A Novel Back-Off Algorithm for the Integration Between Dynamic Optimization and Scheduling of Batch Processes Under Uncertainty

by

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A thesis
presented to the University of Waterloo
in fulfillment of the
thesis requirement for the degree of
Master of Applied Science
in
Chemical Engineering

Waterloo, Ontario, Canada, 2019

Author's Declaration

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.

Statement of Contributions

The content in Chapter 3 of this thesis has been published to Industrial & Engineering Chemistry Research (I&EC) Journal on November 22, 2019. Valdez-Navarro YI, Ricardez-Sandoval LA. A Novel Back-off Algorithm for Integration of Scheduling and Control of Batch Processes under Uncertainty. Ind Eng Chem Res. November 2019:acs.iecr.9b04963. doi:10.1021/acs.iecr.9b04963. That manuscript was written entirely by myself, and was edited by my supervisor, Luis Ricardez-Sandoval. Adapted with permission from Industrial & Engineering Chemistry Research. Copyright 2019, American Chemical Society.

The work in Chapter 4 of this thesis has been partially presented at the 12th IFAC Symposium on Dynamics and Control of Process Systems, including Biosystems (DYCOPS-CAB,2019). Valdez-Navarro YI, Ricardez-Sandoval LA. Integration between Dynamic Optimization and Scheduling of Batch Processes under Uncertainty: A Back-off Approach. 12th IFAC Symp Dyn Control Process Syst Incl Biosyst. 2019;52(1):1-6. doi:10.1016/j.ifacol.2019.06.137. That article was written entirely by myself, and was edited by my supervisor, Luis Ricardez-Sandoval. Permission to use the content for a thesis is granted according to IFAC's Copyright Transfer and Conditions (© 2019, IFAC)

Abstract

Smarter manufacturing decisions need to be made in order to meet the increasing demand of specialty products. Batch processes are ideal in this context, as their flexibility is an attractive property to meet changing market conditions. Scheduling and control are key in the enterprise wide optimization problem, their connection links decisions that occur at the management and production level. This motivates a rethinking of the sequential-based decision making, commonly found in operations management. An integrated decision approach has been shown to provide better quality solutions. Integrated methods are generally casted as mixed-integer dynamic optimization problems (MIDO), which may become computationally intractable for large-scale applications. Moreover, the presence of uncertainty can cause deviation from nominal plant operation. Efforts from the process systems engineering (PSE) community aim to tackle this challenging problem; however, there is still a gap in the literature for integrated methods between the scheduling and control that account for parameter uncertainty.

A novel decomposition algorithm for the integration of scheduling and control of multiproduct, multiunit batch processes under stochastic parameter uncertainty is presented in this thesis. This iterative algorithm solves a scheduling and dynamic optimization problem around a nominal point while approximating uncertainty through back-off terms, embedded in the process constraints. Monte Carlo simulations are performed to propagate uncertainty and to evaluate dynamic feasibility; statistical information is drawn from these simulations to update the back-off terms. Convergence of the algorithm results in a set of scheduling and control decisions that aim to keep the plant dynamically feasible under the effect of uncertainty up to a user-defined tolerance criterion. The performance of the back-off approach is gauged against a fully-integrated approach, with multiscenario-based uncertainty. This integrated method serves as a benchmark, both in solution quality and computational efficiency. Results show that the proposed decomposition algorithm remains computationally attractive, without compromising the quality of the solution. Important interactions between scheduling, control and uncertainty are observed, thus justifying the need for their integration.

Acknowledgments

First, I would like to deeply thank my supervisor, Prof. Luis Ricardez-Sandoval, who supported me with his insightful ideas, his patience and guidance through my Master's degree. And most importantly, the genuine interest he shows everyone in this research group by giving time to every concern that we have, however minute they may be.

I would like to extend my thanks to my Thesis committee, Professor Budman and Professor Erenay. I am grateful for the financial support CONACYT provided, which without it, the opportunity for a Master's degree would not have happened.

To every member of our research group, a sincere thank you is needed for the fun experiences we've had together.

To everyone in my family, who have always unconditionally given me support when I most needed it. Finally, to the love of my life and wife, Cathy, a thesis-long acknowledgement would be needed to express my gratitude for the time we've spent together, thanks.

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List of Acronyms

CHR	Convex hull relaxation
DAE	Differential-algebraic equations
GDP	Generalized disjunctive programming
MC	Monte-Carlo
MIDO	Mixed-integer dynamic optimization
MILP	Mixed integer linear programming
MINLP	Mixed Integer non-linear programming
MLDO	Mixed logic dynamic optimization
NLP	Non-linear programming
PSE	Process systems engineering
STN	State-task-network

List of symbols

Indexes

i	Back-off algorithm master outer-loop index
j	Task index
k	Unit index
l	Mechanistic unit model index
m	Equality constraint index
n	Back-off algorithm inner-loop index
p	Inequality constraint index
s	Material state index
t	Time index
μ	Tray index
γ	Product index
ν	Unit-specific stochastic parameter index
φ	Multi-scenario uncertain parameters combination index

Sets

$\boldsymbol{g_{crit}}$	Matrix storing simulation information
$\boldsymbol{J}$	Set of total tasks
$\boldsymbol{J_k}$	Set of tasks that can be performed in a unit
$\boldsymbol{K_j}$	Set of units that can perform a task
$\boldsymbol{K}$	Set of total units
$\boldsymbol{S}$	Set of total states
$\boldsymbol{S_D}$	Set of scheduling decisions
$\boldsymbol{S_j}$	Set of states that feed into a task
$\boldsymbol{\bar{S}_j}$	Set of states produced by a task
$\boldsymbol{T_s}$	Set of tasks consuming a material state
$\boldsymbol{\bar{T}_s}$	Set of tasks producing a material state
$\boldsymbol{\Delta}$	Set of scenarios
$\boldsymbol{\Theta_{nom}}$	Set of deterministic parameters
$\boldsymbol{\Theta_{unc}}$	Set of uncertain parameters
$\boldsymbol{\Theta^{k,\varphi}}$	Unit specific multi-scenario uncertain parameter combination

$\boldsymbol{\Theta}$	Set of deterministic and uncertain parameters

Variables

$b_{p,t,i}$	Back-off term for constraint *p* at time *t* for iteration *i*
$\boldsymbol{B_{j,k,t}}$	Batch size variable for task *j* performed in unit *k* at time *t*
$\boldsymbol{C_A}$	Concentration of species A
$\boldsymbol{C_B}$	Concentration of species B
$\boldsymbol{C_C}$	Concentration of species C
$\boldsymbol{D}$	Extraction flow variable
$\boldsymbol{D_{tot_\gamma}}$	Total accumulated distillate for product $\boldsymbol{\gamma}$
$\boldsymbol{F}$	Processing costs
$\boldsymbol{f^l}$	Vector of mechanistic unit models of size *l*
$\boldsymbol{g^p}$	Vector of inequality constraints of size *p*
$\boldsymbol{h^m}$	Vector of equality constraints of size *m*
$\boldsymbol{L}$	Returning flow variable
$\boldsymbol{Q}$	Reboiler material variable
$\boldsymbol{R}$	Reflux ratio
$\boldsymbol{Sch_{eq}}$	Vector of additional scheduling equality constraints
$\boldsymbol{Sch_{ineq}}$	Vector of additional scheduling inequality constraints
$S_{s,t}$	Material variable for state *s* at time *t*
$\boldsymbol{u}$	Control trajectory profiles
$\boldsymbol{V}$	Vapor flow
$W_{j,k,t}$	Binary assignment variable for task *j* performed in unit *k* at time *t*
$Y_{k,j,t}$	Boolean logical disjunctive indicator variable
$\boldsymbol{x}$	Model state variables
$\dot{\boldsymbol{x}}$	Model state variables' derivatives
$\boldsymbol{x}_\mu$	Liquid concentration in a tray
$\boldsymbol{x_Q}$	Concentration of species B in reboiler
$\boldsymbol{x_d}$	Concentration of species B in distillate
$\boldsymbol{\bar{x}_{d_\gamma}}$	Product purity variable
$\boldsymbol{y}_\mu$	Vapor concentration in a tray
$\boldsymbol{z}$	Objective function

$\boldsymbol{z_{dyn}}$	Objective function of dynamic optimization problem
$\boldsymbol{z_{sched}}$	Objective function of scheduling problem
$\boldsymbol{\rho_{in}}$	Proportion of material input
$\boldsymbol{\rho_{out}}$	Proportion of material output
$\boldsymbol{\Psi}$	Overall net cost function

Parameters

${B_{j,k}}^{max}$	Upper limit on batch size
${B_{j,k}}^{min}$	Lower limit on batch size
H	Scheduling makespan
MC	Total number of Monte Carlo simulations
N_L	Total number of mechanistic unit equations
N_P	Total number of inequality constraints
N_{ctrl}	Total number of control variables
Φ_k	Total number of parameter realizations for a given unit
N_k	Total number of uncertain parameters for a unit
N_m	Total number of equality constraints
N_{nom}	Total number of deterministic parameters
N_{scn}	Total number of scenarios
N_{st}	Total number of model states
N_{unc}	Total number of uncertain parameters
$PDF_{k,\nu}$	Probability density function for an uncertain parameter
p_d	Column price factor
p_f	Filter unit price factor
p_r	Reactor unit price factor
$T_{op_0}^{j}$	Task initiation indicator
$T_{op_f}^{j}$	Task completion indicator
Tol	Back-off algorithm convergence tolerance
u_{max}	Upper bound on control variables
u_{min}	Lower bound on control variables
${\bar{x}_d}^*{}_{\gamma}$	Product purity set-point
α	Relative volatility

β	Kinetic reaction parameter
$\theta^{k,\nu}$	Unit-specific stochastic uncertain parameter
$\theta_n^{k,\nu}$	Random realization of a stochastic uncertain parameter
λ	Back-off term multiplier
ν	Unit-specific stochastic parameter index
τ_j	Task fulfilment time
$\tau_{j,s}$	Processing time for task output to a state
φ	Multi-scenario uncertain parameters combination index
ω_δ	Weight of scenario
$\mathbf{\Omega}$	Stochastic event space

Chapter 1: Introduction

As global competitiveness increases, industries are driven to meet increasingly restrictive constraints, such as product quality, environmental, or productivity restrictions. When facing a highly volatile and uncertain market, industries seek to operate under robust, optimal manufacturing conditions. For this purpose, batch processes are typically used in conditions where varying product properties and manufacturing flexibility is required[1]. Optimization is then performed to improve the overall efficiency and revenue of the plant while assuring a set of process constraints are met. It has been shown that there are extensive benefits to consider model-based optimization of chemical production plants, such as an overall increase in profitability or more attractive operative decisions.

Traditionally, the layers in enterprise-wide optimization (*i.e.* supply chain management, production planning, scheduling, control, process dynamics, and design) have been considered separately, i.e. a set of sequential problems are solved one after the other. However, it has been shown that this approach although computationally attractive, may result in suboptimal or even infeasible solutions, as it ignores important interactions co-dependent between layers[2]. Consequently, the process systems engineering (PSE) community has focused on the development of solution approaches, which can be categorized into integrated and decomposition algorithms, providing high-quality solutions by considering key linking variables between the different layers. The merit of considering reliable first principles models for flexibility and resilience of a process was discussed in Morari and Grossmann[3]. In that work, case-studies where common rules of thumb for the design of chemical plants fail to provide attractive solutions have been presented. Particularly for the case of large-scale plants, it is not always intuitive the identification of the worst-case condition for operation, which may highly depend on design considerations and would also affect upper manufacturing layers such as scheduling and planning decisions. Therefore, it is of interest to consider comprehensive approaches that combine process control and optimization decisions to identify optimal and controllable design and operation management policies for chemical processes[4] The general idea in the integrated approach is to formulate a single comprehensive model, where decisions encompass multiple layers, regardless of their complexity. A decomposition-based approach seeks to identify complicating variables so as to effectively generate master and primal problems, with the goal of reducing the computational burden of the algorithm [5].

Despite the advances in computer science, obtaining a computationally tractable, globally optimal solution to the integrated problem of large-scale multi-unit, multi-product batch plants is still an open challenge, as it often requires the specification of nonconvex mixed-integer dynamic optimization (MIDO) formulations[6]. As a result, studies that seek to address the integration problem seek to optimize only for a particular combination of the manufacturing layers. A review of the state-of-the-art techniques are presented in several papers [7–9].

In addition of the beforementioned challenges, many of the methods proposed in the literature assume process model parameters to be deterministic in nature; however, this assumption does not hold when considering a real process, as uncertainty has been shown to have important effects on process operation. This is even more stressed when considering the existence of substantial interactions between layers; therefore uncertainty may propagate between them, turning a previously obtained optimal production sequence into a sub-optimal or infeasible operation[10]. Efficient robust methods must, therefore, be developed in order to incorporate uncertainty on the already computationally taxing integrated methods.

Notable contributions that seek to fill that purpose are presented, particularly in the area of integration of design and control [11–13]. A review of challenges in this field are presented in several papers [4,11,14]. However, there is still a gap in the literature regarding integrated methods for scheduling and control when considering model uncertainty. Scheduling and control are key aspects to consider in the enterprise wide optimization problem, their importance stems from the fact that their connection links decisions that occur at the management and production level. Consequently, this thesis develops two distinct methods for considering scheduling and control decisions, the multi-scenario integrated approach and the back-off method, which are expanded upon on the following chapters.

1.1 Research Objectives

The aim of this study is to expand upon the literature by presenting a novel back-off decomposition methodology for the integration of scheduling and control of multi-unit, multi-product batch plants, subject to the effects of stochastic-based process uncertainty.

This thesis explores two different approaches for optimization under uncertainty, an integrated multi-scenario-based approach and a new decomposition-based back-off method. The multi-scenario approach, optimizes an integrated scheduling and control problem for a discrete number of scenarios, so that all realizations considered are accommodated by the solution. The back-off method has the purpose of converging to a robust solution by iteratively solving a decomposition of the scheduling and control problems, stochastic simulations are performed to generate back-off terms. These back-off terms are incorporated into the process operational constraints to approximate the effect of fully stochastic uncertain model parameters.

The novelty of this work is that the proposed back-off algorithm avoids the solution of a computationally expensive stochastic Mixed Logic Dynamic Optimization (MLDO) problem by decomposing scheduling and control decisions. The quality of the obtained solution is validated against a fully integrated problem. The presented methods consider the full non-linear dynamic models, along with parameter uncertainty. Multiple distributions in the uncertain parameters and their effects on the solution were explored in this research. To the authors' knowledge, this is the first study that presents a back-off decomposition algorithm for scheduling and control of batch plants. Previously published works on batch plant scheduling and open-loop optimization have rarely considered stochastic-based parameter uncertainty.

A novel feature of the current work is that the proposed decomposition method is to be compared against a fully integrated problem, obtained from a large scale multi-scenario-based MLDO formulation. The expected contribution is to provide an algorithm capable of obtaining a computationally tractable solution, while retaining its quality. Both, the proposed back-off and fully integrated methods are to be tested on a multi-product, multi-unit batch plant, subject to operational constraints and model parameter uncertainty.

1.2 Structure of Thesis

This thesis is organized into the following chapters:

Chapter 2: This chapter presents a general review of the current state of the art in the integration of scheduling and control, highlighting the different approaches, their advantages, disadvantages and areas for research interest. This latter section emphasizes the contributions made by the presented study. A special focus is placed on methods that incorporate process uncertainty into their optimization framework. Introductory concepts to process scheduling, dynamic optimization and Generalized Disjunctive Programming are also presented in this chapter for completeness.

Chapter 3: In order to gauge the performance of the decomposition algorithm, a simultaneous based approach for the integration of scheduling and control of batch plants is presented. The conceptual definition of a general scheduling and control problem under stochastic uncertainty is presented, outlining limitations and challenges involved with obtaining a globally optimal solution of the problem. Subsequently, the conceptual formulation of the multi-scenario-based optimization problem is described. The content in this chapter has been published to Industrial & Engineering Chemistry Research (I&EC) Journal[15].

Chapter 4: In this section, the back-off decomposition algorithm is presented. The conceptual formulation is explained and a general flowchart of the algorithm is presented, highlighting the definition of the linking variables, assumptions, and characteristics for convergence. This work has been partially presented at the 12th IFAC Symposium on Dynamics and Control of Process Systems, including Biosystems (DYCOPS-CAB,2019)[16].

Chapter 5: This chapter presents the case study and results used to assess the performance of the methods covered in this thesis. A detailed overview of the batch plant is provided. Moreover, this section will discuss in length computational performance of the methods, interaction between scheduling and control decisions and the effects of uncertainty upon them. For illustrative purposes both global and local solvers are implemented for the solution of the resulting optimization problems.

Chapter 6: This section summarizes the key outcomes obtained from the present study and suggest future improvements that can be explored for the present methodology. Furthermore, possible research opportunities in the area of integrated plant operations are provided.

Chapter 2: Literature Review

As mentioned in the previous chapter, methodologies that seek to integrate model-based optimization with scheduling are of high interest to the PSE community due to their benefits upon performance. As such, this chapter presents the current state-of-the-art approaches to accomplish that goal. Furthermore, special emphasis is given to those methods that have incorporated uncertainty into the problem, as it has been shown that their effects have a significant impact upon the performance of chemical manufacturing plants.

The difficulty in determining optimal scheduling and control decisions for a process can vary greatly depending on the approach that is followed. Two common methods (*i.e.* sequential method and the integrated method) are explained in this section, and the contributions of relevant works are summarized.

A focus on studies that have considered a multi-scenario and stochastic based approaches to the uncertainty is given, highlighting their differences, benefits and limitations for their application to the integration of scheduling and control. With this information, the scope of the presented study and its contribution to the literature is exemplified.

2.1 Enterprise Wide Optimization

Uncertain market conditions, continuous process improvement, consideration of environmental constraints and a significant increase in competition are some of the justifications that have pushed the industries and the PSE community to develop novel robust methods that meet the increasingly restrictive constraints upon operations. In consequence, the combined efforts of industries and academia aim to solve the beforementioned challenges through the development of Enterprise Wide Optimization, providing software and computational tools that can serve as means for the maximization of process profitability, responsiveness to demands and optimal assignation of assets[17].

Enterprise-wide optimization combines the knowledge from PSE and operations research. The main purpose of it is to obtain a set of decisions that result in optimal operations in a company. A key major feature of enterprise-wide optimization is the emphasis on maintaining the full non-linear models for the description of the mechanistic manufacturing layers (*i.e.* control/dynamic optimization and the processes)[1]. As shown in Figure 1, the classic top-to-bottom decision-making hierarchy consists of six decision layers, i.e. supply chain management, planning, scheduling, control/real time optimization and the process [14].

