00	5.90E+00	3.30E+00	*5.10E+00*
Vanadium (Elements totals bound to PM)	5.23E-03	6.56E-03	1.17E-02	5.23E-03	1.32E-02
Xylene	1.60E+00	3.50E+00	4.40E+00	1.60E+00	*8.00E-01*
Zinc (Elements totals bound to PM)	7.59E-02	1.76E-02	3.24E-02	7.59E-02	1.36E-01
or PM2.5 (DC)p	1.10E+01	6.00E+00	1.00E+01	1.10E+01	8.00E+00
(from precursors)					
Ammonia	0	0	0	0	0
Nox (NO2, ppb)	17	14	14	17	14
SOx (SO2, ppb)	10	1	6	10	2

Appendix H – Parametric Background Concentrations

Background levels generally:	**High**		**Medium**		**Low**	
Substance Name	*Geometric MEAN*	*Geometric Stdev*	*Geometric MEAN*	*Geometric Stdev*	*Geometric MEAN*	*Geometric Stdev*
1,3-Butadiene	0.21	1.60	0.20	1.44	0.08	2.02
Benzene	2.08	1.38	1.24	1.10	0.72	2.07
Ethylene (as 5% Ethylene Oxide)	3.14	1.44	2.81	1.93	0.85	2.18
Nickel (Elements totals bound to PM)	0.00	1.55	0.00	2.76	0.00	1.79
PAHs (BaP surrogate class) BaP	0.00	3.62	0.00	1.99	0.00	2.97
Formaldehyde	2.60	1.27	2.70	1.28	1.34	1.82
Acetaldehyde	1.78	1.11	1.69	1.09	0.98	1.59
1,2,4-trimethylbenzene	0.64	1.37	0.34	1.45	0.10	2.40
Ammonia	0.00	0.00	0.00	0.00	0.00	0.00
Benzene (as BTEX potentiator)	2.08	1.38	1.15	1.21	0.72	2.07
BTEX	0.00					
Cyclohexane	1.26	2.24	0.73	1.75	0.10	2.40
Dicyclopentadiene	0.00	0.00	0.00	0.00	0.00	0.00
Diethanolamine (and its salts)	0.00	0.00	0.00	0.00	0.00	0.00
Ethylbenzene	1.02	1.51	0.51	1.63	0.18	2.10
Hydrogen Sulphide	0.00	1.09	0.00	1.00	0.00	1.65
Isoprene	0.48	1.97	0.27	1.22	0.10	2.20
Mercury (Elements totals bound to PM)	0.00	1.17	0.00	1.32	0.00	2.35
Methanol	14.27	1.00	14.27	1.00	8.99	1.76
Methyl Ethyl Ketone (MEK)	1.34	1.15	1.68	1.78	0.46	2.12
Methyl Isobutyl Ketone (MIBK)	0.22	1.11	0.28	1.70	0.08	1.88
Methyl Tert-Butyl Ether (MTBE)	0.00	0.00	0.00	0.00	0.00	0.00
Naphthalene	0.68	1.16	0.54	1.55	0.26	2.83
n-Hexane	3.92	1.75	1.40	2.06	0.35	1.92
Phenol	4.05	1.00	4.05	1.00	2.86	1.46
Propylene	1.97	2.28	1.63	2.22	0.83	3.75
Styrene	0.35	1.98	0.00	0.00	0.00	0.00
Sulphuric Acid	0.00	0.00	0.00	0.00	0.00	0.00
Toluene	5.41	1.72	3.96	1.32	1.17	1.93
Vanadium (Elements totals bound to PM)	0.01	1.37	0.01	1.98	0.00	1.70
Xylene	4.29	1.53	1.82	1.69	0.71	2.13
Zinc (Elements totals bound to PM)	0.02	1.45	0.05	3.04	0.01	3.85

Appendix I: Proportion of predicted incidence below the *de minimis* risk level for substances emitted from individual refineries

1. Chevron-Burnaby

Substance	Proportion of predicted incidence below 10^{-6}	Proportion of predicted incidence above 10^{-6}	Relevant outcome (for reference)	Rank here[28] (for validation comparison with other ranking output)
Benzene	1.00	0.00	Leukemia	4
Ethylene (as 5% ethylene oxide)	1.00	0.00	Leukemia	3
Nickel	0.91	0.09	Lung cancer	1
PAH (using Benzo[a] pyrene)	1.00	0.00	Lung cancer	2
1,2,4-trimethylbenzene	1.00	0.00	Moderate anemia	9
BTEX	0.64	0.36	CNS neurotoxicity	1
Cyclohexane	1.00	0.00	Reduced bodyweight	6
Hydrogen sulphide	1.00	0.00	Nose irritation	8
MTBE	1.00	0.00	PNS neurotoxicity	5
Naphthalene	1.00	0.00	Benign lung tumors	10
n-hexane	1.00	0.00	PNS neurotixicity	4
Propylene	1.00	0.00	benign nasal and upper airway tumours	7
Sulphuric Acid	0.99	0.01	Benign nasal and upper airway tumors	3
Vanadium	0.77	0.23	Nasal and upper airway irriatation	2
Zinc	1.00	0.00	Moderate anemia	11

2. Consumer's Co-operative

Substance	Proportion of predicted incidence below 10^{-6}	Proportion of predicted incidence above 10^{-6}	Relevant outcome (for reference)	Rank here (for validation comparison with other ranking output)
Benzene	0.96	0.04	Leukemia	1

---

[28] Rank may be based on differences at the 10^{-8} level or less

Ethylene (as 5% ethylene oxide)	0.98	0.02	Leukemia	2
Nickel	0.98	0.02	Lung cancer	3
1,2,4-trimethylbenzene	1.00	0.00	Moderate anemia	9
Ammonia	1.00	0.00	skin and nose irritation	10
BTEX	0.83	0.17	CNS neurotoxicity	1
Cyclohexane	1.00	0.00	Reduced bodyweight	4
Hydrogen sulphide	0.92	0.08	Nose irritation	2
Naphthalene	0.99	0.01	Benign lung tumors	3
n-hexane	1.00	0.00	PNS neurotoxicity	8
Phenol	1.00	0.00	Mild CNS neurotoxicity	11
Propylene	1.00	0.00	benign nasal and upper airway tumours	7
Sulphuric Acid	1.00	0.00	Benign nasal and upper airway tumors	6
Vanadium	1.00	0.00	Nasal and upper airway irriatation	5