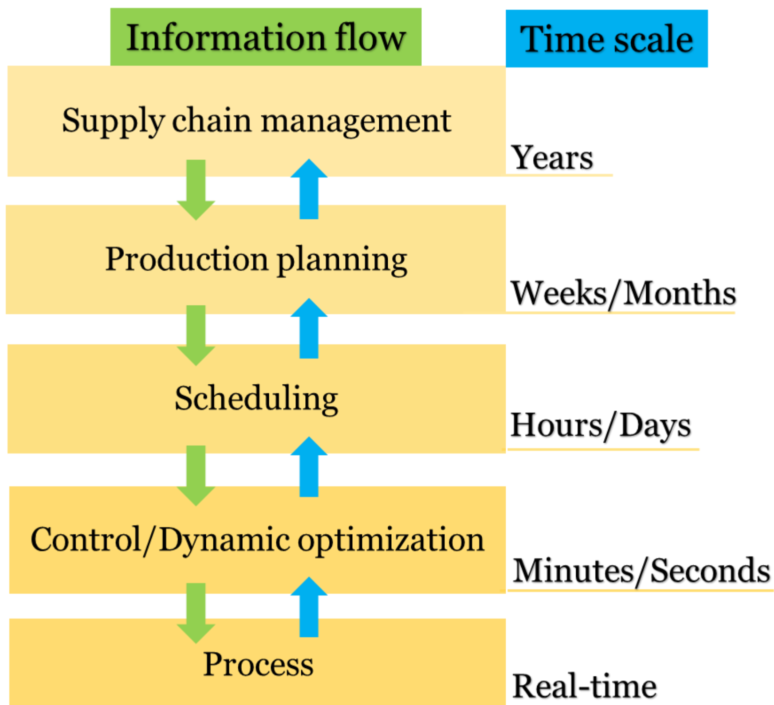

Figure 1: Layers in decision hierarchy in EWO

As shown in Figure 1, typically information flow goes top-to-bottom, while the time scale and frequency of the decisions increase accordingly[18]. At the top, supply chain management, planning and scheduling are long-term decisions. The two layers at the bottom can be considered as short-term decisions.

A brief explanation of the production layers is expanded upon in this section, as defined by Shobrys and White[19].

- Supply chain management define desired changes to the current overall business. Typical decisions found in this layer might relate to contracts, selection of raw material providers, production and distribution capacity. The extension of this layer may encompass global or nation-wide markets.
- Planning is used to create distribution, sales and inventory plans based on customer and market information, thereby setting a target for operating performance. This layer encompasses individual sites, however, industries with multiple manufacturing plants can incorporate regional planning to coordinate activities.
- Scheduling assigns limited resources (process units, materials, utilities, etc.) in a given production facility to create manufacturing sequences for products based on a demand. Typical decisions made in this layer are the time an operation should be initialized, its duration, the equipment which will process said operation and its corresponding amount of material.
- Control/Dynamic optimization involves the manipulation of state variables to reject a form of process disturbances and to meet key manufacturing and product constraints while ensuring that those decisions do not violate the set bounds on the manipulated variables. It may be responsible for keeping an economic production through the determination of optimal operating set-points.
- The process itself is governed by mechanistic models, which are formulated by initially making educated assumptions on the properties of the system in question. The result is the formulation of highly detailed physical and mathematical models to replicate the dynamic behavior of the real phenomenon.

2.2 Sequential vs Integrated Approach

Traditionally, the layers in enterprise-wide optimization have been considered separately, such that a sequential problem is solved for each layer, one after the other. Although this approach is computationally attractive, it has been shown that it may result in suboptimal or even infeasible solutions, as it ignores important interactions co-dependent between layers [2]. Consequently, the PSE community has focused on the development of integrated solution approaches that can provide high-quality solutions by considering key linking variables between the different layers[2,9,14]. The basic idea in the integrated approach is to formulate a single comprehensive model, where decisions encompass multiple layers, regardless of their complexity. Decisions made at each one of these levels differ in terms of time horizon, complexity and objectives. Significant efforts have been done to develop methods that seek to integrate multiple decision layers, recognizing the inherent interconnectivity between them [18,20]. Accordingly, different methodologies can be categorized into two main solution approaches to the complex integrated problem: a simultaneous, fully integrated approach and a decomposition-based approach.

Advantages of the simultaneous decision-approach include the avoidance of infeasibilities or sub-optimal solutions by solving a sparse system. However, a challenge attributed to this methodology comes from addressing the differing time scales of the different models considered in the integrated problem. This previous consideration results in highly complex large-scale optimization problem, which may become computationally intractable[18]. On the other hand, decomposition-based approaches are often developed with the purpose to address the previous challenges. Generally, these methods aim to identify key complicating variables, exploiting certain problem properties to effectively generate a master and primal optimization problem. The purpose is to reduce the computational effort of solving a complex integrated problem without compromising on solution quality[21].

Despite these efforts, obtaining a computationally tractable, globally optimal solution to the integrated problem of large-scale multi-unit, multi-product batch plants is currently an open challenge, as it often requires the specification of nonconvex mixed-integer dynamic optimization (MIDO) formulations [6,22–24]. As a result, studies that aim to address the integration problem seek to optimize only for a particular combination of the manufacturing layers. More recently however, contributions have been made toward the consideration of multiple layers, mainly design, scheduling and control [25–28] or planning, scheduling and control [29–31]. The integration of planning, scheduling, and control results in complex large-scale MINLPs. Due to this complexity, direct solution methods by out-of-the-box MINLP solvers are time-consuming and intractable for large-scale applications[30]. Obtaining solutions to tackle such problems typically require the specification of key linking variables, such that a decomposition framework can be implemented[31]. A recent contribution which presents a comprehensive review of state-of-the-art integrative techniques is presented by Burnak et al.[20], additional assessment of different integration methods are presented elsewhere [7–9,20,32,33].

2.3 Scheduling

In this thesis, the main focus of the decision-making hierarchy is given to scheduling and dynamic optimization. For that end, a brief, introductory explanation to process scheduling is provided.

Scheduling is an important class of optimization problem in the PSE community. In general, they are formulated to determine when, where and how to produce a set of given products subject to particular constraints, such as a make-span or time horizon, consideration of limited resources, capacity or specific manufacturing sequences[34]. Scheduling problems can generally be considered combinatorial in nature due to the discrete decisions involved (i.e. assignment and allocation constraints); hence, they may be challenging from the computational complexity point of view[35]. For this reason, the need to develop efficient solution methods is apparent. Significant efforts have been done to accomplish this goal[35–37].

Scheduling models for the representation of a chemical production plant can have multiple structures. Common classifications include, but are not limited to: time-representation and process-representation [36]. Each of these categories can have significant effects on both computational performance and solution quality of the schedules. In this section, a brief review on important concepts and solution approaches developed for optimal process scheduling is presented.

2.3.1 Time Representation

Time representation is a key classification used to describe a scheduling model. There exist two main categories for approaching the discretization of time in a scheduling formulation, they are the discrete and continuous time representations.

The discrete time representation partitions the scheduling horizon into a known and equidistant number of periods, defining a common time grid for all variables and constraints that may be encountered in a scheduling problem, *i.e.* assignation of tasks/equipment material balance constraints, etc. The start or end of an event can occur only on a period as determined by the discretization. Moreover, processing times are assumed to be constant and generally, are integer multiples of the unit slot duration [35,38] . An important feature of the discrete-time representation is its ease of modeling and interoperability. Moreover, a very fine discretization allows for a high degree of flexibility in the quality solutions. However, a small discretization in turn will require larger number of variables, resulting in larger problem, which may become intractable for large-scale applications or minute discretization periods[38].

The second representation is referred to as the continuous time approach, which as its name implies, introduces a time grid where events (scheduling decisions) can occur at arbitrary time points in a given horizon. The scheduling horizon is then partitioned into periods of unequal and unknown length and tasks can have variable processing times. Often, the continuous time representation requires fewer grid discretizations when compared to the discrete time approach. Continuous-time representation can be further classified into global grid, which adopt a unique time grid for all processes[35] and unit-specific time representation, which considers multiple asynchronized time grids for every unit, allowing different tasks to start at different moments in different units for the same event point[39]. Since the timing and duration of events is not defined *a priori* a smaller optimization problem may result, owing to the fact that no fine discretization is required. Therefore, accurate processing times can be obtained without increasing the size of the problem. However, this formulation may become more challenging to model, leading to a complicated model structure when compared against a discrete-time formulation[35,38], particularly for large-scale applications. Although efforts have been made to extend algorithms for their application to large-scale scheduling of industrial plants[34,40–43].

As per the discussion above, each representation has their own advantages and disadvantages. It is noted that in reality their computational performances are highly problem dependent. Although industry practitioners seem to have mainly adopted the practical discrete-time representation[38,44].

2.3.2 Process Representation

The second method for representing scheduling models is through process representation. In this case, the methods can be divided into two categories[45]:

- Sequential processes: Where multiple products are manufactured using one processing sequence. For this type of process, it is not necessary to consider mass balances explicitly.
- Network processes: This corresponds to a more general case where materials can merge and/or split; therefore, mass balance constraints are required. Two well-known formulations are expanded upon on the section below.
    - State-Task Network (STN): Originally formulated by Kondili et al.[46] as a general framework for representing processes. The STN of a chemical plant can be visualized as a graph with two types of connecting nodes; circles, which represent state nodes (*i.e.* materials, intermediates or products). Rectangles, which represent task nodes (*i.e.* equipment operations). The fraction of a state consumed or produced by a task, if not equal to one, is given beside the arch linking the corresponding state and task nodes.
    - Resource-Task Network (RTN): Originally formulated by Pantelides[47] as an extension to STN. The main feature is that equipment, storage, material and utilities are represented in a unified fashion, and are denominated as resources that can be consumed by tasks.

An in-depth discussion on computational performance of both representations, advantages and disadvantages can be found elsewhere[45,48].

2.4 Dynamic Optimization

Dynamic optimization problems arise in many areas of PSE such as batch plant optimization, optimal grade transition, optimal process control and parameter estimation. It can be defined as an optimization problem, which requires the solution of a system whose behavior is dictated by a set of differential-algebraic-equations, usually in the domain of space or time. These types of systems usually require the definition of an initial value or boundary value problem. The algebraic equations are typically derived from mechanistic equations, where the degrees of freedom available to the system are control and time-independent variables.

The solution of these dynamic optimization problems is formally explored by applying concepts from optimal control theory, however this is only viable for relatively simple problems, for larger more complex systems efficient numerical methods are required. For the purpose of this thesis, the direct transcription approach is preferred. This numerical approach deals with the full discretization of state equations and control paths. A common discretization method is orthogonal collocation on finite elements, a method that has attractive properties, such as, a numerically stable behavior on stiff problems (A-stable) and can handle non-smooth events the boundaries between elements. The resulting discretized set of equations and constraints may be solved with a commercial NLP solver. Extended information on convergence properties, stability and how to exploit the resulting structure of the large NLP problem for good quality and efficient solution may be found elsewhere[49].

2.5 Integration of Scheduling & Control

A traditional approach to solve the problem of scheduling and control is to consider them separately. However, it has been shown there exists key linking variables that interconnect information between the scheduling and control layer. In consequence, to obtain an economically and operationally attractive solution one must consider this problem in an integrated fashion [50]. Consequently, a single optimization formulation that can solve the beforementioned problem simultaneously is desirable. A number of major advantages of the integrated approach are noted by Engell and Harjunkoski[14].

- Reduce maintenance needs and improve equipment life-time.
- Improve the feasibility of schedules for operation.
- Exploit the degrees of freedom of control in plant designs.
- Use more precise and timely information in scheduling.

Although the integrated approach is attractive for the quality of the obtained solution, it has been shown that methods which implement this approach found difficulties on the computational cost[22]. This is mainly because a fully integrated simultaneous approach requires the specification of a sparse MIDO problem[23,51]. Complexities appear with the combination of integer scheduling decisions with highly non-linear dynamic models. A trend is then to develop decomposition based-approaches to improve performance. Nystrom et al.[52] originally proposed an iterative method to solve the integrated problem, sharing key information between layers; Terrazas- Moreno et al.[53] presented a Lagrangean-based decomposition approach for the integration of scheduling and control. Solution to this problem was obtained by iterating between a primal control problem and a master scheduling problem More recently, Generalized Benders Decomposition algorithms were explored by Yisu et al.[54] and Chu and You[5], effectively lowering computational time while maintaining solution quality. Recent state-of-the-art approaches focus on the development of surrogate[55] and multi-parametric[26,56] approaches for the solution of the integrated problem. A recent study by Simkoff and Baldea[57] solved the integrated problem through a novel implementation of complementarity constraints, fully incorporating control decisions into the scheduling model.

Integrated methodologies for scheduling and control were originally applied to case studies that dealt with optimal grade transition of continuous processes. For instance, Nystrom et al.[52] proposed a decoupling method for polymerization processes and parallel polymerization lines with multiple units[58]. Flores-Tlacuahuac and Grossmann [51,59] tested their approach on cyclic productions with CSTR and PFR reactors; Terrazas-Moreno et al.[60] solved the integration of cyclic scheduling and control of two polymerization systems. Zhuge and Ierapetritou[61] explore two case studies, a CSTR and an isothermal tubular reactor when considering closed loop control. The development of integrated methods for scheduling and control were mainly applied to continuous processes, rather than batch processes. This is mainly due to modelling and solution complexities[54].

As stated earlier, a key objective of the integrated method is to be flexible to changing market conditions and customer requirements. Consequently, dynamic batch processing provides additional transient operating freedom, that can stretch the limits of profitability under strict market, facility, and time constraints[62]. Hence, batch processes are typically used in conditions where changing product properties and manufacturing flexibility is required[63]. In addition, batch processes are able to handle unpredictable events from external markets. For the reasons discussed above, this thesis will focus on the development of methods for the integration of scheduling and control of multi-purpose batch plants.

Among the first contributions to this area of research was the work by Bhatia and Biegler[62], which considered the effect of incorporating the non-linear process models to enrich a special formulation of a scheduling problem. That study showcased the merit of considering the optimization of batch plants. Mishra et al.[22] performed a comparison between a fully integrated and a recipe-based approach, which considered fixed control decisions. That study highlighted the merit of considering a fully integrated simultaneous approach, but also outlines the challenges of solving a complex MINLP.

Subsequently progress in this area is observed in the works by Nie et al.[54,64] and Chu and You[21], which showcase a trend for the development of tailored decomposition-based algorithms to solve the complex integrated problem. A study by Capón-García et al.[65] considers full process dynamics, comparing a nominal indirect and direct approach for a multiproduct single stage batch plant. More recently, Zhuge and Ierapetritou[66] developed a method for integration of scheduling and control of batch processes, through the consideration of a multi-parametric scheme, showcasing the potential of the method for on-line applications.

2.6 Model Parameter Uncertainty

In addition of the challenges mentioned above, many of the methods proposed in the literature assume perfect knowledge of the process model parameters; however, this assumption does not hold when considering a real process, as uncertainty has been shown to have important effects on process operation.

This is even more stressed when considering the existence of substantial interactions between layers; thus uncertainty may propagate between them, turning a previously obtained optimal production sequences into sub-optimal or infeasible solutions when implemented online [10]. Therefore, there is a need to develop efficient robust methods that incorporate uncertainty on the already computationally taxing integrated methods. Also, scheduling and control approaches that deal with uncertain process operations and

Table 1: Overview of integration of scheduling and control, for both continuous and batch processes when considering deterministic and uncertain realizations in the model parameters

Plant type	**Approach**	**Author(s)**
Continuous	Without uncertainty	Zhuge and Ierapetritou [50,67], Baldea et al. [8,57], Dias et al.[99], Flores-Tlacuahuac and Grossman[51,59,100]
	With uncertainty	Dias and Ierapetritou[18], Zhuge and Ierapetritou[101], Terrazas-Moreno et al.[102], Burnak et al.[103]
Batch	Without uncertainty	Mishra et al. [22], Bhatia and Biegler [62], Nie and Biegler[64,104], Chu and You[21,68,105], Capón-García [65]
	With uncertainty	Bhatia and Biegler[73], Chu and You[5]

disturbances in real-time have been reported in the literature[29,30,67,68]. Other notable contributions that seek to incorporate uncertainty have been presented, particularly in the area of integration of design and control under uncertainty [12,69–72]. However, there is still a gap in the literature regarding integrated methods for scheduling and control of batch processes when considering model parameter uncertainty, as indicated in

.

An early work on the consideration of model parameter uncertainty for the solution of scheduling and control of batch plant was provided by Bhatia and Biegler [73], who formulated a dynamic optimization problem, where an economic objective function was subject to a dynamic high-fidelity model of the process described by differential algebraic system of equations. Those authors proposed a solution strategy based on discretizing the process model by orthogonal collocation over finite elements. Chu & You [5] presented a two-stage Generalized Benders Decomposition algorithm for considering uncertainty in the scheduling of sequential batch plants. This thesis has the goal of filling the gap in the literature by considering the effect of fully-stochastic uncertain parameters on scheduling and control decisions.

The multi-scenario approach considers multiple different realizations of the process disturbance or parameter uncertainty in the optimization problem. A simple implementation of the multi-scenario approach considers every scenario simultaneously. The work by Chu and You[5] solved the integrated problem with the goal to maximize the overall profit on average over all possible scenarios under discrete realizations in the uncertain parameters. It is considered that as the number of realizations grow, the problem becomes increasingly difficult to solve.

The second method developed in this thesis, the back-off method, is discussed next. The concept of the back-off framework was originally proposed and expanded upon by Perkins and co-workers[74–77]. Our research group has recently developed different implementations of the back-off method for the purpose of design and control under uncertainty[69,78]. The key idea in the back-off approach is to move away in a systematic, iterative fashion from a nominal operating point, which has the properties of being economically attractive but dynamically infeasible in the presence of uncertainty. Convergence of the algorithm results in a set of decisions that most surely remain dynamically feasible in the presence of stochastic uncertainty. The work proposed by Koller & Ricardez-Sandoval [27] successfully implemented the back-off method for design, scheduling and control of continuous multi-purpose production units. A single unit involving the production of multiple products was used in that work to illustrate the main features of their back-off method. This research expands upon that work to consider the simultaneous scheduling and control of multiple units subject to stochastic realizations in the uncertain parameters.

2.7 Generalized Disjunctive Programing

A recent method for consideration of scheduling and control decisions simultaneously is a logical based reformulation of the problem. For this reason, a general overview of Generalized Disjunctive Programming (GDP) is presented next.

The precursor to GDP was presented in a previous study by Balas[79] where they presented a series of linear programming problems that define disjunctions, which are a type of constraints that allow a logical exclusive OR decisions to be performed, meaning that from a given set of constraints only a certain subset may be enforced. Raman and Grossmann[80] expanded upon that work by generalizing the solution algorithm of mixed-integer type problems when considering logical disjunctions and prepositions. Several case studies were considered in that study, including a job-shop scheduling formulation. A comprehensive formulation was presented in a study by Grossmann and Ruiz[81]. The framework is named Generalized disjunctive programming and allows for the representation of a mixture of logical or algebraic constraints. Boolean and continuous type variables may be specified, such that the resulting problem can have MINLP characteristics. GDPs are often reformulated by using either the Big-M or the Convex Hull relaxations, Grossmann and Ruiz[81] compare the quality, size and tightness of the resulting continuous reformulations. In a work by Trespalacios and Grossmann[82], an alternative formulation to the Big-M relaxation was presented. The method assigns more than one big-M term to each constraint involved in their respective disjunction thus resulting in a tighter relaxation. Generally, algorithms employed to solve the resulting MINLP problem assume the function to be convex in nature. A solution algorithm for nonconvex GDP problems was explored by Lee and Grossmann[83], where a lower bound for a global optimum solution may be found initially with the solution from a local optimizer. Recently, Ruiz and Grossmann[84] presented a review for the challenge of finding a global optimal solution to highly non-convex disjunctive formulations.