3. Prince George

Substance	Proportion of predicted incidence below 10^{-6}	Proportion of predicted incidence above 10^{-6}	Relevant outcome (for reference)	Rank here (for validation comparison with other ranking output)
BTEX	0.83	0.17	CNS neurotoxicity	1
Cyclohexane	1.00	0.00	Reduced bodyweight	2
Hydrogen sulphide	1.00	0.00	Nose irritation	4
n-hexane	1.00	0.00	PNS neurotoxicity	5
Propylene	1.00	0.00	benign nasal and upper airway tumours	3

4. Imperial Dartmouth

Substance	Proportion of predicted incidence below 10^{-6}	Proportion of predicted incidence above 10^{-6}	Relevant outcome (for reference)	Rank here (for validation comparison with other ranking output)
Benzene	0.99	0.01	Leukemia	2
Ethylene (as 5%	1.00	0.00	Leukemia	3

ethylene oxide)				
PAH (using Benzo[a] pyrene)	0.98	0.02	Lung cancer	1
1,2,4-trimethylbenzene	1.00	0.00	Moderate anemia	12
Ammonia	1.00	0.00	skin and nose irritation	13
BTEX	0.81	0.19	CNS neurotoxicity	2
Cyclohexane	1.00	0.00	Reduced bodyweight	8
Diethanolamine	1.00	0.00	Throat irritation	9
Hydrogen sulphide	0.99	0.01	Nose irritation	3
Mercury	1.00	0.00	severe CNS neurotoxicity	9
Methanol	1.00	0.00	Benign lung tumors	6
Naphthalene	1.00	0.00	PNS neurotoxicity	4
n-hexane	1.00	0.00	Mild CNS neurotoxicity	5
Phenol	1.00	0.00	Mild CNS neurotoxicity	7
Propylene	1.00	0.00	benign nasal and upper airway tumours	11
Sulphuric Acid	0.68	0.32	Benign nasal and upper airway tumors	1

5. Imperial Nanticoke

Substance	**Proportion of predicted incidence below 10^{-6}**	**Proportion of predicted incidence above 10^{-6}**	**Relevant outcome (for reference)**	**Rank here (for validation comparison with other ranking output)**
Benzene	1.00	0.00	Leukemia	3
Ethylene (as 5% ethylene oxide)	1.00	0.00	Leukemia	2
PAH (using Benzo[a] pyrene)	0.98	0.02	Lung cancer	1
1,2,4-trimethylbenzene	1.00	0.00	Moderate anemia	10
Ammonia	1.00	0.00	skin and nose irritation	12
BTEX	0.83	0.17	CNS neurotoxicity	2
Cyclohexane	1.00	0.00	Reduced bodyweight	4
Diethanolamine	1.00	0.00	Throat irritation	5
Hydrogen sulphide	0.96	0.04	Nose irritation	3
Mercury	1.00	0.00	severe CNS neurotoxicity	6

Methanol	1.00	0.00	physical teratogenesis	9
Naphthalene	1.00	0.00	Benign lung tumors	11
n-hexane	1.00	0.00	PNS neurotoxicity	8
Phenol	1.00	0.00	mild CNS neurotoxicity	13
Propylene	1.00	0.00	benign nasal & upper airway tumours	7
Sulphuric Acid	0.71	0.29	Benign nasal and upper airway tumors	1

6. Imperial Sarnia

Substance	Proportion of predicted incidence below 10^{-6}	Proportion of predicted incidence above 10^{-6}	Relevant outcome (for reference)	Rank here (for validation comparison with other ranking output)
1,3-butadiene	1.00	0.00	Leukemia	4
Benzene	0.96	0.04	Leukemia	3
Ethylene (as 5% ethylene oxide)	1.00	0.00	Leukemia	5
Nickel	0.16	0.84	Lung cancer	1
PAH (using Benzo[a] pyrene)	0.65	0.35	Lung cancer	2
1,2,4-trimethylbenzene	1.00	0.00	Moderate anemia	13
Ammonia	1.00	0.00	skin and nose irritation	14
BTEX	0.81	0.19	CNS neurotoxicity	3
Cyclohexane	1.00	0.00	Reduced bodyweight	11
Hydrogen sulphide	0.97	0.03	Nose irritation	4
Mercury	1.00	0.00	severe CNS neurotoxicity	10
Methanol	1.00	0.00	physical teratogenesis	8
Naphthalene	0.99	0.01	Benign lung tumors	6
n-hexane	0.99	0.01	PNS neurotoxicity	5
Phenol	1.00	0.00	mild CNS neurotoxicity	9
Propylene	1.00	0.00	benign nasal & upper airway tumours	12
Sulphuric Acid	0.54	0.46	Benign nasal and upper airway tumors	2
Vanadium	0.45	0.55	Nasal and upper	1

			airway irriatation	
Zinc	0.99	0.01	Moderate anemia	7

7. Imperial Strathcona

Substance	Proportion of predicted incidence below 10^{-6}	Proportion of predicted incidence above 10^{-6}	Relevant outcome (for reference)	Rank here (for validation comparison with other ranking output)
Benzene	1.00	0.00	Leukemia	3
Ethylene (as 5% ethylene oxide)	1.00	0.00	Leukemia	2
PAH (using Benzo[a] pyrene)	0.99	0.01	Lung cancer	1
1,2,4-trimethylbenzene	1.00	0.00	Moderate anemia	13
Ammonia	1.00	0.00	skin and nose irritation	12
BTEX	0.65	0.35	CNS neurotoxicity	1
Cyclohexane	1.00	0.00	Reduced bodyweight	9
Hydrogen sulphide	1.00	0.00	Nose irritation	5
Mercury	1.00	0.00	severe CNS neurotoxicity	8
MEK	1.00	0.00	developmental retardation	10
MIBK	1.00	0.00	developmental retardation	7
Naphthalene	0.99	0.01	Benign lung tumors	4
n-hexane	0.99	0.01	PNS neurotoxicity	3
Phenol	1.00	0.00	mild CNS neurotoxicity	6
Propylene	1.00	0.00	benign nasal & upper airway tumours	11
Sulphuric Acid	0.71	0.29	Benign nasal and upper airway tumors	2
Zinc	1.00	0.00	Moderate anemia	14