Some of the efforts by the PSE community to solve the integrated problem by considering logical disjunctions have been presented. A study that developed a general framework for the consideration of disjunctive decisions was presented by Oldenburg and Marquardt[85], addressing the modeling and optimal control of hybrid systems that can be described by systems of ordinary differential equations (ODEs). Flores-Tlacuahuac and Biegler[86] presented a MIDO problem for the integration of design and control. Issues such as computational efficiency, quality and different solution characteristics from different GDP formulations were explored in that study. A work by Nie and Biegler[64] presented a formulation that considers operating modes for an equipment as logical disjunctions, solving an integrated scheduling and control problem for multi-purpose batch plants.

2.8 Chapter Summary

In this chapter a comprehensive review of the literature is provided. A common approach to enterprise-wide optimization is the sequential approach, while this method is computationally attractive, it ignores important interactions between the production layer. This consideration may result in sub-optimal or even infeasible solutions. Thus, there is a trend towards implementing an integrated approach to process optimization. This results in much more attractive solutions, with increased plant profitability and optimal operation. However, this method typically results in the definition of a large scale MINLP, which are complex to solve. For this purpose, studies have been focused on the development of decomposition-based approaches. Moreover, a more realistic approach is to consider the effects of uncertainty, which is shown to have significant effect on the optimality of a solution. To that end, different methods have been developed to account for model parameter uncertainty. Often, stochastic uncertain parameter descriptions are not considered in previous publications due to their associated computational challenges. Instead, a small number of discrete realizations in the uncertain parameters have been considered in previous studies leading to the formulation of multi-scenario-based optimization frameworks. A gap in the literature is then noted, in the area of integration of scheduling and control of batch processes under stochastic-based uncertainty. To the author's knowledge, the combination of these aspects has not been previously addressed. This thesis serves the purpose of filling that gap in the literature, by presenting a novel back-off approach which is gauged in performance against an integrated method.

Chapter 3: Multi-Scenario Integrated Approach

In this section, fully integrated scheduling and dynamic optimization algorithm for multi-product, multi-unit batch processes is presented, based upon the methodology originally proposed by Nie & Biegler[64]. An expansion upon that work is presented by accounting for interactions when considering multi-scenario-based model parameter uncertainty. The main purpose of this method is to use it as a benchmark for the decomposition back-off approach, both in computational efficiency and solution quality.

3.1 General Scheduling & Control Formulation under Uncertainty

The mathematical conceptual formulation of the optimization problem that considers the integration of scheduling and control under the effects of stochastic-based parameter uncertainty is presented in this section. The following considerations have been made to define the scope of the integration of scheduling and control problem addressed in this work.

Consider a multi-product, multi-unit batch plant described by a total of N_L mechanistic unit models ($\boldsymbol{f^l}$), N_m equality ($\boldsymbol{h^m}$) and N_P inequality constraints ($\boldsymbol{g^p}$) affected by a set ($\boldsymbol{\Theta}$), which includes deterministic parameters known *a priori* ($\boldsymbol{\Theta_{nom}} \in \mathbb{R}^{1\times N_{nom}}$) and stochastic-based uncertain parameters ($\boldsymbol{\Theta_{unc}} \in \mathbb{R}^{1\times N_{unc}}$). Each parameter $\boldsymbol{\theta^{k,v}}$ in $\boldsymbol{\Theta_{unc}}$ is described by a user-defined probability density function (PDF) over an event space $\boldsymbol{\Omega}$, *i.e.* $\boldsymbol{\Theta_{unc}} = \left\{\boldsymbol{\theta^{k,v}} \middle| \boldsymbol{\theta^{k,v}} = \boldsymbol{PDF_{k,v}}(\boldsymbol{\Omega}),\ \forall k \in \boldsymbol{K}, v \in 1,2 \dots, N_k\right\}$, where $\boldsymbol{K}$ is the set of units comprising the batch plant and N_k is the total number of uncertain parameters considered for unit k. The plant is assumed to operate within a fixed makespan (H), fixed task processing times, no pre-emptive operation, instant material transfer and unlimited intermediate storage. The aim is to seek for a set of scheduling decisions ($\boldsymbol{S_D}$) and optimal control trajectory profiles ($\boldsymbol{u}$), which result in the assignment of tasks, batch sizes and operating cost for each unit, such that an objective function *($\boldsymbol{z}$)* is optimized (e.g. maximization of profits) and constraints maintain dynamic operability in the presence of stochastic realizations in the uncertain parameters. This problem can be conceptually formulated as follows:

$$\max_{\{\boldsymbol{u},\boldsymbol{S_D}\}} \boldsymbol{z}(\boldsymbol{x}(t), \dot{\boldsymbol{x}}(t), \boldsymbol{u}(t), \boldsymbol{\Theta}, \boldsymbol{S_D}) \tag{1}$$

$s.t.$

$$\boldsymbol{f^l}(\boldsymbol{x}(t), \dot{\boldsymbol{x}}(t), \boldsymbol{u}(t), \boldsymbol{\Theta}, \boldsymbol{S_D}) = 0; \qquad \forall t, l \in 1,2 \dots, N_L$$

$$\boldsymbol{g^p}(\boldsymbol{x}(t), \dot{\boldsymbol{x}}(t), \boldsymbol{u}(t), \boldsymbol{\Theta}, \boldsymbol{S_D}) <= 0; \quad \forall t, p \in 1,2 \dots, N_P$$

$$\boldsymbol{h^m}(\boldsymbol{x}(t), \dot{\boldsymbol{x}}(t), \boldsymbol{u}(t), \boldsymbol{\Theta}, \boldsymbol{S_D}) = 0; \qquad \forall t, m \in 1,2 \dots, N_m$$

$$u_{min} \leq \boldsymbol{u}(t) \leq u_{max}; \qquad \forall t$$

$$\boldsymbol{\Theta} = \{\Theta_{nom}, \Theta_{unc}\}$$

$$\boldsymbol{t} \in [0, H]$$

where $\boldsymbol{x(t)} \in \mathbb{R}^{1\times N_{st}}$ represent the system's states and their derivatives $\dot{\boldsymbol{x}}\boldsymbol{(t)} \in \mathbb{R}^{1\times N_{st}}$, where N_{st} is the total number of model states; control variables $\boldsymbol{u(t)} \in \mathbb{R}^{1\times N_{ctrl}}$ and N_{ctrl} is the total amount of control inputs available for each unit; $\boldsymbol{S_D}$ is a set of decisions that results in a production schedule, *e.g.* assignment variables, operational costs or batch sizes. Problem (1) is challenging to solve, i.e. to ensure dynamic feasibility, an infinitely dimensional search space in a continuous time domain would need to be explored, resulting from treating uncertain process parameters as randomly distributed variables. This problem can be casted as a stochastic MIDO, which may be reformulated as a stochastic Mixed Integer Non-Linear Programming (MINLP) problem by discretizing the time domain[49]. Problem complexity still remains since dynamic and integer dependent decisions have to be determined over a discretized time horizon for every possible realization of the uncertain parameters.

In this study, two methods are presented which circumvent the complications arising with problem (1). The first algorithm, explored in this chapter, aims to solve a fully integrated MINLP, but relaxes the assumption of stochastic-based representation of the uncertain model parameters by proposing multi-scenario-based descriptions for the uncertain parameters. The second algorithm, explored in the next chapter, decomposes the problem by searching for scheduling and control decisions in an iterative fashion thus avoiding the need to solve an expensive MINLP. A key feature of the later approach is the consideration of back-off terms, which are used to approximate process variability due to the effect of stochastic realizations in the uncertain parameters. The goal of the proposed back-off algorithm is to search for a set of scheduling and control decisions that most surely remain dynamically feasible in the presence of stochastic-based uncertainty.

3.2 Multi-Scenario Approach: Problem Definition

For the challenges mentioned in the previous section, the original consideration of stochastic-based uncertainty is reconsidered. In its stead, a multi-scenario-based representation is adopted to solve the fully integrated problem, this section will expand upon the definition, assumptions and characteristics of the subsequent approach.

The State-Task-Network representation (STN), adopted from Kondili, et al.[46] and Shah et al.[87] is considered to describe a multi-unit multi-product batch plant. STN is considered here due to its wide applicability for solving scheduling problems in chemical batch plants. This formulation, in combination with task-dependent disjunctive decisions, enable detailed scheduling and dynamic optimization modeling of flowshop batch plants, *i.e.*

$$\max_{\{\boldsymbol{u},\boldsymbol{S_D}\}}/\min \ \boldsymbol{z}(\boldsymbol{x}(t),\dot{\boldsymbol{x}}(t),\boldsymbol{u}(t),\boldsymbol{\Theta},\boldsymbol{S_D},\omega_\delta) \tag{2a}$$

$s.t.$

$$\sum_{j\in J_k}\sum_{t'=t}^{t-\tau_j+1} W_{j,k,t'} \leq 1 \qquad \forall k,t \tag{2b}$$

$$W_{j,k,t}{B_{j,k}}^{min} \leq B_{j,k,t} \leq W_{j,k,t}{B_{j,k}}^{max} \qquad \forall j,k \in K_j,t \tag{2c}$$

$$S_{s,t} = S_{s,t-1} + \sum_{j\in \bar{T}_s}\sum_{\delta\in\Delta}\omega_\delta {\rho_{out}}_{j,s,t,\delta}\sum_{k\in K_j} B_{j,k,t-\tau_{j,s}} - \sum_{j\in T_s}\sum_{\delta\in\Delta}\omega_\delta\, {\rho_{in}}_{j,s,t,\delta}\sum_{k\in K_j} B_{j,k,t} \quad \forall s,t \tag{2d}$$

$$\boldsymbol{Sch_{eq}}(\boldsymbol{x}(t),\dot{\boldsymbol{x}}(t),\boldsymbol{u}(t),\boldsymbol{\Theta},\boldsymbol{S_D}) = 0 \tag{2e}$$

$$\boldsymbol{Sch_{ineq}}(\boldsymbol{x}(t),\dot{\boldsymbol{x}}(t),\boldsymbol{u}(t),\boldsymbol{\Theta},\boldsymbol{S_D}) \leq 0 \tag{2f}$$

$$\begin{bmatrix} Y_{j,k,t} = True \\ W_{j,k,t} = 1 \\ h^{m}_{k,j,\delta}\left(x_{j,k,t,\delta}(\tau^{j}), \dot{x}_{j,k,t,\delta}(\tau^{j}), u_{j,k,t}(\tau^{j}), \Theta, S_D\right) = 0 \ \forall m, \delta \in \Delta \\ g^{p}_{k,j,\delta}\left(x_{j,k,t,\delta}(\tau^{j}), \dot{x}_{j,k,t,\delta}(\tau^{j}), u_{j,k,t}(\tau^{j}), \Theta, S_D\right) \leq 0 \ \forall p, \delta \in \Delta \\ u_{min} \leq u_{k,j,t}(\tau^{j}) \leq u_{max} \\ \rho_{in_{j,s,t,\delta}}\left(x_{j,k,t,\delta}(\tau^{j}), \dot{x}_{j,k,t,\delta}(\tau^{j}), u_{j,k,t}(\tau^{j}), \Theta\right) \forall s \in S_j, \delta \in \Delta \\ \rho_{out_{j,s,t,\delta}}\left(x_{j,k,t,\delta}(\tau^{j}), \dot{x}_{j,k,t,\delta}(\tau^{j}), u_{j,k,t}(\tau^{j}), \Theta\right) \forall s \in \bar{S}_j, \delta \in \Delta \\ F_{k,t,\delta} = F_{j,k,t,\delta}\left(u_{j,k,t}, \tau^{j}, B_{j,k,t}, x_{j,k,t,\delta}\left(T^{j}_{op_f}\right)\right) \ \forall \delta \in \Delta \end{bmatrix} \bigvee \begin{bmatrix} Y_{j,k,t} = False \\ W_{j,k,t} = 0 \\ \rho_{in_{j,s,t,\delta}} = 0 \ \forall s \in S_j, \delta \in \Delta \\ \rho_{out_{j,s,t,\delta}} = 0 \ \forall s \in \bar{S}_j, \delta \in \Delta \\ F_{k,t,\delta} = 0 \ \forall \delta \in \Delta \end{bmatrix}$$

$$\forall t, j \in \boldsymbol{J_k}, k \in \boldsymbol{K} \qquad (2g)$$

$$t \in [0, H],\ \boldsymbol{\Delta} = \{\delta_1, \delta_2 \ldots \delta_{N_{scn}}\}, \boldsymbol{\Theta} = \{\Theta_{nom}, \Theta_{unc}\},\ Y_{j,k,t} \in \{True, False\},\ \tau^{j} \in \left[T^{j}_{op_0}, T^{j}_{op_f}\right] \ \forall j \in J \qquad (2h)$$

Equation (2a) states the objective function of the integrated formulation; that is, the optimization of a function dependent on mechanistic states (x), its derivatives ($\dot{x}$), control actions (u), model parameters (Θ) and scheduling decisions, which include assignment variables, batch sizes and production costs ($\boldsymbol{S_D} = \{W_{j,k,t}, B_{j,k,t}, F_{k,t,\delta}\}$). Relevant sets are denoted as $\boldsymbol{K}$ (available units), $\boldsymbol{J_k}$ (tasks that can be performed in unit *k*), $\boldsymbol{K_j}$ (units capable of performing task *j*), $\boldsymbol{\bar{T}_s}$ (tasks producing *s*), $\boldsymbol{T_s}$(tasks consuming *s*) and $\boldsymbol{\Delta}$ (total scenarios). The time required to produce material *s* from task *j* is assumed fixed and denoted as $\tau_{j,s}$. Note that task fulfilment time is defined as τ^{j}, and is composed of two indicators, a task initiation ($T^{j}_{op_0}$) and completion time ($T^{j}_{op_f}$).

3.3 Unified Time-Grid

The multi-scenario integrated algorithm seeks to tie the scheduling model with the process dynamics, with the aim to perform simultaneous scheduling and control. A time grid that showcases the main structure of the proposed integrated approach is shown in Figure 2.

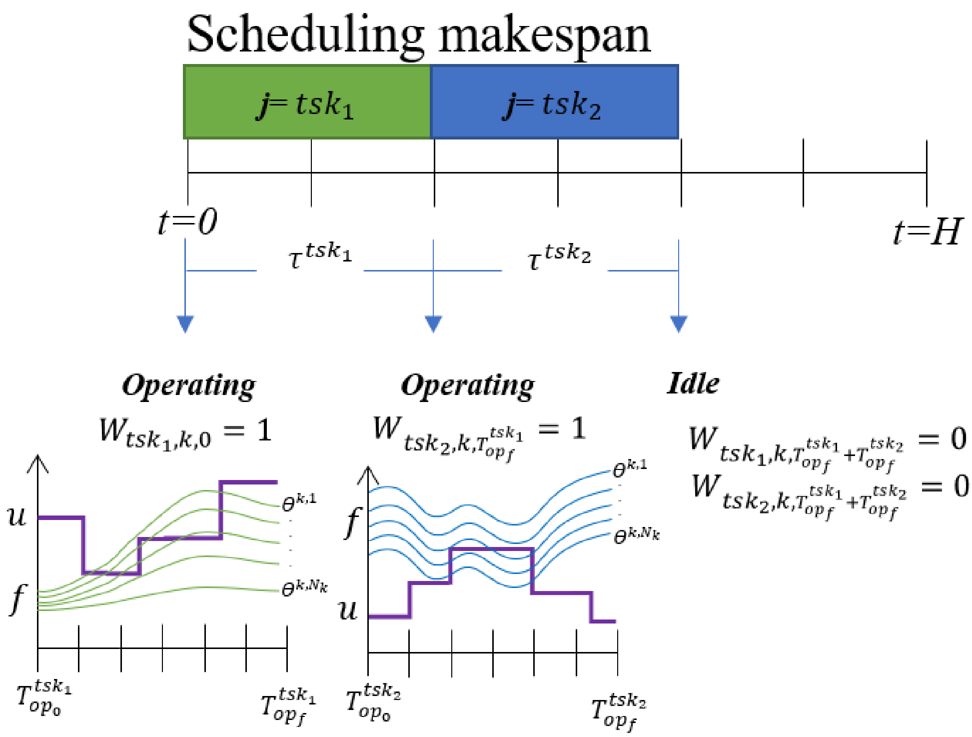

Figure 2: Visual representation of the multi-scenario integrated algorithm.

As shown in problem (2), the production makespan is discretized ($t \in [0, H]$) following the STN framework. Scheduling decisions can be performed at each t discretization of the horizon. Assignment constraints (Equation 2b) are related to the binary variable $W_{j,k,t}$ to assign an operating state ($W_{j,k,t} = 1$) or idle state ($W_{j,k,t} = 0$); specifically, $W_{j,k,t}$ determines that, at any point in time t, an equipment k can only operate a single task j for the duration of τ^j. Capacity constraints (Equation 2c) limit the batch size $B_{j,k,t}$ within a given bound if an equipment is operating a certain task. The material balance constraint (Equation 2d) describes the net change in material $S_{s,t}$ at any time t for every state s. Material balance for any state is dictated by their proportion of material input ($\rho_{in_{j,s,t,\delta}}$) for each state which feed task j ($\boldsymbol{S_j}$) and output ($\rho_{out_{j,s,t,\delta}}$) for each state which task j produces ($\boldsymbol{\bar{S}_j}$). A weight ω_δ is considered for every effect of scenario δ in $\boldsymbol{\Delta}$, such that the sum of all weights is equal to the unity. Equations (2e-f) include additional equality and inequality constraints that may be considered for a scheduling framework, such as non-preemptive operation, product demands, state capacity, etc.

3.4 Task-Dependent Disjunctive Decisions

Moreover, at each t discretization, an exclusive task and unit-dependent logical disjunctive decision is performed, as shown in Equation (2g). The latter aims to engage the non-linear dynamic equations with the multi-period scheduling constraints. These logical selective decisions typically found in Generalized Disjunctive Programming (GDP) are posed by implementing different relaxation methods [81]. Therefore, a GDP modeling strategy is followed to recast the optimization problem into a logic-based model, offering a robust modeling method for cases where exclusive constraints have to be enforced. This means that task and unit assignment can be simultaneously considered by the scheduling and dynamic constraints.