8. Irving Saint John

Substance	Proportion of predicted incidence below 10^{-6}	Proportion of predicted incidence above 10^{-6}	Relevant outcome (for reference)	Rank here (for validation comparison with other ranking output)
1,3-butadiene	1.00	0.00	Leukemia	4
Benzene	0.98	0.02	Leukemia	1
Ethylene (as 5% ethylene oxide)	1.00	0.00	Lung cancer	2

Nickel	0.88	0.12	Lung cancer	2
1,2,4-trimethylbenzene	1.00	0.00	Moderate anemia	7
BTEX	0.83	0.17	CNS neurotoxicity	1
Cyclohexane	1.00	0.00	Reduced bodyweight	3
Hydrogen sulphide	1.00	0.00	Nose irritation	8
MTBE	1.00	0.00	PNS neurotoxicity	4
Naphthalene	1.00	0.00	Benign lung tumors	9
n-hexane	1.00	0.00	PNS neurotoxicity	6
Propylene	1.00	0.00	benign nasal & upper airway tumours	5
Styrene	0.98	0.02	mild developmental retardation	2
Vanadium	1.00	0.00	Nasal and upper airway irriatation	7

9. North Atlantic Refining

Substance	Proportion of predicted incidence below 10^{-6}	Proportion of predicted incidence above 10^{-6}	Relevant outcome (for reference)	Rank here (for validation comparison with other ranking output)
Benzene	0.96	0.04	Leukemia	2
Nickel	0.27	0.73	Lung cancer	1
PAH (using Benzo[a] pyrene)	1.00	0.00	Lung cancer	3
1,2,4-trimethylbenzene	1.00	0.00	Moderate anemia	8
BTEX	0.82	0.18	CNS neurotoxicity	2
Cyclohexane	1.00	0.00	Reduced bodyweight	4
Diethanolamine	1.00	0.00	Throat irritation	6
Hydrogen sulphide	0.99	0.01	Nose irritation	3
MTBE	1.00	0.00	PNS neurotoxicity	5
n-hexane	1.00	0.00	PNS neurotoxicity	7
Phenol	1.00	0.00	mild CNS neurotoxicity	10
Vanadium	0.48	0.52	nasal and upper airway irritation	1
Zinc	1.00	0.00	Moderate anemia	9

10. Nova Corunna

Substance	Proportion of predicted incidence below 10^{-6}	Proportion of predicted incidence above 10^{-6}	Relevant outcome (for reference)	Rank here (for validation comparison with other ranking output)
1,3-butadiene	0.97	0.03	Leukemia	3
Benzene	0.92	0.08	Leukemia	1
Ethylene (as 5% ethylene oxide)	0.97	0.03	Leukemia	2
PAH (using Benzo[a] pyrene)	1.00	0.00	Lung cancer	4
1,2,4-trimethylbenzene	1.00	0.00	Moderate anemia	12
BTEX	0.80	0.20	CNS neurotoxicity	2
Cyclohexane	1.00	0.00	Reduced bodyweight	8
Dicyclopentadiene	1.00	0.00	chronic renal disease	10
Hydrogen sulphide	1.00	0.00	Nose irritation	7
Isoprene	1.00	0.00	benign lung tumours	5
Mercury	1.00	0.00	severe CNS neurotoxicity	6
Naphthalene	0.99	0.01	Benign lung tumors	3
n-hexane	1.00	0.00	PNS neurotoxicity	4
Phenol	1.00	0.00	mild CNS neurotoxicity	9
Propylene	1.00	0.00	benign nasal & upper airway tumours	11
Sulphuric Acid	0.67	0.33	Benign nasal and upper airway tumors	1

11. Parkland Bowden

Substance	Proportion of predicted incidence below 10^{-6}	Proportion of predicted incidence above 10^{-6}	Relevant outcome (for reference)	Rank here (for validation comparison with other ranking output)
1,2,4-trimethylbenzene	1.00	0.00	Moderate anemia	
BTEX	0.83	0.17	CNS neurotoxicity	1
Cyclohexane	1.00	0.00	Reduced bodyweight	
n-hexane	1.00	0.00	PNS neurotoxicity	

12. Petro-Canada - Edmonton

Substance	Proportion of predicted incidence below 10^{-6}	Proportion of predicted incidence above 10^{-6}	Relevant outcome (for reference)	Rank here (for validation comparison with other ranking output)
Benzene	1.00	0.00	Leukemia	4
Ethylene (as 5% ethylene oxide)	1.00	0.00	Leukemia	2
Nickel	1.00	0.00	Lung cancer	3
PAH (using Benzo[a] pyrene)	1.00	0.00	Lung cancer	1
1,2,4-trimethylbenzene	1.00	0.00	Moderate anemia	10
BTEX	0.65	0.35	CNS neurotoxicity	1
Cyclohexane	1.00	0.00	Reduced bodyweight	7
Diethanolamine	1.00	0.00	Throat irritation	5
Hydrogen sulphide	1.00	0.00	Nose irritation	8
Mercury	1.00	0.00	severe CNS neurotoxicity	6
n-hexane	0.99	0.01	PNS neurotoxicity	4
Propylene	1.00	0.00	benign nasal & upper airway tumours	9
Sulphuric Acid	0.78	0.22	Benign nasal and upper airway tumors	2
Vanadium	0.96	0.04	nasal and upper airway irritation	3
Zinc	1.00	0.00	Moderate anemia	11

13. Petro-Canada - Mississauga

Substance	Proportion of predicted incidence below 10^{-6}	Proportion of predicted incidence above 10^{-6}	Relevant outcome (for reference)	Rank here (for validation comparison with other ranking output)
Benzene	1.00	0.00	Leukemia	1
1,2,4-trimethylbenzene	1.00	0.00	Moderate anemia	9
BTEX	0.81	0.19	CNS neurotoxicity	1
Cyclohexane	1.00	0.00	Reduced bodyweight	5
Diethanolamine	1.00	0.00	Throat irritation	4
Hydrogen sulphide	1.00	0.00	Nose irritation	6
MEK	1.00	0.00	developmental retardation	7
Naphthalene	0.99	0.01	Benign lung	3

			tumors	
n-hexane	1.00	0.00	PNS neurotoxicity	10
Propylene	1.00	0.00	benign nasal & upper airway tumours	8
Sulphuric Acid	0.90	0.10	Benign nasal and upper airway tumors	2