In the embedded dynamic optimization problem, mechanistic process models are affected by the selection of the scheduling tasks, *e.g.* manufacture products A, B or C. The relationship between scheduling and process dynamics are reflected as a possible variation of product and task-specific operational constraints or model parameters. This co-dependence justifies the reason for the integration of transient mechanistic unit models and scheduling. As described earlier, the STN formulation regards different operating configurations as alternating tasks that may be assigned to a unit, as shown in Figure 2. Therefore, the total logical disjunctions of a unit comprise the different tasks (dynamics) that the unit may perform; this information is described in the set $\boldsymbol{J_k}$, such that, a unit will have as much disjunctions as elements in $\boldsymbol{J_k}$. If the disjunction indicator variable is active (*i.e.* $Y_{j,k,t} = True$), an operating state is considered, thus the mechanistic task-dependent process equations and constraints (i.e. $h^m_{j,k,\delta}$ and $g^p_{j,k,\delta}$) are enforced. Control trajectories $u_{j,k,t}$ are obtained while maintaining the control variable within pre-specified bounds. Moreover, proportion of material input and output are calculated based on initial and final conditions, respectively. Operating cost ($F_{k,t,\delta}$) is a key variable in the formulation that depends on control profiles, operating time of the current active equipment performing a given task τ^j, batch size $B_{j,k,t}$, or ending conditions of mechanistic state variables $x_{j,k,t,\delta}\left(T^j_{op_f}\right)$.

An additional disjunct is considered to account for equipment idling (*i.e.* $Y_{j,k,t} = False$). In this idle state, no dynamic equations are enforced to describe the behavior of the unit, and all of the variables relevant for the integration, such as process costs, proportion of material production and consumption, are set to zero.

Moreover, dynamic time discretization has to be selected, as a means to correctly incorporate the scheduling time slots, with the reformulated time-dependent equations. For the purpose of generalization, discretization can easily accommodate different schemes, *i.e.* finite differences or finite elements schemes.

3.5 Multi-Scenario Uncertainty

Problem (2) considers a multi-scenario approach to handle process parameter uncertainty. That is, process variables and constraints, sensitive to uncertainty, are evaluated for every scenario $\boldsymbol{\delta}$, exploring a total of N_{scn} scenarios. The definition of a scenario is presented in Figure 3.

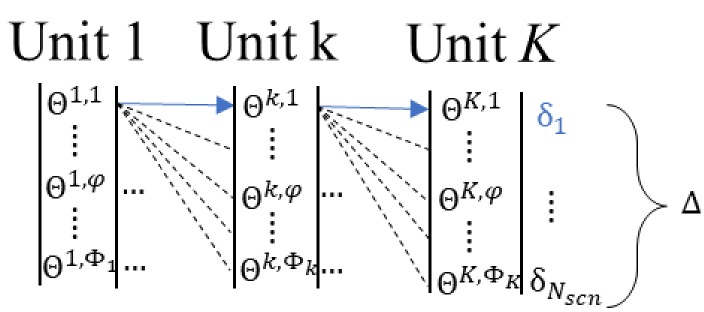

Figure 3:Illustrative definition of a scenario, for simplicity, connections to consequent realizations of uncertainty are represented by three dots.

A limitation of the integrated approach is that, due to computational limits, it is unable to represent fully stochastic model parameters. For this reason and for better representation of the analysis, the original formulation presented in problem (1) is modified, instead of a PDF, each uncertain parameter is now composed by a combination of different discrete realizations, *i.e.* $\boldsymbol{\Theta^{k,\varphi}} = \{\theta^{k,1}, \theta^{k,2}, \ldots \theta^{k,N_k}\}$, $\forall k \in \boldsymbol{K}, \varphi \in 1,2 \ldots, \Phi_k$, where Φ_k is the total number of uncertain parameter realizations considered for a unit.

Each unit k may be affected by a certain number of uncertain parameters (N_k), each of these parameters and their different combinations ($\boldsymbol{\Theta^{k,\varphi}}$), will generate different trajectories for the mechanistic states $x_{j,k,t,\delta}$, and therefore different realizations on variables and constraints sensitive to uncertainty ($i.e. h, g, \rho_{in}, \rho_{out}, F$). Thus, for every combination of uncertain realizations considered, a single control trajectory for each unit needs to be obtained which meets the enforced constraints.

Propagation of uncertainty is considered to be non-preemptive, meaning that control decisions for each unit considers the cumulative effects of uncertainty up to that unit itself. This can be exemplified with Figure 3; consider unit 1, a unique control trajectory is determined for the net effects of all the realizations in the uncertain parameters, i.e. $\boldsymbol{\Theta}^{1,1}$ to $\boldsymbol{\Theta}^{1,\Phi_1}$. In consequence, to find a control profile for unit *k* several scenarios must be considered involving all the possible combinations in the realizations of the uncertain parameters from unit 1 up until unit k. As shown in Figure 3, scenario δ_1 for unit *k* considers the combined effects of $\boldsymbol{\Theta}^{1,1}$, $\boldsymbol{\Theta}^{k-1,1}$ up until $\boldsymbol{\Theta}^{k,1}$. Hence, scenario $\boldsymbol{\delta_1}$ for unit *K* would then need to consider the cumulative effects of all previous uncertainty realizations (i.e. $\boldsymbol{\Theta}^{1,1}$, $\boldsymbol{\Theta}^{K-1,1}$ up until $\boldsymbol{\Theta}^{K,1}$). This implies the problem grows exponentially as more units and uncertain parameters are considered.

3.6 Model Convergence

The integrated problem generally contains non-convex terms from the dynamic and disjunctive models. The existence of non-convexities can be time-consuming in converging to a solution of a highly-dimensional MINLP problem. In this study, locally optimal solutions identified by local solvers are accepted, within reasonable CPU times. However, the decomposition method can take advantage of the problem structure to reduce the overall computational time (see Chapter 6).

In the multi scenario-based representation of uncertainty, the probability density function of the uncertain parameters is represented and approximated by a finite set of scenarios, each correlated to a particular probability of occurrence ω_δ. A large number of scenarios have to be explored for this approach to yield results that converge to a stochastic representation. In practice, it would be desired to select a sufficiently large number of selected scenarios such that any addition of a discrete realization within a given uncertainty bound does not significantly change the solution quality. However, problem complexity and computational costs may limit the maximum allowed number of realizations. Furthermore, to aid convergence to a locally optimum solution, an initialization phase is required. This is achieved by obtaining the optimal solution of the recipe-based case (MILP), where scheduling parameters are obtained from a steady-state analysis of the plant. The previously obtained MILP solution is used to fix a production sequence (binary variables) so that a nonlinear optimization of the dynamic unit models is performed (NLP), considering uncertainty realizations to be at their expected value[64]. The integrated MINLP model is solved departing from the solution generated by the previous step.

3.7 Chapter Summary

In this section, the fully integrated MLDO methodology is described. Given the optimization problem in (2), the scheduling time region is discretized into global equidistant discretizations by following the STN framework. This formulation allows for the detailed design of a batch schedule through the definition of material states, equipment and tasks. However, that formulation alone does not contain important dynamic information and optimal control strategies to maximize the batch plant's performance. Consequently, at each of the discretizations, logical disjunctive decisions are performed. This results in a mixed-logic dynamic optimization (MLDO) problem. By applying discretization and relaxation techniques, the problem can be casted as an MINLP. Two possible operating states are explored, if an indicator variable is active, a set of dynamic model and operational constraints are enforced. The activation of these constraints allows for imposing dynamic dependency on the scheduling parameters, therefore, linking the control and scheduling layers. If the binary indicator is inactive, then said scheduling parameters are set to zero. Disjunctive selective decisions are performed, with the goal of enforcing product specific quality constraints. Incorporation of stochastic-based uncertain parameters would tax the computational performance of an already challenging problem to solve, as such, multi-scenario-based uncertainty is proposed. The main purpose of this method is for it to serve as a benchmark for the decomposition approach, both in computational efficiency and in solution quality.

Chapter 4: Back-Off Decomposition Algorithm

This section presents the back-off decomposition algorithm proposed to address the integration of scheduling and control of batch plants under stochastic realizations in the uncertain parameters. This method was adopted from the methodology previously presented by Koller et al.[27], where it was shown to be successfully applied to the integration of design, scheduling, and control of a continuous multi-purpose unit.

An expansion upon this methodology is presented, a decomposition approach for the integration and dynamic optimization of multi-unit, multi-product batch plants. The proposed algorithm is expected to converge to an economically attractive solution while incorporating fully stochastic distributions of parameter uncertainty and avoiding the solution of a complex MLDO problem, which is the key feature of this method.

The main difference between the proposed algorithm and that presented by Koller et al.[27] is that the latter requires the formulation and solution of an MINLP at each iteration step for a single production unit. Applying that approach to multiple units may become a daunting task, e.g. computationally taxing for large-scale and complex applications; hence, the proposed approach avoids the need to solve such intensive problems by decomposing the scheduling and control layers into two optimization formulations.

As shown in Figure 4, the proposed algorithm consists of a master outer loop, which includes scheduling and dynamic optimization (control) decisions, and an inner loop, which aims to propagate model parameter uncertainty into the dynamic process by solving feasibility-based problems. Each of the steps involved in the proposed back-off decomposition algorithm is explained next.

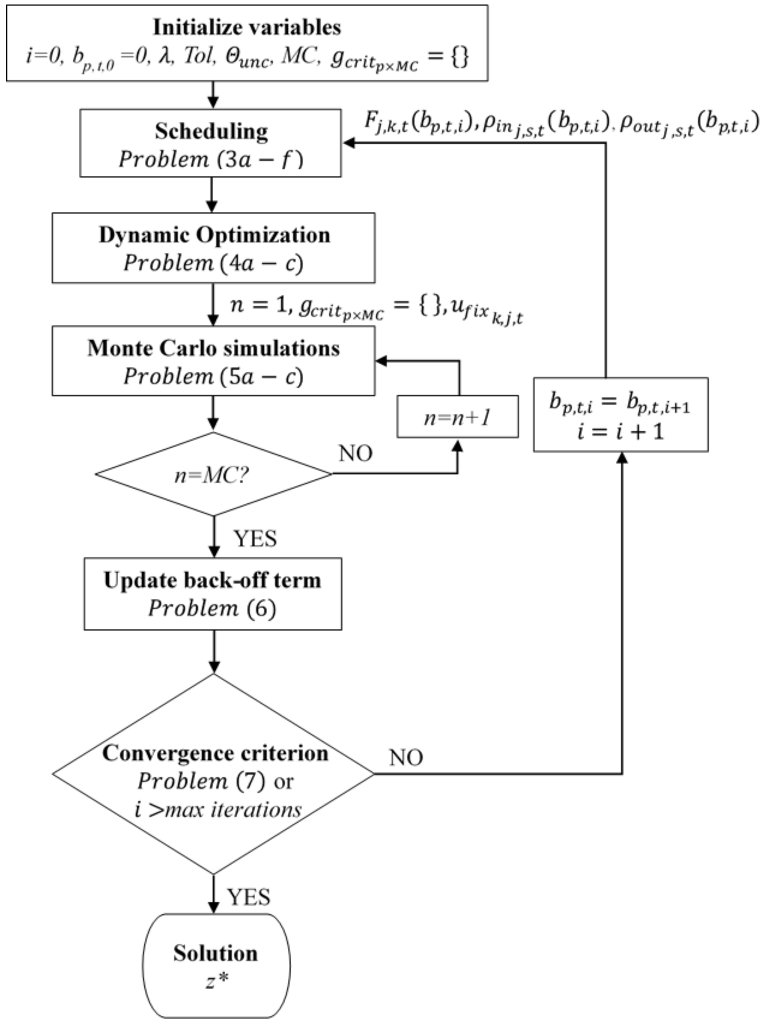

Figure 4: Flowchart of the decomposition back-off algorithm

4.1 Initialize Variables

The first stage consists of initializing relevant algorithm parameters, *i.e.* an iteration index (*i=0*), maximum number of iterations, a user-defined criterion for the tolerance of convergence (*Tol*), and a multiplier for the back-off terms (λ), which shapes the conservativeness of the solution. Also, the present method requires the specification of the set of probability density functions that describe each of the realizations of the uncertain parameters (Θ_{unc}) and the number of Monte Carlo simulations (*MC*), which have to be large enough so that an accurate representation of the distribution for each parameter in Θ_{unc} is achieved. Similarly, an empty matrix, g_{crit}, needs to be initialized and used to store relevant information extracted from the *MC* simulations. At the first iteration (*i=0*), no uncertainty in the model parameters is considered in the scheduling and dynamic optimization stage, this case is referred to as the *nominal* solution. Consequently, back-off terms $b_{p,t,i}$ are set to zero for the first iteration (*i=0*); for all discretizations in time t and $p \in 1,2 \dots, N_P$, where N_P represents the total number of constraints considered in the formulation, as shown in Problem 1.

4.2 Scheduling

A general scheduling formulation, which allows for the definition of states and tasks resulting in a multi-product manufacturing recipe for chemical batch plants is specified as follows:

$$\max_{\{S_D\}} z_{sched_i}\left(F_{j,k,t}(b_{p,t,i}), \rho_{in\,j,s,t}(b_{p,t,i}), \rho_{out\,j,s,t}(b_{p,t,i}), H\right) \tag{3a}$$

$$s.t. \sum_{j \in J_k} \sum_{t'=t}^{t-\tau_j+1} W_{j,k,t'} \leq 1 \qquad \forall k, t \tag{3b}$$

$$W_{j,k,t} B_{j,k}{}^{min} \leq B_{j,k,t} \leq W_{j,k,t} B_{j,k}{}^{max} \qquad \forall j, t, k \in K_j \tag{3c}$$

$$S_{s,t} = S_{s,t-1} + \sum_{j \in \overline{T}_s} \rho_{out\,j,s,t}(b_{p,t,i}) \sum_{k \in K_j} B_{j,k,t-\tau_{j,s}} - \sum_{j \in T_s} \rho_{in\,j,s,t}(b_{p,t,i}) \sum_{k \in K_j} B_{j,k,t} \qquad \forall s, t \tag{3d}$$

$$\boldsymbol{Sch_{eq}}(x(t), \dot{x}(t), u(t), \Theta, S_D) = 0 \tag{3e}$$

$$\boldsymbol{Sch_{ineq}}(x(t), \dot{x}(t), u(t), \Theta, S_D) \leq 0 \tag{3f}$$

Problem (3a-f) is typically formulated as a mixed-integer linear problem (MILP). At each iteration step *i*, the resulting schedule is generated by solving problem (Equation 3a-f), which consist of maximizing a user-defined objective function z_{sched_i} (Equation 3a) subject to a set of allocation (Equation 3b), capacity (Equation 3c) and material balance (Equation 3d) constraints. Equations (3e-f), as in section 2, represent placeholder constraints which may represent additional scheduling considerations, e.g. temporary unavailability of equipment, unit cleaning, etc. Global uniform discretization was applied to the scheduling makespan (*H*), i.e. scheduling decisions occur at specific equidistant points in time t using a time-scale which is shared by all units. Variable definitions remain the same as in problem (2a-h). Note that in the present method the variables may change at each iteration of the master outer loop. Moreover, variables that for the full integration problem were indexed by uncertainty (*i.e.* $\rho_{in_{j,s,t,\delta}}$, $\rho_{out_{j,s,t,\delta}}$, $F_{j,k,t,\delta}$) are now redefined such that process variability is captured explicitly through the consideration of back-off terms. Note that at each iteration of the master outer loop, new back-off terms $b_{p,t,i}$ are calculated. Consequently, uncertainty dependent linking variables (*i.e.* operating costs, proportion of material consumption/production) are updated accordingly, as a means of effectively propagating process variability into the scheduling problem. As indicated in the *Initialize variables* stage, $b_{p,t,0}=0$, *i.e.* no uncertainty is considered for $i=0$; hence, all the scheduling parameters shown in Equation (3a-f) can be obtained *a priori* or calculated from a steady-state analysis of the batch plant for the first iteration.

4.3 Dynamic Optimization

The solution from (3) provides the production parameters and the manufacturing sequence to follow, *i.e.* S_D. This information is the key input used to search for optimal open-loop control profiles on the batch units that are expected to maintain the plant on specification and dynamically operable in the presence of uncertainty. The optimal control profiles can then be calculated from a discretized dynamic optimization problem (NLP). As shown in (4), an objective function z_{dyn} needs to be optimized over the time horizon H. Mechanistic process variables $x_{j,k,t}$ are to follow a trajectory specified by the optimized control profiles $u_{j,k,t}$. For this stage, a key consideration is made, every uncertain parameter is assumed to be set at their expected values, *i.e.* $\widehat{\boldsymbol{\Theta}}_{\boldsymbol{unc}} = \{\theta^{k,\nu} | \theta^{k,\nu} = E[PDF_{k,\nu}(\Omega)]\}$. This assumption however, may produce constraint violations should the nominal solution be subjected to any other possible realization in the uncertain model parameters. To address this problem, back-off terms ($b_{p,t,i}$) are explicitly considered into the inequality constraints ($g_{p,t}$) at any time t to approximate the effects of process variability due to uncertainty, as shown in Equation (4c). Back-off terms are not static or obtained from a single optimization problem. The terms carry important statistical information regarding the effect of stochastic process variability on the corresponding process constraints, and they are refined at each iteration of the master loop. Hence, these back-off (penalty) terms are being updated at each iteration in the present algorithm. This is a key difference with respect to penalty-based methods, which penalize deviations from a desired behavior through the implementation of sum of errors (i.e. sum of squares) directly into the objective function[30,65,88]. The reformulation of the inequality constraints implies that, by shifting away from the nominal operation of the plant (*i.e.* when $\widehat{\Theta}_{unc}$ is considered), dynamic operability of the plant may be ensured, even under the effects of stochastic realizations in the uncertain parameters. Robustness of the solution can be fine-tuned by modifying the user-defined weight parameter λ_p, which determines the amount of variability (*i.e.* back-off terms) that is considered on each constraint $g_{p,t}$ due to model uncertainty.

$$\max z_{dyn_i}\left(\boldsymbol{x}(t), \dot{\boldsymbol{x}}(t), \boldsymbol{u}(t), \boldsymbol{\Theta_{nom}}, \widehat{\boldsymbol{\Theta}}_{\boldsymbol{unc}}\right) \tag{4a}$$

$s.t.$

$$f_{l,t}\left(x_{j,k,t}, \dot{x}_{j,k,t+1}, u_{j,k,t}, \Theta_{nom}, \widehat{\Theta}_{unc}\right) = 0 \qquad \forall t, j \in \boldsymbol{J_k}, k, l \in 1,2 \ldots N_L \tag{4b}$$

$$g_{p,t}\left(x_{j,k,t}, \dot{x}_{j,k,t}, u_{j,k,t}, \Theta_{nom}, \widehat{\Theta}_{unc}\right) + \lambda_p b_{p,t,i} \leq 0 \qquad \forall t, j \in \boldsymbol{J_k}, k, p \in 1,2 \ldots N_P \tag{4c}$$