14. Petro-Canada - Montreal

Substance	Proportion of predicted incidence below 10^{-6}	Proportion of predicted incidence above 10^{-6}	Relevant outcome (for reference)	Rank here (for validation comparison with other ranking output)
1,3-butadiene	1.00	0.00	Leukemia	4
Benzene	0.98	0.02	Leukemia	2
Ethylene (as 5% ethylene oxide)	1.00	0.00	Leukemia	5
Nickel	0.76	0.24	Lung cancer	1
PAH (using Benzo[a] pyrene)	0.99	0.01	Lung cancer	3
1,2,4-trimethylbenzene	1.00	0.00	Moderate anemia	9
BTEX	0.64	0.36	CNS neurotoxicity	1
Cyclohexane	1.00	0.00	Reduced bodyweight	6
Hydrogen sulphide	1.00	0.00	Nose irritation	5
Mercury	1.00	0.00	severe CNS neurotoxicity	6
Methanol	1.00	0.00	physical teratogenesis	12
Naphthalene	1.00	0.00	Benign lung tumors	10
n-hexane	1.00	0.00	PNS neurotoxicity	4
Propylene	1.00	0.00	benign nasal & upper airway tumours	8
Sulphuric Acid	0.74	0.26	Benign nasal and upper airway tumors	3
Vanadium	0.72	0.28	nasal and upper airway irritation	2
Zinc	1.00	0.00	Moderate anemia	11

15. Petro-Canada - Oakville

Substance	Proportion of predicted incidence below 10^{-6}	Proportion of predicted incidence above 10^{-6}	Relevant outcome (for reference)	Rank here (for validation comparison with other ranking

				output)
1,3-butadiene	1.00	0.00	Leukemia	3
Benzene	1.00	0.00	Leukemia	5
Ethylene (as 5% ethylene oxide)	1.00	0.00	Leukemia	4
Nickel	0.92	0.08	Lung cancer	2
PAH (using Benzo[a] pyrene)	0.29	0.71	Lung cancer	1
1,2,4-trimethylbenzene	1.00	0.00	Moderate anemia	11
Ammonia	1.00	0.00	skin and nose irritation	5
BTEX	0.64	0.36	CNS neurotoxicity	1
Cyclohexane	1.00	0.00	Reduced bodyweight	8
Diethanolamine	1.00	0.00	Throat irritation	6
Hydrogen sulphide	1.00	0.00	Nose irritation	9
Mercury	1.00	0.00	severe CNS neurotoxicity	7
Naphthalene	1.00	0.00	Benign lung tumors	12
n-hexane	1.00	0.00	PNS neurotoxicity	4
Propylene	1.00	0.00	benign nasal & upper airway tumours	10
Sulphuric Acid	0.71	0.29	Benign nasal and upper airway tumors	2
Vanadium	0.80	0.20	nasal and upper airway irritation	3

16. Shell-Montreal

Substance	**Proportion of predicted incidence below 10^{-6}**	**Proportion of predicted incidence above 10^{-6}**	**Relevant outcome (for reference)**	**Rank here (for validation comparison with other ranking output)**
Benzene	1.00	0.00	Leukemia	2
Ethylene (as 5% ethylene oxide)	1.00	0.00	Leukemia	3
PAH (using Benzo[a] pyrene)	0.95	0.05	Lung Cancer	1
1,2,4-trimethylbenzene	1.00	0.00	Moderate anemia	14
Ammonia	1.00	0.00	skin and nose irritation	13
BTEX	0.64	0.36	CNS neurotoxicity	1
Cyclohexane	1.00	0.00	Reduced bodyweight	8
Diethanolamine	1.00	0.00	Throat irritation	8

Hydrogen sulphide	1.00	0.00	Nose irritation	11
Mercury	1.00	0.00	severe CNS neurotoxicity	6
MEK	1.00	0.00	developmental retardation	10
MIBK	1.00	0.00	developmental retardation	7
Naphthalene	1.00	0.00	Benign lung tumors	4
n-hexane	0.99	0.01	PNS neurotoxicity	3
Phenol	1.00	0.00	mild CNS neurotoxicity	5
Propylene	1.00	0.00	benign nasal & upper airway tumours	12
Sulphuric Acid	0.74	0.26	Benign nasal and upper airway tumors	2

17. Shell Sarnia

Substance	Proportion of predicted incidence below 10^{-6}	Proportion of predicted incidence above 10^{-6}	Relevant outcome (for reference)	Rank here (for validation comparison with other ranking output)
Benzene	0.95	0.05	Leukemia	2
Ethylene (as 5% ethylene oxide)	1.00	0.00	Leukemia	4
Nickel	0.43	0.57	Lung Cancer	1
PAH (using Benzo[a] pyrene)	0.95	0.05	Lung Cancer	3
1,2,4-trimethylbenzene	1.00	0.00	Moderate anemia	10
Ammonia	1.00	0.00	skin and nose irritation	6
BTEX	0.80	0.20	CNS neurotoxicity	3
Cyclohexane	1.00	0.00	Reduced bodyweight	7
Diethanolamine	1.00	0.00	Throat irritation	9
Hydrogen sulphide	0.99	0.01	Nose irritation	4
Mercury	1.00	0.00	severe CNS neurotoxicity	8
Methanol	1.00	0.00	physical teratogenesis	13
Naphthalene	1.00	0.00	Benign lung tumors	5
n-hexane	1.00	0.00	PNS neurotoxicity	12
Propylene	1.00	0.00	benign nasal & upper airway tumours	11
Sulphuric Acid	0.48	0.52	Benign nasal	1

			and upper airway tumors	
Vanadium	0.55	0.45	nasal and upper airway irritation	2

18. Shell Scotford

Substance	Proportion of predicted incidence below 10^{-6}	Proportion of predicted incidence above 10^{-6}	Relevant outcome (for reference)	Rank here (for validation comparison with other ranking output)
Benzene	1.00	0.00	Leukemia	2
Nickel	1.00	0.00	Lung Cancer	3
PAH (using Benzo[a] pyrene)	0.75	0.25	Lung Cancer	1
1,2,4-trimethylbenzene	1.00	0.00	Moderate anemia	7
Ammonia	1.00	0.00	skin and nose irritation	8
BTEX	0.64	0.36	CNS neurotoxicity	1
Cyclohexane	1.00	0.00	Reduced bodyweight	4
Hydrogen sulphide	1.00	0.00	Nose irritation	5
Mercury	1.00	0.00	severe CNS neurotoxicity	3
Naphthalene	1.00	0.00	Benign lung tumors	8
n-hexane	1.00	0.00	PNS neurotoxicity	2
Propylene	1.00	0.00	benign nasal & upper airway tumours	6