$t \in [0, H]$

4.4 Monte Carlo Simulations

The aim of this stage is to test the dynamic feasibility of the schedule and control profiles obtained from the previous stages under the effects of fully stochastic uncertain parameters in $\boldsymbol{\Theta_{unc}}$, as defined in Problem (1). For this purpose, a feasibility problem is posed in Equation (5a-b), where the objective function is set to be constant *c*. Dynamic process model equations for each batch unit (5b) are the only set of constraints enforced. Whereas in problem (4) control variables ($u_{j,k,t}$) were optimized using fixed back-off terms and nominal realizations in the uncertain parameters ($\widehat{\boldsymbol{\Theta}}_{\boldsymbol{unc}}$), this stage keeps the control actions fixed such that the set of control decisions calculated in (4) *i.e.* $u_{j,k,t}$ remain as inputs to problem (5), as shown in Figure 4. For the sake of clarity, the set of fixed control inputs obtained from problem (4) are referred to as ${u_{fix}}_{j,k,t}$. Thus, by enforcing a set of specific control trajectories, mechanistic process variables are sensitive only to different realizations in $\theta^{k,\nu}$. Each of the uncertain model parameters in $\boldsymbol{\Theta_{unc}}$ are to be described by a number of *MC* realizations, which follow a user-defined probability distribution that are defined *a priori* (*i.e.* in the initialization stage). Monte Carlo sampling techniques are used to obtain a random realization *n* of the ν^{th} element in the set $\boldsymbol{\Theta_{unc}}$ (referred to as $\theta_n^{k,\nu}$) which together with the control profile ${u_{fix}}_{j,k,t}$, represent the key inputs to problem (5).

$$\max c \tag{5a}$$

$$s.t.\, f_t^l\left(x_{j,k,t}, \dot{x}_{j,k,t}, {u_{fix}}_{j,k,t}, \boldsymbol{\Theta_{nom}}, \theta_n^{k,\nu}\right) = 0 \qquad \forall t, j \in \boldsymbol{J_k}, k, \nu \in 1,2 \ldots, N_{unc}, l \in 1,2 \ldots N_L \tag{5b}$$

The solution from (5a-b) for current inner-loop iteration *n*, allows for the evaluation of every inequality constraint $g_{p,t}$. The measured value at iteration *n* of each constraint $g_{p,t}$ is added to the p^{th} row, n^{th} column of matrix g_{crit}; thus, each *p* row in g_{crit} contains an approximation of the variability of each g_p due to the stochastic effect of the uncertain parameters Θ_{unc}, as shown in problem (5c).

$$g_{crit_{p,t,n}} \cup g_{p,t,n}\left(x_{j,k,t}, \dot{x}_{j,k,t}, {u_{fix}}_{j,k,t}, \boldsymbol{\Theta_{nom}}, \theta_n^{k,\nu}\right)$$

$$\forall t, j \in \boldsymbol{J_k}, k, n \in 1,2 \ldots MC, \nu \in 1,2 \ldots N_{unc}, \forall p \in 1,2 \ldots N_P \tag{5c}$$

The procedure considered for solving (5a-b) to (5c) is systematically repeated until *MC* feasibility problems have been solved (*n=MC*). The outcome from this stage is to draw statistical information from the inequality constraints contained in $\boldsymbol{g_{crit}} \in \mathbb{R}^{p\times t\times MC}$.

4.5 Update back-off terms

With the statistical data obtained from the Monte Carlo simulations, back-off terms at each t for each constraint $g_{p,t}$ are updated using Equation (6), which is the formal definition of the standard deviation for each output distribution $g_{crit_{p,t}}$. Therefore, the updated back-off terms $(b_{p,t,i+1})$ represent the variability (measured in terms of the standard deviation) of the p^{th} inequality constraint due to the effect of *MC* realizations for every parameter in $\boldsymbol{\Theta_{unc}}$ at time *t*. Moreover, λ_p can be considered for each constraint $g_{p,t}$, as a user-defined multiplier of the expected standard deviation on process variability. As shown in Equation (4c), an increase in magnitude of the multipliers λ_p can be regarded as an increase in the robustness of the solution.

$$b_{p,t,i+1} = \sqrt{\frac{1}{MC}\sum_{n=1}^{MC}\left[g_{crit_{p,t,n}} - \frac{1}{MC}\sum_{n=1}^{MC} g_{crit_{p,t,n}}\right]^2} \qquad \forall t, p \in 1, 2, \dots, N_p \tag{6}$$

4.6 Convergence Criterion

As shown in (7), the back-off terms from successive iterations are compared to determine if convergence has been achieved. If criterion (7) is not met, $b_{p,t,i}$ is updated with the value of $b_{p,t,i+1}$, as shown in Figure 4. Updated scheduling parameters are calculated and used as inputs to Equation (3) for the next iteration $i+1$, as shown in Figure 4. Convergence is achieved if the difference between successive back-off terms is less than a user-defined tolerance criterion (*Tol*). Accordingly, a solution z^* composed by a set of scheduling decisions and control profiles that remain dynamically feasible under the effects of uncertainty has been found. The algorithm is also terminated if a maximum number of iterations is reached.

$$\left|\frac{(b_{p,t,i+1} - b_{p,t,i})}{b_{p,t,i+1}}\right| \leq Tol \quad \forall t, p \in 1,2 \dots N_p \tag{7}$$

The back-off algorithm proposed in this work follows a similar structure to equation (2); however, a separation of the MINLP into its MILP and NLP components is performed; moreover, no disjunctive decisions are required. The iterative nature of the algorithm can decrease computational costs of the problem when gauged in performance against an MINLP that attempts to perform scheduling and control simultaneously. Moreover, the proposed algorithm gives the user the freedom to fine-tune solution conservativeness by modifying λ_p. In addition, the MINLP formulation handles uncertainty using a multi-scenario approach, which may require a sufficiently large number of uncertainty realizations to return an acceptable solution that may be immune to uncertainty. Some inherent limitations of the decomposition algorithm exist due to the stochastic nature of the model parameters. If the selected number of MC simulations is not sufficiently large, then uncertainty might not be fully captured by the back-off terms; hence, multiple runs of the algorithm over the same case study may yield to different results or to convergence issues. Moreover, convergence of the algorithm may be inhibited if either the multiplier λ_p, or the back-off terms are sufficiently large in magnitude, *i.e.* large process variability. This may manifest as dynamic infeasibilities when solving problem (4). However, this issue can be resolved if relaxation on the bounds of the control variables is a possibility since infeasibilities are mainly due to limited degrees of freedom. We recognize that convergence to the optimal back-off solution cannot be guaranteed, unless the back-off terms are proven to be insensitive to the optimization variables. Moreover, if first order KKT optimality conditions for the integrated optimization hold, and critical realizations in the uncertain parameters are active at the solution, the present back-off calculation is equivalent to the integrated problem[89]. More details about convergence issues with the present back-off method are described in Koller et al.[27]

4.7 Chapter Summary

This section presented the novel back-off decomposition algorithm for integration of scheduling and control. The proposed methodology offers an iterative approach to the solution of scheduling and control of sequential batch plants, subject to stochastic model-parameter uncertainty. The solution of a complex

MLDO problem is thus avoided by iteratively solving between a scheduling formulation (MILP) and an optimal open-loop control strategy (NLP). The key idea of this method is to approximate process variability through Monte Carlo simulations, so as to move away from an economically attractive though dynamically infeasible operation policy to obtain robust scheduling and control decisions. The proposed algorithm can accommodate different probabilistic distributions in the uncertain model parameters, which are propagated into the process model through feasibility simulations obtaining a resulting output distribution on key process constraints. From this output, back-off terms are calculated and incorporated into the dynamic optimization problem, conditions from this modified problem allow for the calculation of key scheduling parameters. This process is repeated until a convergence criterion is met. The solutions obtained by this method are able to accommodate robustness up to a user-defined level of process variability. Convergence of the algorithm is discussed, namely the selection of a large enough number of feasibility problems to approximate variability. A case study illustrating the features and limitation of this algorithm is presented in the next chapter.

Chapter 5: Case Study & Results

In this chapter the previously presented methods are applied to a multi-product, multi-unit batch plant. Equipment, materials and scheduling representation are all expanded upon in the section below. Results from the application are presented, discussing in depth computational performance, effects of uncertainty upon the solution, advantages and disadvantages of both the integrated and decomposition-based approaches.

5.1 Flowshop Batch Plant

The performance of the algorithms presented in sections 3 and 4 were tested on a case study involving the optimal scheduling and control of a multiproduct flowshop batch plant adapted from Nie and Biegler[64]. The main goal of the sequential batch plant is to maximize the overall profit in the production of two chemical species, *ProdB1* and *ProdB2*, differing only in their economic attractiveness and their purity. The process flow diagram of the multi-product multi-unit batch plant is shown in Figure 5.

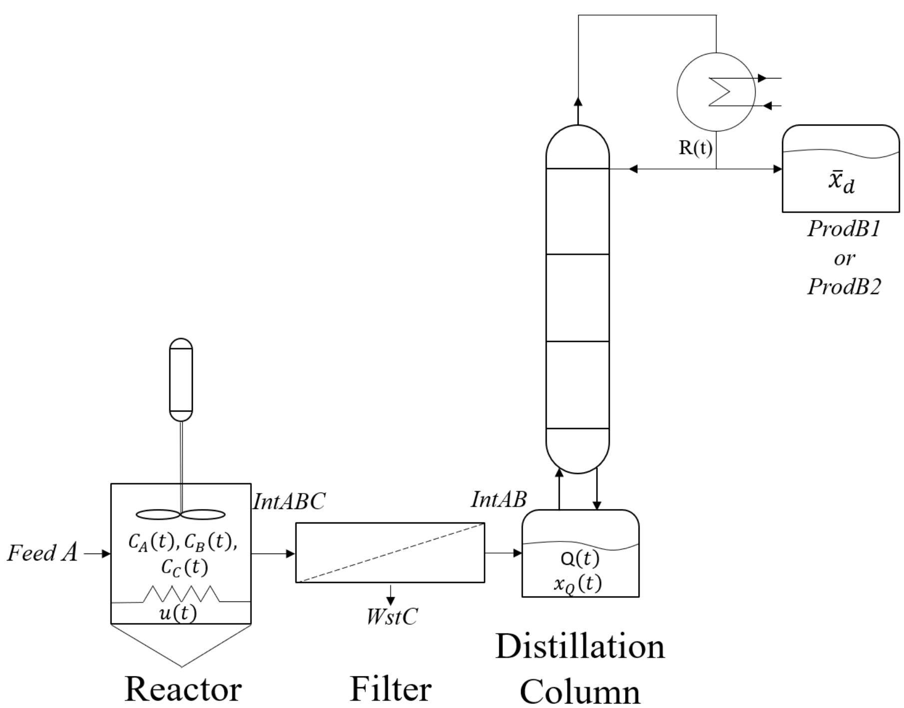

Figure 5: Process flow chart of case study

The batch plant consists of three main processing units, a reactor, a filter and a distillation column. The process starts with a material inlet to a reactor (*FeedA*). Material output from the reactor (*IntABC*) is a mixture of three species *A*, *B* and *C*, respectively. This material serves as an input to the filter, whose main task is to separate the undesired species *C* (*WstC*) to yield a material composed of only *A* and *B* (*IntAB*), which is then fed as an input to the distillation column. The final step in the production sequence consists of the binary distillation of light species B from heavy *A* to yield either *ProdB1* or *ProdB2*. The production of either product, *i.e.* $Prod\gamma$ ($\gamma \in \boldsymbol{\Gamma} = \{B1, B2\}$), depends on factors such as process economics, scheduling and control decisions.

Scheduling

The state-task sequence for this plant is presented in Figure 6. Following the STN formulation presented in the previous sections, the set $\boldsymbol{K}$ represent the available units (*i.e.* $\boldsymbol{K} = \{r, f, d\}$); similarly, four tasks need to be defined for this process, *i.e.* $\boldsymbol{J} = \{Rct, Fil, DisB1, DisB2\}$. The former tasks $Dis\gamma$ ($\gamma \in \boldsymbol{\Gamma}$) correspond to the selection of either desired product within the distillation unit (*ProdB1* or *ProdB2*), as shown in Figure 6. Therefore, this decision may be considered as a switching condition. In addition, eight material states are defined for this process as shown in Figure 6, *i.e.* **S**= {*Feed A*, *IntABC*, *WstC*, *IntAB*, *RcyB1*, *RcyB2*, *ProdB1*, *ProdB2*}.

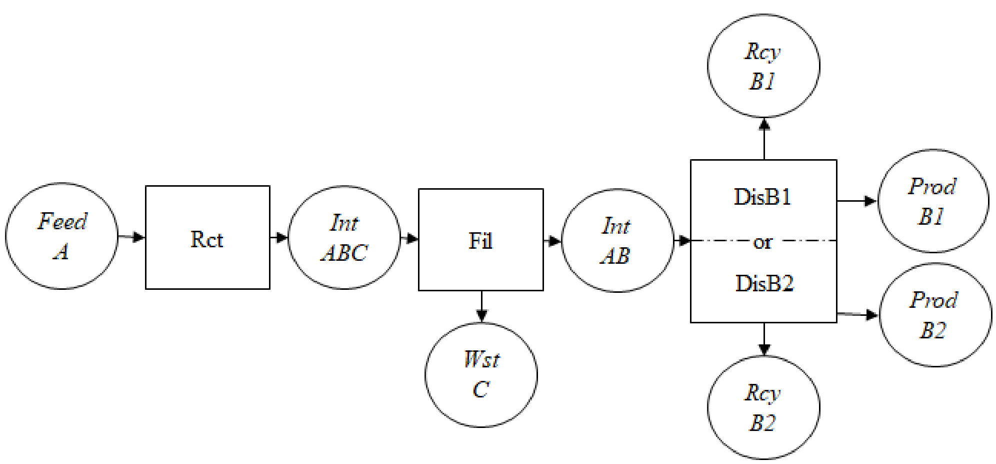

Figure 6: STN representation of the proposed case-study

To simplify the analysis, the operational time τ^j for the tasks performed by the reactor, filter and distillation is assumed to be fixed and equal to 2 hours each. Processing units described in the case study are assumed to have a batch size limit of 60 kg. Considerations for each equipment are described next.

Reactor

As shown in Figure 5 and 6, input to the reactor comes from material state *Feed A*. The main function of this unit is to produce species *B* through an irreversible reaction of *A*. In a similar fashion, *B* degrades into waste species *C*. Ending conditions of this unit propagate and affect initial conditions of the following units, therefore affecting the production of $Prod\gamma$. The reactor dynamics (Equations 8a-c) are assumed to be accurately driven by the transformed temperature control variable, *u(t)* (m^3/kg·hr).

$$\dot{C}_A = -u(t)C_A^2(t) \qquad C_A(0) = 1 \qquad (8a)$$
$$\dot{C}_B = u(t)C_A^2(t) - \beta u^2(t)C_B(t) \qquad C_B(0) = 0 \qquad (8b)$$
$$\dot{C}_c = \beta u^2(t)C_B(t) \qquad C_C(0) = 0 \qquad (8c)$$

$\dot{C}_A, \dot{C}_B$ and $\dot{C}_C$ represent the change in each species concentration with respect to time, initial conditions state that initially there is only species *A* in the reactor, kinetics will be affected by β, a reaction parameter. The operating cost of the reactor is assumed a function of the batch size processed in the unit $B_{Rct,r,t}$ and the heating utility, given a unit price factor p_r (\$0.3/kg), i.e.

$$F_{Rct,r,t} = p_r B_{Rct,r,t} \int_0^{\tau^{Rct}} u(t)dt \qquad (9)$$

For the purpose of this equipment, having only one material input and one output means that variables ${\rho_{in}}_{Rct,FeedA,t}$ and ${\rho_{out}}_{Rct,IntABC,t}$ are equal to the unity for any time *t*.

Filter

The goal of filtration is to eliminate any trace of waste species *C* from the reactor material output, *IntABC*. No inherent dynamics are considered for this unit. The operating cost for this unit is dependent on the amount of material *IntAB* produced ($S_{IntAB,t}$), a penalization on the production of waste species $WstC$ ($S_{WstC,t}$), and a unit price factor p_f ($1/kg), i.e.

$$F_{Fil,f,t} = p_f(S_{IntAB,t} + 4S_{WstC,t}) \qquad \forall t \tag{10}$$

Having two outputs, material balance on task *Fil* consists of two variables $\rho_{out_{Fil,IntAB,t}}$ and $\rho_{out_{Fil,WstC,t}}$, which define the proportion of the processed batch fed into states *IntAB* and *WstC*. As shown in Equation (11a-b), these variables are dependent on the final conditions of the reactor.

$$\rho_{out_{i,Fil,WstC,t}} = C_c(\tau^{\mathrm{Rct}})/\left[C_A\left(\tau^{\mathrm{Rct}}\right) + C_B\left(\tau^{\mathrm{Rct}}\right) + C_C(\tau^{\mathrm{Rct}})\right] \tag{11a}$$

$$\rho_{out_{i,Fil,IntAB,t}} = \left[C_B\left(\tau^{\mathrm{Rct}}\right) + C_A\left(\tau^{\mathrm{Rct}}\right)\right]/\left[C_A\left(\tau^{\mathrm{Rct}}\right) + C_B\left(\tau^{\mathrm{Rct}}\right) + C_C(\tau^{\mathrm{Rct}})\right] \tag{11b}$$

Distillation Column

As shown in Figure 5 and 6, the binary distillation column aims to further purify the filter material output *IntAB*. This material is fed into the reboiler, with an initial charge equivalent to $B_{Dis\gamma,d,t}$. Change in the reboiler's material over time is dictated by $\dot{Q}$ as shown in Equation (12a). Change of concentration of species *B* in the reboiler is described by $\dot{x}_Q$, with an initial concentration of η_B (Equation 12b).

$$\dot{\boldsymbol{Q}} = \boldsymbol{L} - \boldsymbol{V} \qquad Q(0) = B_{Dis\gamma,d,t}\ (kg) \quad \forall\gamma \in \boldsymbol{\Gamma} = \{B1, B2\}) \tag{12a}$$

$$\dot{\boldsymbol{x}}_{\boldsymbol{Q}} = \frac{V\left(x_Q - x_d\right)}{[(R+1)\cdot Q]} \qquad x_Q(0) = \eta_B\ \ (kg/kg) = C_B(\tau^{\mathrm{Rct}})/[C_A(\tau^{\mathrm{Rct}}) + C_B(\tau^{\mathrm{Rct}})] \tag{12b}$$

$\boldsymbol{L}$ is the flow returning to the column, **V** is the vapor flow, $\boldsymbol{x_d}$ the distillate concentration and $\boldsymbol{R}$ the reflux ratio. The dynamics of the distillation column are solved using the shortcut batch distillation model without holdup and a constant relative volatility α. Equilibrium between liquid ($\boldsymbol{x}_\mu$) and vapor phases ($\boldsymbol{y}_\mu$) in each μ tray, which impacts distillation purity, is as follows:

$$\boldsymbol{y}_\mu = \frac{\alpha\boldsymbol{x}_\mu}{\left[1 + (\alpha - 1)\cdot\boldsymbol{x}_\mu\right]} \qquad \forall\mu = 1 \ldots 4 \tag{12c}$$

Moreover, the adjustable variable for control in this unit is the reflux ratio *R*, which represents a relationship between flow returning to the column (*L*) and the amount drawn from to distillate (*D*), as shown in Equation (13). As depicted in Equation (14), both *L* and *D* hold a relationship with the vapor flow *V*, which is assumed to be a function of batch size $B_{j,d,t}$ and parameter κ_{d} (1.646).

$$\boldsymbol{R}(\boldsymbol{t}) = \boldsymbol{L}(\boldsymbol{t})/\boldsymbol{D}(\boldsymbol{t}) \tag{13}$$

$$\boldsymbol{L}(\boldsymbol{t}) + \boldsymbol{D}(\boldsymbol{t}) = \mathrm{V} = \kappa_{\mathrm{d}} B_{Dis\gamma,d,t} \qquad \forall \gamma \in \Gamma \tag{14}$$

The manufacturing constraint for the batch plant is as follows:

$$\bar{x}_{d_{\gamma}} = \frac{\mathrm{Q}(0)x_{\mathrm{Q}}(0) - \mathrm{Q}(\tau^{Dis\gamma})x_{\mathrm{Q}}(\tau^{Dis\gamma})}{\int_0^{\tau^{Dis\gamma}} D dt} \qquad \forall \gamma \in \Gamma \tag{15}$$

$$\bar{x}_{d_{\gamma}} \geq \bar{x}_{d}{}^{*}{}_{\gamma} \qquad \forall \gamma \in \Gamma \tag{16}$$

where $\bar{x}_{d}{}^{*}{}_{\mathrm{B1}}$ and $\bar{x}_{d}{}^{*}{}_{\mathrm{B2}}$ represent the critical product purity for *ProdB1* (0.995) and *ProdB2* (0.997), respectively. Therefore, an optimal reflux ratio must be determined to keep the unit on spec, according to the task selected. The operational cost function for this equipment is a function of vapor flow, unit price p_d (\$1.5/m^3·hr), and the task completion time, *i.e.*

$$F_{Dis\gamma,d,t} = \tau^{Dis\gamma} p_d V \qquad \forall \gamma \in \Gamma \tag{17}$$

Material output proportion variables are defined in Equation (18a-b), where the total amount of accumulated distillate ($D_{tot_{\gamma}}$) dictates the net quantity of manufactured product. Initial reboiler charge $\mathrm{Q}(0)$ is given in Equation (12a).

$$\rho_{out_{i,Dis\gamma,Prod\gamma,t}} = D_{tot_{\gamma}}/\mathrm{Q}(0) \qquad \forall \gamma \in \Gamma \tag{18a}$$

$$\rho_{out_{i,Rcy\gamma,Prod\gamma,t}} = \mathrm{Q}(\tau^{Dis\gamma})/\mathrm{Q}(0) \qquad \forall \gamma \in \Gamma \tag{18b}$$

The overall net cost function considered for this plant for a given production horizon is as follows:

$$\Psi(\$) = \sum_{k}^{K} \sum_{j}^{K_j} \sum_{t=0}^{H} F_{j,k,t} \tag{18}$$

5.2 Results

In this section, results are presented, obtained from applying the algorithms presented above to three different scenarios of the case study. The Python package, Pyomo 5.6.1[90,91], was chosen to solve the resulting optimization problems. A computer with an Intel® Core™ i7-7770HQ 3.8GHz and 16GB of RAM was used to run all the optimization problems. Solvers were selected based on performance. For the back-off decomposition algorithm, CPLEX was used for the MILP scheduling problem and ipopt with the ma57 HSL linear solver for the dynamic optimization problem. Several open-source MINLP solvers were tested for the integrated formulation; however, better performance was found when using the Pyomo/GAMS interface. The solvers SBB[92] and DICOPT[93] are selected for the multi-scenario integrated problem, CONOPT[94] was used as the non-linear sub-solver in both MINLP solvers.

Several modules within Pyomo were used to complete the implementation of the proposed algorithms. The Generalized Disjunctive Programming (GDP) module facilitated the definition of logical disjunctions, which are needed for the integrated approach. To recast the multi-scenario MLDO into a MIDO, this module provides two methods to reformulate logical disjunctions, the Big-M method and the convex hull relaxation (CHR). The latter generally leads to a tighter relaxed problem at the cost of larger problem size, compared with the Big M method. In the proposed algorithm, the dynamic models that describe operating tasks are nonlinear and nonconvex, such that applying the CHR might risk cutting off the feasible search space [84]. Moreover, since the problem is already highly dimensional due to the multi-scenario uncertainty, consequent growth in the size of the problem is highly undesirable, for this purpose the Big-M method was selected. Furthermore, Pyomo's GDP module is capable of considering non-identical M multipliers for linear constraints. This method, also referred to as Multiple Parameter Big-M methodology[82], can use different values for the M multipliers with their respective constraint. An optimal value of M is found, such that, good quality, tighter relaxations can be achieved.

Moreover, the differential-algebraic equations (DAE)[95] module was chosen for its versatility when obtaining the discretization of time-dependent equations. This allows for the reformulation of the MIDO problem into an MINLP. For the purpose of this study, and to guarantee numeric stability, a discretization based on orthogonal collocation on finite elements is selected. In this case study, eight finite elements are considered, each having four collocation points, which provided accurate results in reasonably short computational times.

Scenario 1: Nominal Conditions

For comparison purposes, a scenario where the uncertain parameters are set to their expected value (nominal conditions) is considered first, which is then be compared against the decomposition approach. This scenario is equivalent to solving the optimization problems presented in appendix A considering only one realization in the uncertain parameters, corresponding to the relative volatility (Equation 12c) and the reactor kinetic coefficient (Equation 8b-c).

For illustrative purposes, an attempt at solving the integrated approach to global optimality is performed. BARON [96] was used to solve the resulting MINLP problem. A locally optimal solution is found in the pre-solve stage, corresponding to the same objective as SBB and DICOPT (Shown in Table 2). However, given a computational time limit of 86,400 seconds, it failed to close the upper bound on the problem (relative gap of 31%) even when providing the solver with lower and upper bounds on all variables and an initialization based on locally optimal conditions. Efficient implementation of techniques for ensuring a global optimal solution of non-convex generalized disjunctive formulations still remains an open research question [84].

Table 2: Comparison between the integrated and decomposition approach when considering a nominal realization in the uncertain parameters

Approach	*Integrated*	*Back-off decomposition*
Integer Variables	66	66
Continuous Variables	2,823	1,770
Number of constraints	3,029	1,852
Process revenue ($)	1,694 (SBB, DICOPT, BARON)	1,578
CPU time (s)	295 (SBB), 540 (DICOPT), 86,400 (BARON)	0.76

In comparison, local MINLP solvers provide a solution with a relatively low computational time. A feasible integer solution is found by the branch and bound algorithm, closing the relative optimality gap to 0.1%. Differences between dynamic decisions and objective function obtained with SBB and DICOPT are negligible, as shown in Table 2. Computational time of DICOPT, although almost two times greater than SBB, still remains attractive; however, this property diminishes as the problem increases in size, as it will be shown in the next scenarios. A different schedule, which yields the same objective value is obtained for each solver; however, the only difference stems from the order of the production sequence, batch sizes and material balance remained the same for both solvers.

For the case of the decomposition algorithm, a nominal solution is obtained by first solving the scheduling problem, which accounts for all of the integer variables for this approach. Relevant scheduling parameters are obtained from a steady-state, recipe-based operation of the batch plant and are calculated *a priori*. Consequently, the dynamic optimization problem aims to find the optimal control trajectory when no uncertainty or process variability is considered for the resulting production sequence. This case is one which has not received any feed-back from the back-off terms, and can be considered equivalent to a sequential-based optimization. For this scenario, the integrated formulation exploits the linking of scheduling and dynamic decisions to achieve around 9% greater objective value than the decomposition approach. Comparison of solutions for both methodologies are shown in Table 2.

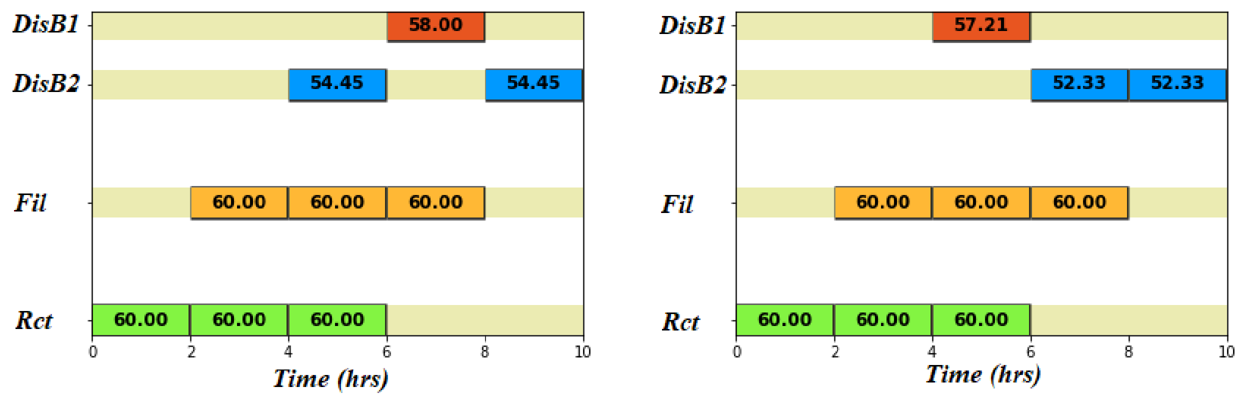

Figure 7: Scenario 1: Schedules for the back-off decomposition (left) and SBB-BARON integrated approach (right)

Figure 7 shows the production sequences obtained from the back-off and integrated approaches, respectively. In both cases, two events on the distillation column are dedicated to the production of *ProdB2* (blue), while only one is used for the production of *ProdB1* (red). This suggests that *ProdB2* is considered to be the most economically relevant product when the nominal case is considered. SBB and BARON converged to the same schedule. Scheduling decisions, however, are not necessarily unique. There may exist multiple production sequences that yield the same value in the objective function[46], which was observed on the resulting schedules obtained by SBB and DICOPT, where the latter allocates the production of *ProdB1* to the last possible slot (at t=8), however converging to the same objective and dynamic decisions. Note that the integrated approach utilizes its interconnectivity between layers to achieve a greater purity of species *B* in intermediate material *IntAB*; a greater initial concentration of species B in the initial distillation column batch indicates that a greater amount of *ProdB1* or *ProdB2* may be produced. Moreover, smaller batch sizes processed by the distillation column translate into lower operational costs.

As mentioned in the previous section, average purity (Equation 15) is the critical operational constraint of the plant. Since *ProdB2* has a higher purity requirement (*i.e.* 0.997) than *ProdB1* (*i.e.* 0.995), keeping the average purity of *ProdB2* above its minimum threshold (Equation 16) requires an overall larger reflux ratio, when compared to the production of *ProdB1*. Therefore, *ProdB2* is the product which limits the degrees of freedom of the overall problem and is of the most interest for the presentation of the results. The optimal control profile for the reflux ratio in the production of *ProdB2* is shown in Figure 8 for both the integrated (SBB, DICOPT) and sequential back-off approach. As a consequence of processing smaller batch sizes, the integrated problem is able to meet the operational constraint with a smaller reflux ratio, which indicates that more product is accumulated as distillate thus producing higher revenues for this process.

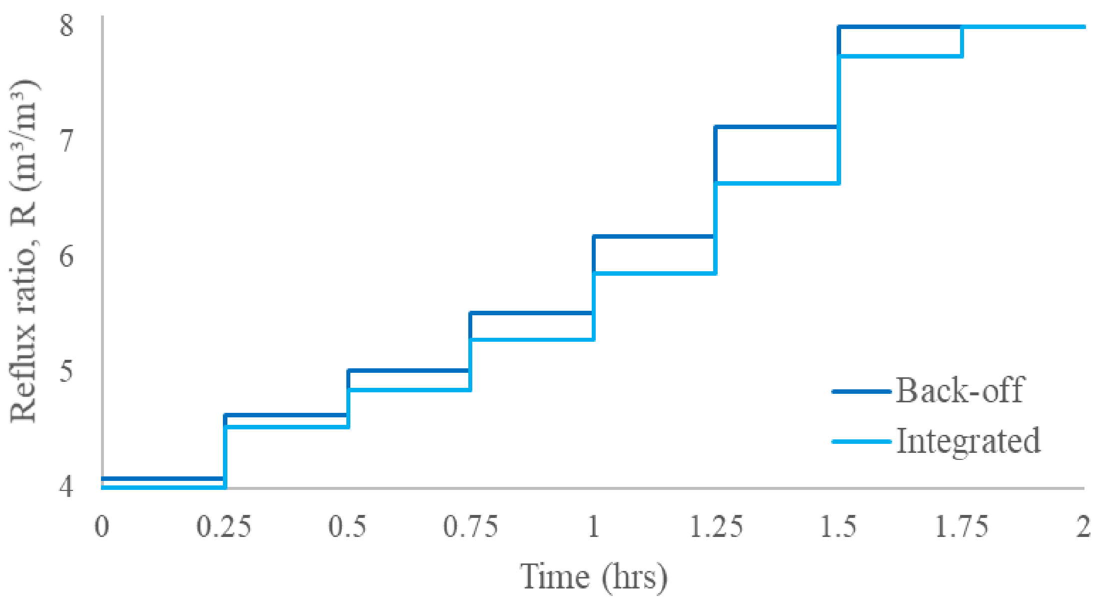

Figure 8: Resulting reflux ratio control profiles for the manufacturing of ProdB2, considering the nominal case for the integrated (SBB, DICOPT), and back-off approach

Scenario 2: Uncertainty in the Distillation Unit

The aim of this scenario is to test the performance of both the integrated and back-off approach under the effects of an uncertain parameter in the distillation unit. For this scenario, uncertainty in the relative volatility (α) is considered. Consider that the uncertain parameter α is normally distributed, *i.e.*

$$\Theta_{unc} = \alpha \sim N(2.515, 0.0683^2)$$

For the integrated approach, a vector of normalized weights is calculated, which are assigned to each discrete realization of the uncertain parameter. Nineteen realizations of α are considered; preliminary simulations were used to determine that this number of realizations is enough so that any addition does not change the objective function by more than 0.5%, the range of possible values are within 4 standard deviations of the previously defined PDF. This case is equivalent to solving the optimization problem in Appendix A.1, exploring 19 different discrete realizations affecting Equation (19d). Although uncertain realizations do not increase the number of integer variables in the integrated formulation, added constraints have significant impact on problem size, e.g. by an order of magnitude when compared to the nominal case (Table 2) thus affecting the overall algorithm performance (see Table 3).

Table 3: Comparison of problem size between integrated and back-off approach when considering one stochastic parameter in the process model

Approach	*Integrated*	*Back-off decomposition*
Integer Variables	66	66
Continuous Variables	23,996	1,770
Number of constraints	24,464	1,852

Next, the proposed scenario is solved by following the back-off decomposition approach. The initial procedure is similar to that described for Scenario 1. However, for this case, by considering a stochastic representation of the uncertain parameter, MC simulations have to be performed to capture the variability of the batch plant. It was determined, through *a priori* simulations tests, that the number of Monte Carlo simulations should be *MC*=1,000 to obtain consistent output distributions.

For each resulting feasibility problem, we evaluate 1,126 variables and 1,374 constraints, as described in section 4. This stage evaluates *MC* realizations on inequality constraint (Equation 15), so as to obtain a process PDF output, due to the stochastic effect of α on the distillation process.

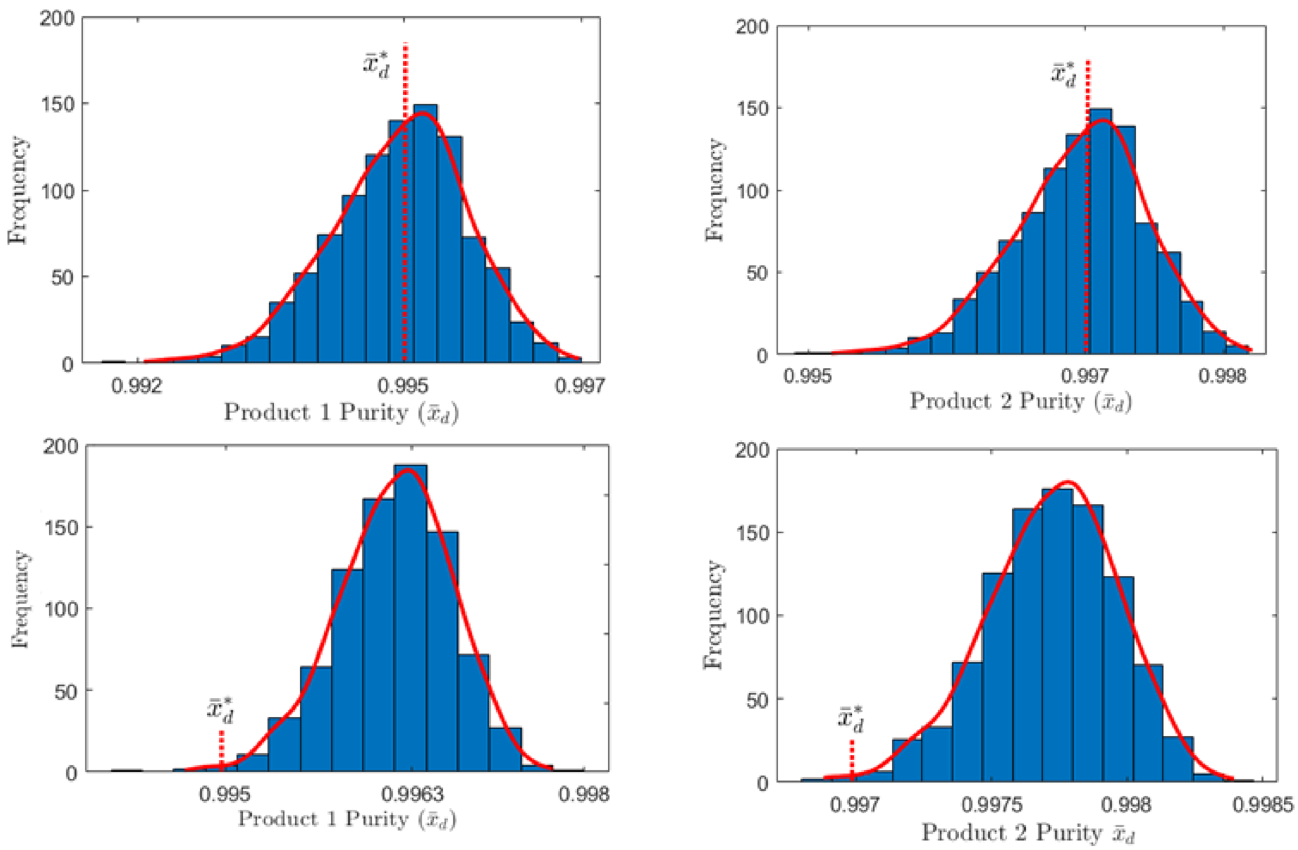

Figure 9: Output distributions of the operational constraint when subject to uncertainty when considering (top) no back-off, (bottom) λ=3. Dotted line represents the required purity constraint on both products

Figure 9 (top), show the resulting PDFs which correspond to output of the first master outer-loop iteration ($i=0$) of the back-off approach. This iteration, due to not receiving variability feed-back in the form of the back-off parameters, creates an output distribution scenario where the key purity constraint is most surely violated during operation. Therefore, a "shift" in the purity constraint must be considered if the plant is to be kept on spec due to the effect of uncertainty. That "shift" can be tuned in the present approach by setting the multiplier in the back-off terms (λ) to a sufficiently large value. In this scenario, λ=3, which implies that three standard deviations on the output purity variability are incorporated as variability, as explained in section 4. The algorithm converged in four iterations generating a solution that most surely satisfies the required operational constraint, as shown in Figure 9 (bottom).