19. Sunoco

Substance	Proportion of predicted incidence below 10^{-6}	Proportion of predicted incidence above 10^{-6}	Relevant outcome (for reference)	Rank here (for validation comparison with other ranking output)
Benzene	0.95	0.05	Leukemia	3
PAH (using Benzo[a] pyrene)	0.93	0.07	Lung Cancer	1
Formaldehyde	0.94	0.06	nasal and lung cancer	2
1,2,4-trimethylbenzene	1.00	0.00	Moderate anemia	8
BTEX	0.80	0.20	CNS neurotoxicity	2
Cyclohexane	1.00	0.00	Reduced bodyweight	5
Hydrogen sulphide	1.00	0.00	Nose irritation	6

Naphthalene	1.00	0.00	Benign lung tumors	3
n-hexane	1.00	0.00	PNS neurotoxicity	4
Propylene	1.00	0.00	benign nasal & upper airway tumours	7
Sulphuric Acid	0.75	0.25	Benign nasal and upper airway tumors	1

20. Ultramar St. Romuald

Substance	Proportion of predicted incidence below 10^{-6}	Proportion of predicted incidence above 10^{-6}	Relevant outcome (for reference)	Rank here (for validation comparison with other ranking output)
Benzene	1.00	0.00	Leukemia	1
Ethylene (as 5% ethylene oxide)	1.00	0.00	Leukemia	3
PAH (using Benzo[a] pyrene)	1.00	0.00	Lung Cancer	2
1,2,4-trimethylbenzene	1.00	0.00	Moderate anemia	9
Ammonia	1.00	0.00	skin and nose irritation	7
BTEX	0.81	0.19	CNS neurotoxicity	1
Cyclohexane	1.00	0.00	Reduced bodyweight	6
Hydrogen sulphide	0.98	0.02	Nose irritation	3
Mercury	1.00	0.00	severe CNS neurotoxicity	5
Naphthalene	1.00	0.00	Benign lung tumors	10
n-hexane	1.00	0.00	PNS neurotoxicity	4
Propylene	1.00	0.00	benign nasal & upper airway tumours	7
Sulphuric Acid	0.87	0.13	Benign nasal and upper airway tumors	2

21. Hypothetical Worst-Case Refinery

Substance	Proportion of predicted incidence below 10^{-6}	Proportion of predicted incidence above 10^{-6}	Relevant outcome (for reference)	Rank here (for validation comparison with other ranking output)
1,3-Butadiene	0.97	0.03	Leukemia	6
Benzene	0.92	0.08	Leukemia	3
Ethylene (as 5% ethylene oxide)	0.97	0.03	Leukemia	5

Nickel	0.24	0.76	Lung Cancer	1
PAH (using Benzo[a] pyrene)	0.26	0.74	Lung Cancer	2
Formaldehyde	0.96	0.04	nasal and lung cancer	4
1,2,4-trimethylbenzene	0.99	0.01	Moderate anemia	7
Ammonia	1.00	0.00	skin and nose irritation	20
BTEX	0.64	0.36	CNS neurotoxicity	3
Cyclohexane	1.00	0.00	Reduced bodyweight	12
Dicyclopentadiene	1.00	0.00	chronic renal disease	17
Diethanolamine	1.00	0.00	Throat irritation	16
Hydrogen sulphide	0.94	0.06	Nose irritation	4
Isoprene	1.00	0.00	benign lung tumours	9
Mercury	1.00	0.00	severe CNS neurotoxicity	14
Methanol	1.00	0.00	physical teratogenesis	8
MEK	1.00	0.00	developmental retardation	13
MIBK	1.00	0.00	developmental retardation	10
MTBE	1.00	0.00	PNS neurotoxicity	11
Naphthalene	0.99	0.01	Benign lung tumors	6
n-hexane	0.98	0.02	PNS neurotoxicity	5
Phenol	1.00	0.00	mild CNS neurotoxicity	15
Propylene	1.00	0.00	benign nasal & upper airway tumours	19
Styrene	1.00	0.00	mild developmental retardation	18
Sulphuric Acid	0.57	0.43	Benign nasal and upper airway tumors	2
Vanadium	0.43	0.57	nasal and upper airway irritation	1
Zinc	1.00	0.00	Moderate anemia	21

Appendix J: Predicted Case Incidence and Rates for Class 3 Substances at Each of Canada's Refineries

Substance	**5th percentile**	**Mean**	**95th percentile**	**Mean (predicted) cases**
Refinery: Chevron Burnaby (population = 1 694 061)				
PM from SOx - Mortality	0.8	8.2	15.7	4.9E-06
Chronic bronchitis	1.5	15.4	29.3	9.2E-06
Asthma hospitalizations	0.1	1.0	1.8	5.7E-07
Asthma ER visits	0.2	1.7	3.3	1.0E-06
PM from NOx - Mortality	0.3	3.1	5.9	1.8E-06
Chronic bronchitis	0.6	5.7	10.8	3.4E-06
Asthma hospitalizations	0.0	0.4	0.7	2.3E-07
Asthma ER visits	0.1	0.6	1.1	3.6E-07
Primary PM - Mortality	0.2	2.1	3.9	1.2E-06
Chronic bronchitis	0.4	3.9	7.4	2.3E-06
Asthma hospitalizations	0.0	0.2	0.5	1.5E-07
Asthma ER visits	0.0	0.4	0.8	2.5E-07
Refinery: Consumer's Co-operative (population = 193 214)				
PM from SOx - Mortality	0.2	2.0	3.8	1.0E-05
Chronic bronchitis	0.4	4.0	7.6	2.1E-05
Asthma hospitalizations	0.0	0.2	0.4	1.2E-06
Asthma ER visits	0.0	0.4	0.7	2.0E-06
PM from NOx - Mortality	0.1	0.6	1.1	3.0E-06
Chronic bronchitis	0.1	1.1	2.1	5.7E-06
Asthma hospitalizations	0.0	0.1	0.1	3.9E-07
Asthma ER visits	0.0	0.1	0.2	6.1E-07
Primary PM - Mortality	0.0	0.3	0.5	1.3E-06
Chronic bronchitis	0.1	0.5	1.0	2.8E-06
Asthma hospitalizations	0.0	0.0	0.1	1.6E-07
Asthma ER visits	0.0	0.1	0.1	2.9E-07
Refinery: Husky Prince-George				
No emissions reported				
Refinery: Imperial-Dartmouth (population = 317 113)				
PM from SOx - Mortality	0.7	7.0	13.4	2.2E-05
Chronic bronchitis	1.3	13.3	25.2	4.2E-05
Asthma hospitalizations	0.1	0.9	1.7	2.8E-06
Asthma ER visits	0.1	1.5	2.8	4.6E-06
PM from NOx - Mortality	0.4	3.9	7.4	1.2E-05
Chronic bronchitis	0.8	8.1	15.4	2.6E-05
Asthma hospitalizations	0.0	0.4	0.9	1.4E-06
Asthma ER visits	0.1	0.7	1.4	2.3E-06
Primary PM - Mortality	0.3	2.6	5.0	8.3E-06
Chronic bronchitis	0.5	5.0	9.4	1.6E-05
Asthma hospitalizations	0.0	0.3	0.6	9.5E-07
Asthma ER visits	0.1	0.5	1.0	1.7E-06
Refinery: Imperial Nanticoke (population = 47 143)				
PM from SOx - Mortality	0.1	1.1	2.0	2.2E-05
Chronic bronchitis	0.2	2.0	3.7	4.1E-05
Asthma hospitalizations	0.0	0.1	0.2	2.5E-06
Asthma ER visits	0.0	0.2	0.4	4.3E-06

PM from NOx - Mortality	0.0	0.3	0.7	7.3E-06
Chronic bronchitis	0.1	0.7	1.4	1.5E-05
Asthma hospitalizations	0.0	0.0	0.1	8.0E-07
Asthma ER visits	0.0	0.1	0.1	1.4E-06
Primary PM - Mortality	0.01	0.13	0.25	2.8E-06
Chronic bronchitis	0.02	0.24	0.45	5.0E-06
Asthma hospitalizations	0.00	0.01	0.03	3.1E-07
Asthma ER visits	0.00	0.02	0.05	5.3E-07
Refinery: Imperial Sarnia (population = 98 730)				
PM from SOx - Mortality	1.0	10.1	19.2	1.0E-04
Chronic bronchitis	2.0	19.8	37.6	2.0E-04
Asthma hospitalizations	0.1	1.2	2.3	1.2E-05
Asthma ER visits	0.2	2.0	3.8	2.0E-05
PM from NOx - Mortality	0.1	1.1	2.1	1.1E-05
Chronic bronchitis	0.2	2.0	3.7	2.0E-05
Asthma hospitalizations	0.0	0.1	0.2	1.2E-06
Asthma ER visits	0.0	0.2	0.4	2.0E-06
Primary PM - Mortality	0.2	2.0	3.7	2.0E-05
Chronic bronchitis	0.4	3.6	6.9	3.7E-05
Asthma hospitalizations	0.0	0.2	0.4	2.2E-06
Asthma ER visits	0.0	0.4	0.8	4.2E-06
Refinery: Imperial Strathcona (population = 929 299)				
PM from SOx - Mortality	1.7	17.1	32.5	1.8E-05
Chronic bronchitis	3.2	32.4	61.5	3.5E-05
Asthma hospitalizations	0.2	1.9	3.6	2.0E-06
Asthma ER visits	0.3	3.4	6.5	3.7E-06
PM from NOx - Mortality	0.5	5.0	9.5	5.4E-06
Chronic bronchitis	1.0	9.6	18.3	1.0E-05
Asthma hospitalizations	0.1	0.5	1.0	5.9E-07
Asthma ER visits	0.1	1.0	1.9	1.1E-06
Primary PM - Mortality	0.5	4.8	9.2	5.2E-06
Chronic bronchitis	0.9	9.0	17.1	9.7E-06
Asthma hospitalizations	0.1	0.5	1.0	5.9E-07
Asthma ER visits	0.1	1.0	1.9	1.1E-06
Refinery: Irving Saint-John (population = 109 203)				
PM from SOx - Mortality	0.2	2.3	4.4	2.1E-05
Chronic bronchitis	0.4	4.4	8.3	4.0E-05
Asthma hospitalizations	0.0	0.3	0.6	2.7E-06
Asthma ER visits	0.0	0.4	0.8	4.0E-06
PM from NOx - Mortality	0.1	1.4	2.8	1.3E-05
Chronic bronchitis	0.3	2.8	5.3	2.6E-05
Asthma hospitalizations	0.0	0.2	0.3	1.5E-06
Asthma ER visits	0.0	0.3	0.5	2.6E-06
Primary PM - Mortality	0.08	0.81	1.54	7.4E-06
Chronic bronchitis	0.14	1.44	2.73	1.3E-05
Asthma hospitalizations	0.01	0.10	0.19	9.0E-07
Asthma ER visits	0.02	0.16	0.31	1.5E-06
Refinery: North Atlantic Come-by-Chance (population = 4710)				
PM from SOx - Mortality	0.0	0.3	0.6	7.2E-05
Chronic bronchitis	0.1	0.7	1.2	1.4E-04
Asthma hospitalizations	0.0	0.0	0.1	8.0E-06
Asthma ER visits	0.0	0.1	0.1	1.4E-05
PM from NOx - Mortality	0.0	0.0	0.1	6.0E-06