Table 4: Comparison in solution quality and computational cost for integrated and back-off methodology when considering one uncertain parameter

Approach	*Integrated*	*Back-off λ=1*	*Back-off λ=2*	*Back-off λ=3*
Process revenue ($)	979	1,431	1,211	1,016
Iterations	-	3	4	4
CPU time (s)	4,509 (SBB), 6,024 (DICOPT)	2,783	3,691	3,937

Accounting for process variability however, comes at a necessary profit loss, as shown in Table 4. When λ=3, the most conservative case for the back-off approach is explored; as much as a 40% decrease in profits is observed when compared against the nominal solution (see Tables 2 and 4). This loss in profit is mainly attributed to the increasingly conservative reflux ratios, as shown in Figure 10. This is mostly due to the addition of the back-off terms into the purity constraint, which have effectively "backed-off" from the nominal set-points, i.e. 0.995 for *ProdB1* and 0.997 for *ProdB2*, to accommodate the uncertainty in α. As mentioned in the previous section, a larger value for λ accounts for a larger effect of the process variability.

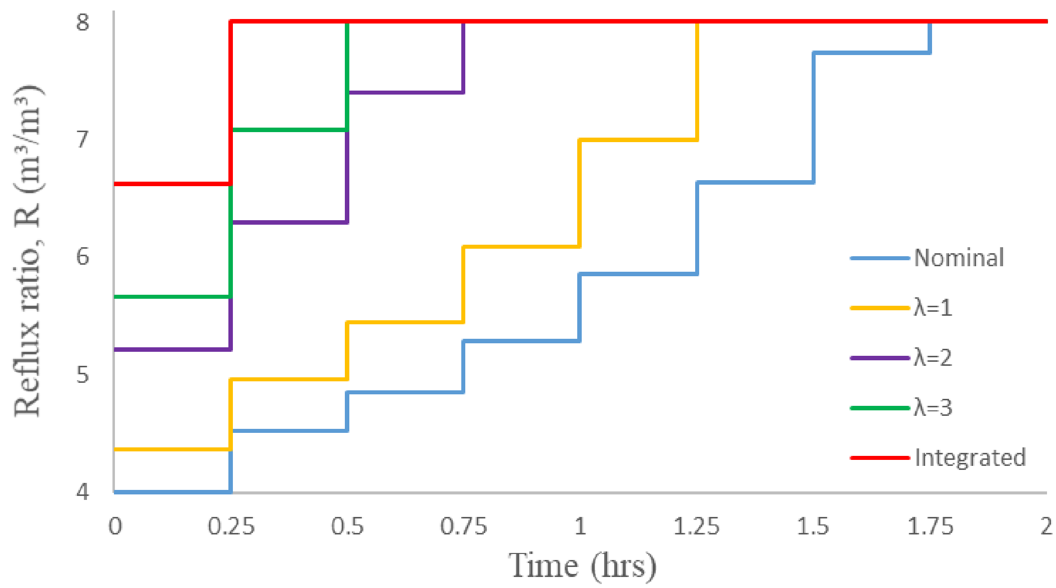

Figure 10: Reflux ratio control profiles for maintaining ProdB2 on spec when considering an integrated approach and different lambda multipliers for the back-off terms

For this particular formulation, the performance of DICOPT started to deteriorate as the problem grows in size. When compared to scenario 1, as much as an order of difference is needed in computational time to converge, as seen in Table 4. Moreover, with each main iteration, the size of the master MILP problem for DICOPT increases, making the successive solution of the master problem progressively expensive[97].

Discrepancies between the integrated and decomposition approach are noted due the inherent calculation of the back-off terms, which assumes output distributions to follow a normal distribution, however, due to the non-linearity of the process, resulting PDFs are slightly skewed. Moreover, due to the stochastic nature of the parameters, there may be critical uncertain realizations for which dynamic feasibility cannot guaranteed, accounting for those unlikely but critical realizations ensure robustness against parameter uncertainty at the expense of generating conservative solutions. The integrated approach, by solving a sparse problem, guarantees that every realization considered is accommodated by the particular dynamic decisions found, which is reflected as a more conservative reflux ratio is obtained for this case, as shown in Figure 10, and a lower process revenue relative to the back-off approach, as shown in Table 4.

Computational costs for the integrated approach are observed to increase with problem size, where DICOPT is noted to have already a difference of 33% in performance with respect to SBB. The back-off approach avoids the explicit solution of the MINLP by iteratively solving the MILP and NLP separately; however, the main bottleneck of this approach will be the MC simulations stage, where most of the computational time is spent.

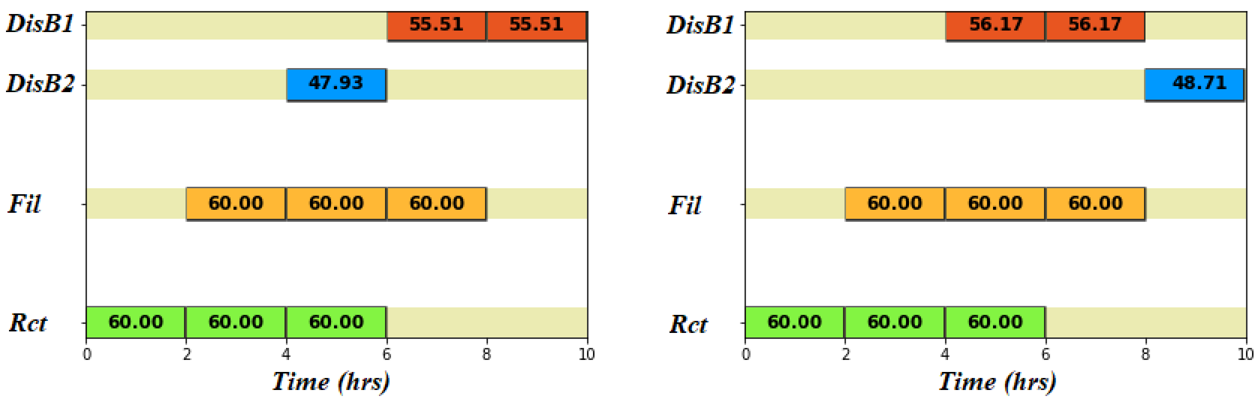

Figure 11: Resulting schedules for the integrated (Left) and back-off decomposition (Right), considering λ=3, when subjected to the effects of a normal probability distribution in a single uncertain parameter

As shown in Figure 11, there exists a critical threshold where *ProdB2* ceases to be the most economically attractive material; instead, production of *ProdB1* is incentivised. This is mainly due to the increasingly conservative reflux ratios, which are reflected as less material output (*i.e.* less overall revenue) at the cost of keeping the purity constraint on spec; therefore, for *ProdB2*, the trade-off between incurring a cost for operating the distillation column and obtaining material sales, is not as profitable as it is for *ProdB1*. Product manufacturing priority, then, has been observed to be sensitive to model parameter uncertainty.

As larger values for λ are considered, decisions made by the back-off methodology seem to converge to that achieved by the integrated approach. This can be observed in Figure 11, where a comparison for the back-off case (λ=3) and the integrated approach is considered. In both cases scheduling decisions led to the allocation of the maximum material capacity in the reactor (60 kg); although this means a larger processing cost is incurred (Equation 9), this also allows for the distillation column to process a larger batch leading to the maximization of product sales.

If *ProdB2* is to remain on spec, a greater initial purity of species *B* is required, which is achieved by minimizing the amount of species *A* in the intermediate material *IntAB.* This however, comes with a trade-off, by reducing the amount of species *A,* production of waste species *C* (*WstC*) increases. As a result, the initial batch size in the column for the production of *ProdB2* is smaller than that specified in the nominal case. This large interaction between uncertainty, dynamic and scheduling decisions serves as a justification for their simultaneous consideration.

Scenario 3: Uncertainty in the Reactor and Distillation Units

For this scenario, the operation of both the distillation and the reactor units are subject to uncertainty. The reaction kinetic parameter (β) in conjunction with α are considered uncertain model parameters. In the following sections, the effects of different PDFs are considered.

Scenario 3.a: Uniform Probability

For the integrated approach, 6 realizations in the reaction kinetic parameter are considered, which remain within a 15% variation from its nominal value while considering 19 realizations in the relative volatility. As shown in Table 5, considering six realizations of equal probability of occurrence in the reactor combined with 19 realizations in α were enough so that any other additional realization does not change the overall objective function by more than 0.5%.

Table 5: Objective function change when considering additional realizations in the additional reactor uncertain parameter and nineteen realizations in α

No. of realizations in uncertain reactor parameter	3	5	6	7
Objective function	923.6	869.82	863.3	865.78
Number of constraints	71,933	119,237	142,889	166,541
Number of variables	71,151	118,041	141,486	164,931

As indicated above, the increase in the number of uncertain realizations does not constitute an increase in the number of integer variables, however a significant growth is observed in the number of nonlinear algebraic equations and degrees of freedom in the optimization problems, when gauged against Scenario 1, as shown in Table 6. This is mainly due to the combinatorial nature in the problem, where the combination of the effects for each different realization in uncertain parameters have to be considered. For the back-off approach, it was found that setting MC=1,000 returned sufficiently accurate approximations to the process output distributions.

Table 6: Problem size comparison for the integrated and back-off approach, when considering a uniform distribution and two uncertain parameters

Approach	*Integrated*	*Back-off decomposition*
Integer Variables	66	66
Continuous Variables	141,420	1,770
Number of constraints	142,889	1,852

Table 7: Overall process revenue of the batch plant for integrated and back-off approach, when subject to two uncertain parameters which follow a uniform distribution

Approach	*Integrated (SBB)*	*Integrated (DICOPT)*	*Back-off λ=1*	*Back-off λ=2*	*Back-off λ=3*
Process revenue ($)	776.9 LB 863.3 UB	863.3	1,403	1,021	934
Iterations	-	-	3	5	5
CPU time (s)	11,283	61,334	2,878	4,472	4,909

A comparison of the results for this scenario is shown in Table 7. Having equal probability of occurrence, the overall profit decreases for all cases so as to account for the high process variability. Compared with the nominal case (Table 2), as much as a 50% reduction in profit has to be incurred to account for the effects on uniform probability on the uncertain parameters. The proposed back-off decomposition algorithm was able to converge within reasonable computational times, i.e. as much as 2 times faster than SBB and an order of magnitude faster with respect to DICOPT. For the integrated approach, the trend of increasingly large computational costs is observed, as more uncertain realizations are considered (See Table 2 and Table 7). However, obtaining a robust solution is guaranteed by ensuring constraints are met for all uncertain parameter combinations considered. A possible reformulation of this approach needs to be considered for its applicability on large-scale batch multi-product multi-unit plants. However, the problem size for the back-off decomposition approach remains unchanged, *i.e*. no additional variables or constraints need to be added since it relies on the feasibility stage to propagate an approximation of process variability into the optimization problem. Therefore, the back-off method converges in shorter computational times than those required by the integrated approach when considering the effects of multiple uncertain parameters, as shown in Table 7.

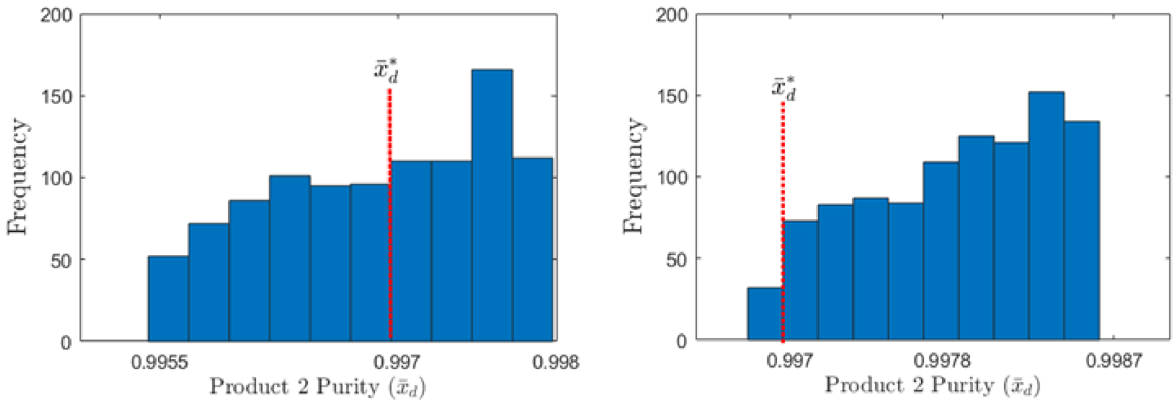

Figure 12: Output distributions of purity for ProdB2 when subjected to the effects of two uncertain parameters which follow a uniform distribution. Images correspond to the specific case of λ=3 for i=0 (Left) and i=5 (Right)

For the present scenario, process non-linearities are more noticeable for the output distribution of the resulting purity when considering a uniform distribution on the uncertain parameters. This in turn, affects the accuracy of the calculated variability (back-off terms). However, the algorithm is able to converge within 5 iterations for the most conservative case (*i.e.* Table 7, λ=3), while still accommodating the specified variability successfully, as shown in Figure 12.

Scenario 3.b: Non-Gaussian Distribution

For this scenario, the effect of having non-gaussian distributions on the reaction kinetic parameter (β) and the relative volatility (α) is considered. This was done to test the performance of the present back-off algorithm under highly nonlinear probability distribution functions.

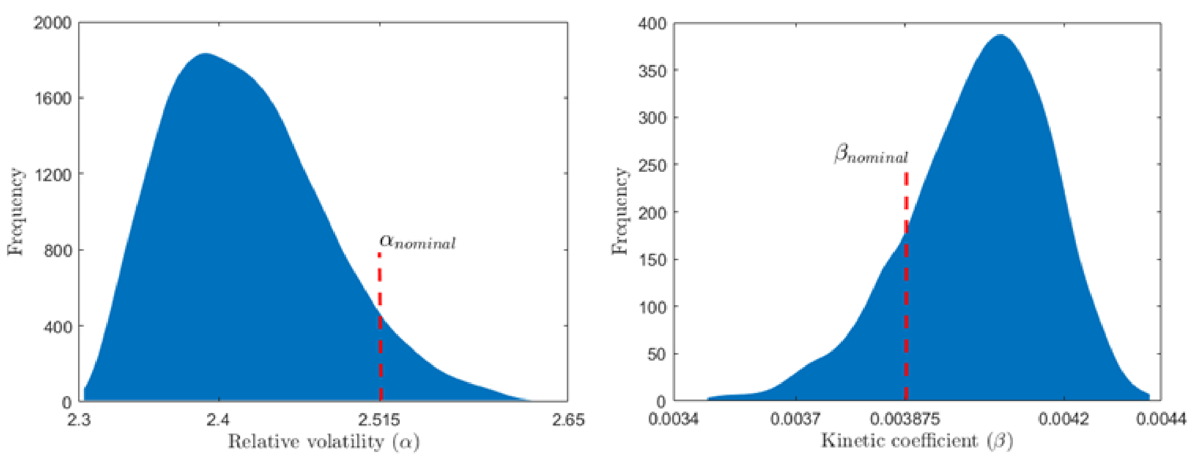

Figure 13: Uncertain parameter non-gaussian distributions

The distributions considered are presented in Figure 13. These distributions were generated by using a Weibull distribution with a shape parameter equal to 10 and 2 for the reactor parameter and relative volatility, respectively.

The results for this scenario indicate that it became computationally limiting to accurately represent such a distribution with the current integrated approach. By considering the same amount of realizations (19) for both the kinetic parameter and the relative volatility, the problem size grows considerably, when compared to the nominal case (Table 2), as shown in Table 8.

Table 8: Model size comparison for the integrated and back-off approach. 19 discrete realizations for the integrated problem were considered for both uncertain parameters.

Approach	*Integrated*	*Back-off decomposition*
Integer Variables	66	66
Continuous Variables	446,271	1,770
Number of constraints	450,365	1,852

From this non-gaussian distribution, note that the back-off algorithm struggles with capturing the variability; as many as 8 iterations were required for the convergence of the algorithm, as shown in Table 9.

Table 9: Results comparison between integrated and back-off approach when considering non-gaussian distributions on the uncertain parameters

Approach	*Integrated*	*Back-off* $\lambda=1$	*Back-off* $\lambda=2$	*Back-off* $\lambda=3$
Process revenue ($)	-	1,288	916	731
Iterations	-	4	8	7
CPU time (s)	>86,000	3,792	7,448	6,846

When capturing a large amount of process variability (i.e. λ=3) a significant decrease in the profits is observed, i.e. more than 50% in revenue when compared against a nominal solution. One of the benefits of the back-off algorithm is its versatility to adjust the conservativeness of the solution. It is possible to accept a certain amount of error in the solution and implement a less conservative λ. Given a computational limit of 86,000 seconds, neither SBB or DICOPT were able to close the set relative optimality criterion; moreover, no feasible solution was found within the given time limit, which is already an order of magnitude when compared against the back-off decomposition approach (Table 9).