Chronic bronchitis	0.0	0.1	0.1	1.1E-05
Asthma hospitalizations	0.0	0.0	0.0	6.6E-07
Asthma ER visits	0.0	0.0	0.0	1.1E-06
Primary PM - Mortality	0.0	0.1	0.1	1.3E-05
Chronic bronchitis	0.0	0.1	0.2	2.4E-05
Asthma hospitalizations	0.0	0.0	0.0	1.4E-06
Asthma ER visits	0.0	0.0	0.0	2.3E-06
Refinery: NOVA Corunna (population = 102 094)				
No reported emissions				
Refinery: Parkland-Bowden (population = 25 933)				
Missing reported emissions				
Refinery: Petro-Canada Edmonton (population = 929 431)				
PM from SOx - Mortality	0.8	7.6	14.5	8.2E-06
Chronic bronchitis	1.4	14.5	27.5	1.6E-05
Asthma hospitalizations	0.1	0.9	1.8	1.0E-06
Asthma ER visits	0.1	1.5	2.8	1.6E-06
PM from NOx - Mortality	0.4	4.4	8.4	4.7E-06
Chronic bronchitis	0.8	7.9	15.0	8.5E-06
Asthma hospitalizations	0.0	0.5	0.9	5.1E-07
Asthma ER visits	0.1	0.9	1.7	9.4E-07
Primary PM - Mortality	0.2	2.4	4.5	2.5E-06
Chronic bronchitis	0.4	4.3	8.1	4.6E-06
Asthma hospitalizations	0.0	0.3	0.5	2.9E-07
Asthma ER visits	0.0	0.5	0.9	5.0E-07
Refinery: Petro-Canada Mississauga (population= 1 572 665)				
PM from SOx - Mortality	0.9	9.1	17.4	5.8E-06
Chronic bronchitis	1.8	18.1	34.3	1.1E-05
Asthma hospitalizations	0.1	1.1	2.1	7.0E-07
Asthma ER visits	0.2	1.7	3.2	1.1E-06
PM from NOx - Mortality	0.3	3.5	6.6	2.2E-06
Chronic bronchitis	0.7	6.8	12.9	4.3E-06
Asthma hospitalizations	0.0	0.4	0.8	2.8E-07
Asthma ER visits	0.1	0.7	1.3	4.4E-07
Primary PM - Mortality	0.2	2.1	3.9	1.3E-06
Chronic bronchitis	0.4	3.6	6.8	2.3E-06
Asthma hospitalizations	0.0	0.2	0.4	1.5E-07
Asthma ER visits	0.0	0.4	0.7	2.5E-07
Refinery: Petro-Canada Montreal (population = 2 560 328)				
PM from SOx - Mortality	3.6	35.5	67.5	1.4E-05
Chronic bronchitis	6.7	66.7	126.8	2.6E-05
Asthma hospitalizations	0.4	4.2	8.0	1.7E-06
Asthma ER visits	0.7	6.8	12.9	2.7E-06
PM from NOx - Mortality	1.1	10.9	20.7	4.3E-06
Chronic bronchitis	2.1	21.2	40.4	8.3E-06
Asthma hospitalizations	0.1	1.2	2.3	4.7E-07
Asthma ER visits	0.2	2.1	3.9	8.0E-07
Primary PM - Mortality	0.7	6.8	13.0	2.7E-06
Chronic bronchitis	1.3	13.0	24.8	5.1E-06
Asthma hospitalizations	0.1	0.8	1.5	3.1E-07
Asthma ER visits	0.1	1.4	2.6	5.3E-07
Refinery: Petro-Canada Oakville (population = 1 095 580)				
PM from SOx - Mortality	2.3	23.1	43.9	2.1E-05
Chronic bronchitis	4.2	42.3	80.5	3.9E-05

Asthma hospitalizations	0.3	3.0	5.7	2.7E-06
Asthma ER visits	0.5	5.0	9.5	4.6E-06
PM from NOx - Mortality	0.2	2.3	4.3	2.1E-06
Chronic bronchitis	0.4	4.2	7.9	3.8E-06
Asthma hospitalizations	0.0	0.3	0.5	2.5E-07
Asthma ER visits	0.0	0.5	0.9	4.1E-07
Primary PM - Mortality	0.4	4.3	8.2	3.9E-06
Chronic bronchitis	0.9	8.5	16.2	7.8E-06
Asthma hospitalizations	0.1	0.5	1.0	4.6E-07
Asthma ER visits	0.1	0.9	1.7	8.1E-07
Refinery: Shell Montreal (population = 2 612 269)				
PM from SOx - Mortality	8.7	86.7	164.7	3.3E-05
Chronic bronchitis	16.1	160.9	305.6	6.2E-05
Asthma hospitalizations	1.1	11.3	21.4	4.3E-06
Asthma ER visits	1.6	16.5	31.3	6.3E-06
PM from NOx - Mortality	2.5	24.7	46.9	9.4E-06
Chronic bronchitis	4.5	44.7	85.0	1.7E-05
Asthma hospitalizations	0.3	2.6	5.0	1.0E-06
Asthma ER visits	0.4	4.4	8.4	1.7E-06
Primary PM - Mortality	1.5	14.8	28.2	5.7E-06
Chronic bronchitis	2.5	25.2	47.8	9.6E-06
Asthma hospitalizations	0.2	1.5	2.9	5.8E-07
Asthma ER visits	0.3	2.6	4.9	9.9E-07
Refinery: Shell Sarnia (population = 96 725)				
PM from SOx - Mortality	0.6	5.7	10.9	5.9E-05
Chronic bronchitis	1.1	10.8	20.5	1.1E-04
Asthma hospitalizations	0.1	0.7	1.3	7.0E-06
Asthma ER visits	0.1	1.1	2.1	1.1E-05
PM from NOx - Mortality	0.1	0.6	1.2	6.4E-06
Chronic bronchitis	0.1	1.2	2.2	1.2E-05
Asthma hospitalizations	0.0	0.1	0.1	7.1E-07
Asthma ER visits	0.0	0.1	0.2	1.2E-06
Primary PM - Mortality	0.1	1.3	2.4	1.3E-05
Chronic bronchitis	0.2	2.2	4.2	2.3E-05
Asthma hospitalizations	0.0	0.1	0.3	1.4E-06
Asthma ER visits	0.0	0.2	0.4	2.4E-06
Refinery: Shell Scotford (population = 31 231)				
PM from SOx - Mortality	0.0	0.0	0.1	8.8E-07
Chronic bronchitis	0.0	0.0	0.1	1.6E-06
Asthma hospitalizations	0.0	0.0	0.0	1.2E-07
Asthma ER visits	0.0	0.0	0.0	1.8E-07
PM from NOx - Mortality	0.0	0.1	0.2	2.5E-06
Chronic bronchitis	0.0	0.2	0.3	5.0E-06
Asthma hospitalizations	0.0	0.0	0.0	3.1E-07
Asthma ER visits	0.0	0.0	0.0	5.5E-07
Primary PM - Mortality	0.0	0.0	0.0	3.1E-07
Chronic bronchitis	0.0	0.0	0.0	5.5E-07
Asthma hospitalizations	0.0	0.0	0.0	4.0E-08
Asthma ER visits	0.0	0.0	0.0	6.2E-08
Refinery: Sunoco Sarnia (population = 96 977)				
PM from SOx - Mortality	0.1	1.1	2.0	1.1E-05
Chronic bronchitis	0.2	2.0	3.8	2.1E-05
Asthma hospitalizations	0.0	0.1	0.2	1.3E-06

Asthma ER visits	0.0	0.2	0.4	2.3E-06
PM from NOx - Mortality	0.0	0.4	0.7	3.7E-06
Chronic bronchitis	0.1	0.7	1.3	7.2E-06
Asthma hospitalizations	0.0	0.0	0.1	4.2E-07
Asthma ER visits	0.0	0.1	0.2	8.2E-07
Primary PM - Mortality	0.0	0.5	0.9	4.9E-06
Chronic bronchitis	0.1	0.9	1.7	9.5E-06
Asthma hospitalizations	0.0	0.1	0.1	5.2E-07
Asthma ER visits	0.0	0.1	0.2	8.8E-07
Refinery: Ultramar St. Romuald (population = 631 211)				
PM from SOx - Mortality	1.1	10.7	20.3	1.7E-05
Chronic bronchitis	1.9	18.7	35.5	3.0E-05
Asthma hospitalizations	0.1	1.2	2.2	1.9E-06
Asthma ER visits	0.2	1.9	3.7	3.1E-06
PM from NOx - Mortality	0.4	3.7	6.9	5.8E-06
Chronic bronchitis	0.7	7.3	13.9	1.2E-05
Asthma hospitalizations	0.0	0.4	0.8	6.3E-07
Asthma ER visits	0.1	0.7	1.4	1.1E-06
Primary PM - Mortality	0.2	1.8	3.4	2.9E-06
Chronic bronchitis	0.3	3.4	6.5	5.4E-06
Asthma hospitalizations	0.0	0.2	0.4	3.3E-07
Asthma ER visits	0.0	0.3	0.7	5.4E-07
Refinery: Hypothetical Worst-Case (population = 2 612 269)				
PM from SOx - Mortality	34.9	348.9	662.9	1.3E-04
Chronic bronchitis	71.0	709.5	1348.1	2.7E-04
Asthma hospitalizations	3.8	37.8	71.8	1.4E-05
Asthma ER visits	6.5	64.7	123.0	2.5E-05
PM from NOx - Mortality	3.3	33.3	63.3	1.3E-05
Chronic bronchitis	6.5	64.5	122.6	2.5E-05
Asthma hospitalizations	0.4	3.8	7.2	1.5E-06
Asthma ER visits	0.6	6.5	12.3	2.5E-06
Primary PM - Mortality	2.8	28.0	53.1	1.1E-05
Chronic bronchitis	5.4	53.9	102.4	2.1E-05
Asthma hospitalizations	0.3	3.2	6.2	1.2E-06
Asthma ER visits	0.6	5.5	10.5	2.1E-06

Glossary

ADI	Acceptable Daily Intake
ATSDR	Agency for Toxic Substances and Disease Registry
BTEX	Benzene, Toluene, Ethylbenzene and Xylene
CAC	Criteria Air Contaminants
CalEPA	California Environmental Protection Agency
CB	Crystal Ball^{TM}
CCME	Canadian Council for Ministers of the Environment
CDF	Cumulative Distribution Function
CEPA	Canadian Environmental Protection Act
CPPI	Canadian Petroleum Producers Institute
CNS	Central Nervous System
C-R	Concentration-Response Parameter
CWS	Canada-Wide Standards
DALY	Disability Adjusted Life Years
DALYp	DALYs per person
ED05	Estimated Dose Affecting 5% of the Population
GIS	Geographic Information System
GSD	Geometric Standard Deviation
HEAST	Health Effects Assessment Summary Tables
HEIDI	Health Effects Indicators Decision Index
HPS	Health Prioritization Subgroup
IARC	International Agency for Research on Cancer
ILSI	International Life Science Institute
IRIS	Integrated Risk Information System
IUPAC	International Union of Pure and Applied Chemistry
k	Rate Constant for Reaction with OH (substance-specific)
LCA	Life Cycle Analysis
LCIA	Life Cycle Impact Analysis
LHS	Latin Hypercube Sampling
LOAEL	Lowest Observed Adverse Effect Level
MEK	Methyl Ethyl Ketone
MIBK	Methyl iso-butyl Ketone
MTBE	Methyl tert-butyl Ether

NAPS	National Air Pollutant Survey (Network)
NERAM	Network for Environmental Risk Assessment and Management
NFPRER	National Framework for Petroleum Refinery Emissions Reductions
NIST	National Institute of Science and Technology
NOAEL	No-Observed Adverse Effects Level
NPRI	National Pollutant Release Inventory
OH	Ambient Concentration of OH
PAH	Polycyclic Aromatic Hydrocarbons
PDF	Probability Density Function
PM	Particulate Matter
PSL	Priority Substances List
RfC	Reference Concentration
SETAC	Society of Environmental Toxicology and Chemistry
SR	Sensitivity Ratio
TC05	Tolerable Concentration Affecting 5% of the Population
TERA	Toxicology Excellence for Risk Assessment
TRACI	Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts
USEPA	United States Environmental Protection Agency
WTP	Willingness to Pay
YLD	Years of Life Disabled
YLL	Years of Life Lost