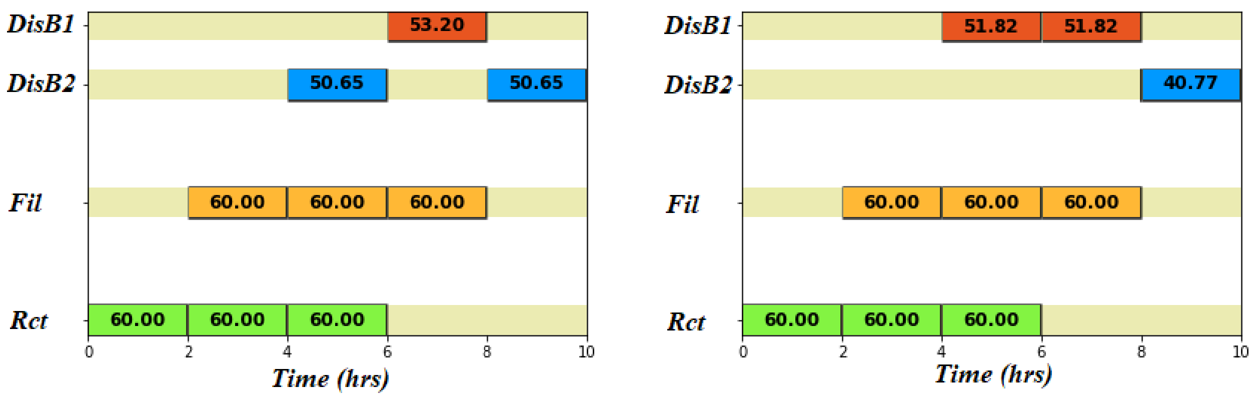

Figure 14: Schedule comparison between different lambda multipliers, λ=1 (Left) and λ=3 (Right), when considering a non-gaussian distribution

Scheduling decisions change due to the different distributions on the uncertain parameters, as mentioned above, originally *ProdB2* was the economically attractive product. This decision shifts to benefit the production of *ProdB1* when considering a stochastic distribution in the uncertain parameters. For the present nonlinear distribution scenario, this shift remains, as shown in Figure 14. However, batch sizes decrease so as to keep the batch plant on spec. A smaller initial batch size on the distillation column implies a larger amount of *WstC* was removed during the filtering stage, this is mainly due to the effects of the uncertainty which are propagated through the reactor into the filter.

As shown in Figure 15, the effects of multipliers (λ) are reflected on the control decisions and the overall conservatism of the solution. It is noted that the effect is more strongly observed in the distillation column; this is expected since this unit is critical for meeting the purity constraint. Moreover, this highly conservative profile (*i.e.* λ>3) is reflected as much less material is drawn from the distillate, affecting overall revenue of the plant. The slight increase in the transformed temperature control profiles for the reactor is mainly attributed to the decision of minimizing the concentration for species *A*. This trade-off generates a larger cost of operation in the reactor, according to Equation (9). Moreover, as the concentration of *A* decreases, a potential increase in the concentration of waste species *C* is observed, also producing an increase in the operation of the filter. Nevertheless, this is done so that the batch plant meets the required operational constraints.

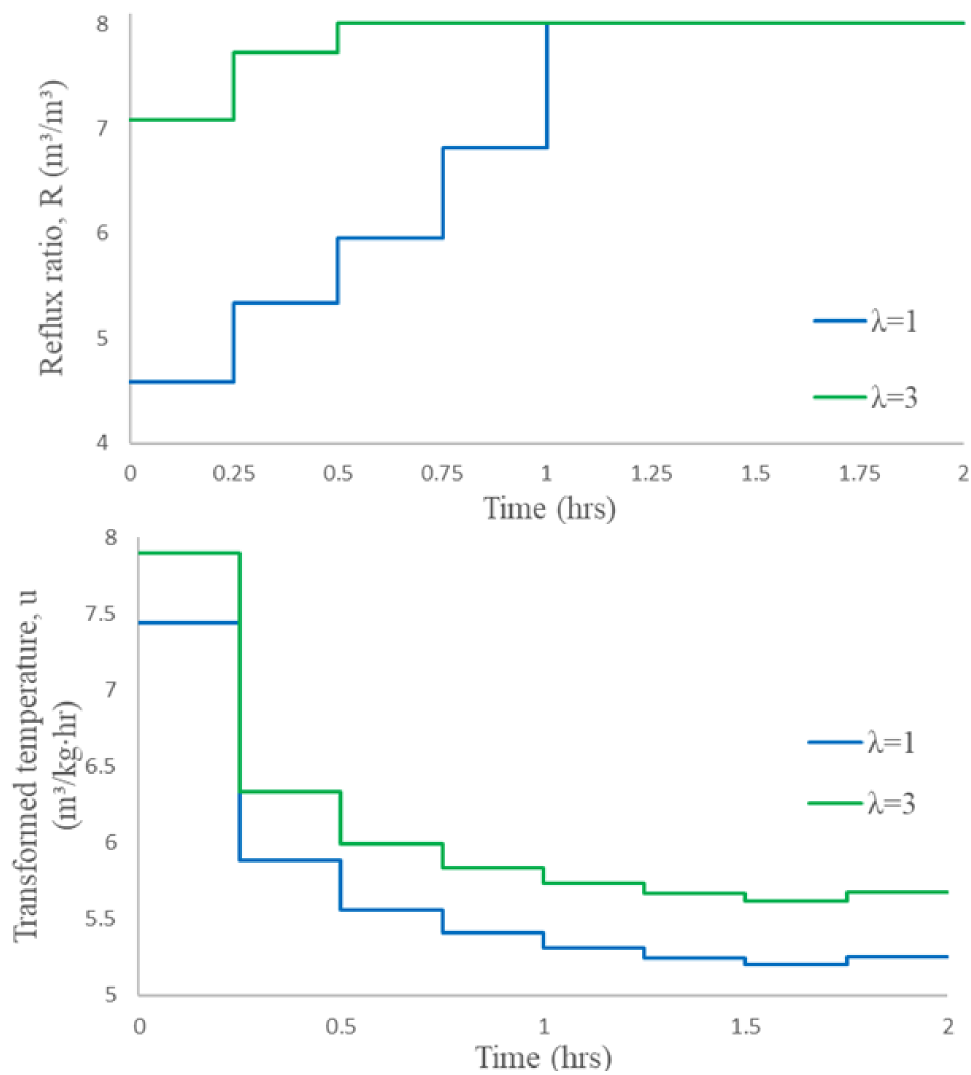

Figure 15: Resulting control decisions when subject to non-gaussian distribution for the back-off approach, when considering different lambda multipliers.

Chapter 6: Conclusions

In this chapter a summary of the contributions of this thesis is presented, highlighting the novelty of the research and expanding upon limitations of the algorithms developed in this study. Based upon the previous considerations, several points are presented for recommendations and possible future research opportunities.

6.1 Summary of Contributions

The research contributes with the development of two algorithms for the integration of scheduling and control of multi-purpose batch plants: an integrated and a decomposition-based approach. The contributions of this study highlight the use of a decomposition algorithm, shown to successfully accommodate stochastic-based model parameter uncertainty. The effect of this uncertainty is shown to significantly impact scheduling and control decisions.

The integrated multi-scenario-based algorithm was shown to obtain robust solutions. This method guarantees to find a local-optimal set of scheduling and control decisions, which remain feasible for all the considered effects of uncertain parameter combinations. However, the computational cost of this algorithm is shown to exponentially grow in size as one considers more realizations in the uncertain parameters, limiting its application to medium-scale plants with a very limited number of uncertain parameters. The resulting complexity of the problem is also highly dependent on the number of discretizations in the scheduling horizon, this is mainly due to the disjunctive task-dependent decisions that have to be performed for each unit at each point in time. For this reason, scalability of this method is limited when considering large number of units with a considerable production make-span. Guaranteeing a globally optimal solution still remains a challenge when considering large-scale non-convex MINLP problems.

The back-off decomposition algorithm was shown to successfully obtain solutions which approximate the objective function of a locally optimal MINLP. A key feature of this algorithm is giving the user the freedom to fine-tune conservativeness of the solution, such that it seeks for scheduling and control solutions that will most-surely remain dynamically feasible under the effect of stochastic uncertainty. However, due to the stochastic nature of the process, there exists certain realizations of the uncertain parameters for which dynamic operability is not guaranteed. The computational benefits of this approach are emphasized, avoiding a combinatorial growth in problem size by approximating multiple effects of process variability. The Monte Carlo simulation stage still remains a bottleneck for this approach; however, possible future improvements may be considered to accurately and efficiently approximate the output distribution of process variability due to uncertainty.

Both the multi-scenario and the back-off algorithms were applied to a multi-product multi-unit batch plant. Considering an open loop control scheme, with the objective of maximizing overall process revenue under the effect of uncertainty. Key decisions include utility costs, material balance constraints, optimal assignation of units and product-dependent constraints. For the decomposition (back-off) approach, a convergence to the local optimal MINLP solution is observed when considering a high enough multiplier on the back-off terms. The effect of back-off terms was observed as a decrease in the overall process revenue when compared against the nominal case; however, optimal open-loop control and scheduling decisions are made, able to mitigate the effects of parameter uncertainty. The effect of different probability density functions on the solution was assessed. When accounting for process variability, a threshold was observed where one product will become more economically attractive. This is reflected as a change in scheduling decisions, favoring the manufacture of the most profitable product.

The scenarios tested in this study showed that the proposed decomposition algorithm remains computationally tractable when compared against an integrated MINLP, without compromising on solution quality. It is observed that conservative solutions are obtained when requiring to incorporate a large magnitude of variability in the process operational constraints, there may be cases where the back-off algorithm becomes a dynamically infeasible problem if limited in control actions (*i.e.* degrees of freedom). A decrease in computational time can be achieved if one chooses to relax the convergence criterion at the expense of lowering the solution quality.

Based on the results obtained in this study, it is shown that there exists important interactions between stochastic effects of parameter uncertainty on scheduling and control decisions. Therefore, there is merit in the consideration for their integration.

6.2 Recommendations and Research Opportunities

On the basis of the previously discussed conclusions, several considerations can be made to improve the efficiency and accuracy of the presented algorithms.

- One main venue for modification of the algorithm would be to consider processing time as a decision variable. This would require however, a complete reformulation of the scheduling scheme into a non-uniform discrete or continuous formulation. This would allow for the exploration of how this new decision variable is sensitive with respect to the uncertain process parameters at the expense of solving more complex optimization formulations.

- Calculation of the back-off terms are based upon a standard deviation, which is adjusted depending of the assumed input distribution of the uncertain process model parameters. This assumption was seen to deviate from reality, as the output distribution is often nonlinear resulting from the non-linearities of the process model. This implies that a re-formulation for updating the back-off terms is necessary, as this will most likely improve the convergence of the algorithm when considering non-gaussian distributions.

- The inclusion of process design and planning decisions would result in a more challenging problem to solve. Although the work presented by Koller et al.[27] includes process design decisions, there is currently no study that explores the solution of planning, design, scheduling and control of batch processes under uncertainty.

- Gauging the performance of the presented back-off decomposition algorithm when solving larger scale, more complex problems is still an aspect that that needs to be explored in detail.

- A more effective method of uncertainty propagation could be implemented, as has been shown in the study presented by Kimaev & Ricardez-Sandoval[98], it is possible to increase the computational performance by implementing polynomial chaos expansions to approximate the distribution of the operational constraints due to the effect of uncertainty, rather than perform expensive MC simulations to obtain the distribution in the process outputs.

- Future research will compare the performance of the proposed back-off approach to other decomposition methods presented in the literature, e.g. Benders decomposition[5,54] or Lagrangian decomposition[53].

- A reformulation would have to be considered for the proposed back-off algorithm to be valid for real-time on-line applications. Integrated reactive scheduling and control under stochastic parameter uncertainty would require information about sensitivities of decisions variables to the effects of uncertainty, so that performing MC simulations to obtain this information might be eliminated altogether.

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Appendix A. Optimization Formulations for the Case Study

A.1 Integrated Approach

In this section the overall optimization problem used for the solution of integrated approach is presented. Several sets used in the formulation correspond to the ones defined on section 4. That is: $K = \{r, f, d\}$), $J = \{Rct, Fil, DisB1, DisB2\}$ and *S= {Feed A, IntABC, WstC, IntAB, RcyB1, RcyB2, ProdB1, ProdB2}*. Task processing time is considered constant, and equal to two hours.

The overall optimization problem consists of 3 main disjunctions (one for each unit considered), within each disjunction, there are J_k modes of operation and one idle state for each unit. This means that equipment which can only perform one task ($J_r = Rct$, $J_f = Fil$) have 2 possible disjunctive decisions, as shown in Equation (19b) for the reactor and (19c) for filter, respectively. Meanwhile, the distillation column ($J_d = DisB1, DisB2$) has three disjunctive decisions (Equation 19d), including its idle state.

$$\max \sum_{\gamma}^{\Gamma} C_{Prod_\gamma} S_{Prod_\gamma,H} - \sum_{\delta=\delta_1}^{\delta_{Nscn}} \omega_\delta \Psi \tag{19a}$$

$s.t.$

$Equations\ (2b - 2d)$

$$\begin{bmatrix} Y_{r,Rct,t} = True \\ W_{r,Rct,t} = 1 \\ Equations\ (8a - c)\ \forall \delta \in \Delta \\ 1.8 \le u_{r,Rct,t}(\tau^j) \le 8.0 \\ \rho_{out_{Rct,IntABC,t,\delta}} = 1\ \ \forall \delta \in \Delta \\ F_{Rct,t,\delta} = Equation\ (9)\ \ \forall \delta \in \Delta \end{bmatrix} \bigvee \begin{bmatrix} Y_{r,Rct,t} = False \\ W_{r,Rct,t} = 0 \\ \rho_{out_{Rct,IntABC,t,\delta}} = 0\ \ \forall \delta \in \Delta \\ F_{Rct,t,\delta} = 0\ \forall \delta \in \Delta \end{bmatrix} \quad \forall t \tag{19b}$$

$$\begin{bmatrix} Y_{f,Fil,t} = True \\ W_{f,Fil,t} = 1 \\ \rho out_{Fil,WstC,t} = Equation\ (11a)\ \forall \delta \in \Delta \\ \rho out_{Fil,IntAB,t} = Equation\ (11b)\ \forall \delta \in \Delta \\ F_{Fil,t,\delta} = Equation\ (10)\ \forall \delta \in \Delta \end{bmatrix} \bigvee \begin{bmatrix} Y_{f,Fil,t} = False \\ W_{f,Fil,t} = 0 \\ \rho out_{Fil,WstC,t} = 0\ \forall \delta \in \Delta \\ \rho out_{Fil,IntAB,t} = 0\ \forall \delta \in \Delta \\ F_{Fil,t,\delta} = 0\ \forall \delta \in \Delta \end{bmatrix} \quad \forall t \qquad (19c)$$

$$\begin{bmatrix} Y_{d,DisB1,t} = True \\ W_{d,DisB1,t} = 1 \\ W_{d,DisB2,t} = 0 \\ Equations\ (12a - 16) \\ 1.8 \leq R \leq 8.0 \\ \rho out_{DisB1,ProdB1,t} = Equation\ (18a)\ \forall \delta \in \Delta \\ \rho out_{DisB1,RcyB1,t} = Equation\ (18b)\ \forall \delta \in \Delta \\ F_{DisB1,t,\delta} = Equation\ (17)\ \forall \delta \in \Delta \end{bmatrix} \bigvee \begin{bmatrix} Y_{d,DisB1,t} = True \\ W_{d,DisB1,t} = 1 \\ W_{d,DisB2,t} = 0 \\ Equations\ (12a - 16) \\ 1.8 \leq R \leq 8.0 \\ \rho out_{DisB2,ProdB2,t} = Equation\ (18a)\ \forall \delta \in \Delta \\ \rho out_{DisB2,RcyB2,t} = Equation\ (18b)\ \forall \delta \in \Delta \\ F_{DisB2,t,\delta} = Equation\ (17)\ \forall \delta \in \Delta \end{bmatrix}$$

$$\bigvee \begin{bmatrix} Y_{d,Dis\gamma,t} = False \\ W_{d,Dis\gamma,t} = 0\ \forall \gamma \in \Gamma \\ \rho out_{Dis\gamma,Prod\gamma,t} = 0\ \forall \gamma \in \Gamma, \delta \in \Delta \\ \rho out_{Dis\gamma,Rcy\gamma,t} = 0\ \forall \gamma \in \Gamma, \delta \in \Delta \\ F_{Dis\gamma,t,\delta} = 0\ \forall \gamma \in \Gamma, \delta \in \Delta \end{bmatrix} \quad \forall t \qquad (19d)$$

$$t \in [0,10], \Delta = \{\delta_1, \delta_2 \dots \delta_{N_{scn}}\}, \Theta_{unc} = \{\alpha, \beta\}, \tau^j \in \left[T^j_{op_0}, T^j_{op_f}\right]\ \forall j$$

A.2 Back-Off Approach

In this section the optimization problems used for the solution of the back-off decomposition approach are presented

Scheduling

$$\max \sum_{\gamma}^{\Gamma} C_{Prod_\gamma} S_{i,Prod_\gamma,H} - \Psi \qquad (20)$$

$s.t.\ Allocation\ Constraints\ (3b)$

$Capacity\ Constraints\ (3c)$

$Material\ Balance\ Constraints\ (3d)$

As shown in Equation (20), the goal of the scheduling problem is to maximize the overall process revenue, given a fixed makespan H and product and specific sale prices ($C_{Prod_{\gamma}}$). The solution to the scheduling problem relates to the dynamics of the plant by sharing the following parameters. The operational cost at each iteration *i* of unit *k* that executes task *j* in time *t* ($F_{j,k,t}$), and material input/output proportion ($\rho_{in\,j,s,t}$ and $\rho_{out\,j,s,t}$). These parameters can be affected by uncertainty and therefore may change at each iteration i.

Dynamic Optimization

Equation (21) presents the overall dynamic optimization problem considered for this case study, where C_{γ} represents the sale price of *ProdB1* 30 (\$/kg) and *ProdB2* 45 (\$/kg), respectively.

$$\max \sum_{\gamma} C_{\gamma} D_{tot_{\gamma}} - \Psi \qquad \forall \gamma \in \Gamma \tag{21}$$

$$s.t.\ \ Equations\ (8) - (15), (17), (18)$$

$$t \in [0, H]$$

The inequality constraint shown in Equation (16) is affected by the uncertain parameters; therefore, these constraints are reformulated as described by the back-off methodology, *i.e.*

$$\bar{x}_{d_{\gamma}} - \lambda b_{i_{\gamma}} \geq \bar{x}_{d_{\gamma}}{}^{*} \qquad \forall \gamma \in \Gamma \tag{22}$$

where $b_{i_{\gamma}}$ represents the back-off term for each product γ estimated at iteration *i*; as described in the previous section. These back-off terms capture the variability in product purity due to the combined stochastic effects of the uncertain kinetic parameter (β) and the relative volatility (α). Thus, resulting scheduling and control decisions obtained from the present analysis are expected to most surely satisfy Equation (16) in the presence of stochastic realizations in the uncertain parameters. To simplify the analysis, a single weighting parameter (λ) for the back-off terms is used in constraint (22) and remains fixed during the execution of the proposed decomposition algorithm.

Note Equation (16) is not considered for the back-off decomposition approach, rather Equation (22) is used in its stead. Through the consideration of the back-off terms, an approximation of the process variability due to stochastic effects of uncertain parameters is achieved. However, in the integrated approach a unique solution is found, which completely satisfies every constraint in the presence of discrete realizations of uncertainty. Equation (22) then, is unnecessary for the integrated formulation.