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Data Article

Data on removal kinetics of pharmaceutical compounds, artificial sweeteners, and perfluoroalkyl substances from water using a passive treatment system containing zero-valent iron and biochar

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ABSTRACT

The data presented in this paper relate to the research paper "Removal of pharmaceutical compounds, artificial sweeteners, and perfluoroalkyl substances from water using a passive treatment system containing zero-valent iron and biochar" [1]. Four columns packed with different ratios of reactive media, including silica sand (SS), zero-valent iron (ZVI), and biochar (BC), were evaluated for simultaneous removal of 14 emerging contaminants from water. The target emerging contaminants included eight pharmaceuticals (carbamazepine, caffeine, sulfamethoxazole, 3,4-methylenedioxyamphetamine, 3,4-methylenedioxymethamphetamine, ibuprofen, gemfibrozil, and naproxen), four artificial sweeteners (acesulfame-K, sucralose, saccharin, and cyclamate), and two perfluoroalkyl substances (perfluorooctanoic acid and perfluorooctane sulfonic acid). The samples for target contaminant analysis were collected from the influent, effluent, and profile (along the flow direction) ports of each column. The removal data (concentration vs. residence time) for each target contaminant were fitted to the first-order (exponential decay equation) or zero-order (linear equation) model using SigmaPlot. The removal rate, removal rate constant (k_{obs}), mass normalized rate constant (k_M), surface area

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normalized rate constant (k_{SA}, specific reaction rate constant), and half-life ($t_{0.5}$) of target contaminants in Columns *ZVI*, *BC*, and *(ZVI + BC)* were calculated and summarized in this dataset.

Specifications Table

Subject	Chemistry
Specific subject area	Organic chemistry, removal kinetics
Type of data	Table
How data were acquired	Software SigmaPlot
Data format	Analyzed
Parameters for data collection	The first-order kinetic data were obtained through the exponential decay fitting in the Regression Wizard in SigmaPlot; the zero-order kinetic data were obtained through the linear fitting in Regression Wizard in SigmaPlot.
Description of data collection	The removal kinetic data were collected through the data analysis (Regression Wizard) in SigmaPlot.
Data source location	University of Waterloo, Waterloo, Ontario Canada
Data accessibility	Data are available in this article
Related research article	YingYing Liu, David W. Blowes, Carol J. Ptacek, and Laura G. Groza Removal of pharmaceutical compounds, artificial sweeteners, and perfluoroalkyl substances from water using a passive treatment system containing zero-valent iron and biochar Science of the Total Environment https://doi.org/10.1016/j.scitotenv.2019.06.450

Value of the Data

- The data in this article provide important information on degradation kinetics such as removal rates and half-lives for 14 emerging contaminants treated by zero-valent iron (ZVI) and biochar (BC).
- Researchers working in the field of remediation of emerging contaminants in water can benefit from the data in this article.
- The data present in this article can provide useful information and guidelines for selecting the appropriate types of reactive media to remove specific emerging contaminants.
- The removal kinetic data (removal rate and half-life) can be used to design reactors or permeable reactive barriers (PRBs) for future large-scale field applications.

1. Data

The dataset showed the removal kinetic parameters, including removal rate constant (k_{obs}), mass normalized rate constant (k_M), surface area normalized rate constant (k_{SA}, specific reaction rate constant), and half-life ($t_{0.5}$), for 14 target emerging contaminants in Column *ZVI*, Column *BC*, and Column *(ZVI + BC)*. The kinetic parameters for each contaminant are summarized in separate tables (Tables 1–14). The raw data (concentration vs. residence time) of each contaminant can be found in the related research article [1].

2. Experimental design, materials, and methods

2.1. Materials

The native analyte compounds carbamazepine (CBZ), caffeine (CAF), sulfamethoxazole (SMX), ibuprofen (IBU), gemfibrozil (GEM), naproxen (NAP), cyclamate (CYC), and saccharin (SAC) for calibration standards and input stock solution were obtained from Sigma-Aldrich (Oakville, ON, Canada).

Table 1
First-order removal rate constant (k_{obs}), mass normalized rate constant (k_M), surface area normalized rate constant (k_{SA}, specific reaction rate constant), and half-life ($t_{0.5}$) of pharmaceutical ***carbamazepine*** in Column *ZVI*, Column *BC*, and Column *(ZVI + BC)*. k_{obs} is calculated using least-squares regression during two experimental stages. ^{t}C is the carbamazepine concentration.

Column	Stage	PV	Removal rate^{t}, μmol L^{-1} d^{-1} (μg L^{-1} d^{-1})	k_{obs}, d^{-1}	k_M, L g^{-1} d^{-1}	k_{SA}, L m^{-2} d^{-1}	$t_{0.5}$, d	R^2
Column 2 (ZVI)	1	1	1.1E+01 × C	1.1E+01	2.6E-03	2.8E-04	0.06	0.999
		13	4.9 × C	4.9	1.1E-03	1.2E-04	0.14	0.975
		25	4.4 × C	4.4	1.0E-03	1.1E-04	0.16	0.965
	2	53	1.2 × C	1.2	2.9E-04	3.0E-05	0.56	0.931
Column 3 (BC)	1	1	5.4 × C	5.4	1.2E-02	1.8E-04	0.19	0.998
		13	2.5 × C	2.5	5.3E-03	8.2E-05	0.28	0.998
		25	1.9 × C	1.9	4.2E-03	6.4E-05	0.36	0.996
	2	53	0.7 × C	0.7	1.5E-03	2.3E-05	1.0	0.970
Column 4 (ZVI + BC)	1	1	8.2 × C	8.2	7.2E-03	2.1E-04	0.09	0.999
		13	4.5 × C	4.5	3.9E-03	1.2E-04	0.16	0.966
		25	4.0 × C	4.0	3.5E-03	1.0E-04	0.17	0.970
	2	53	1.3 × C	1.3	1.1E-03	3.3E-05	0.55	0.992

Table 2
First-order removal rate constant (k_{obs}), mass normalized rate constant (k_M), surface area normalized rate constant (k_{SA}, specific reaction rate constant), and half-life ($t_{0.5}$) of pharmaceutical ***caffeine*** *in* Column *ZVI*, Column *BC, and* Column *(ZVI + BC)*. k_{obs} is calculated using least-squares regression during two experimental stages. ^{t}C is the caffeine concentration.

Column	Stage	PV	Removal rate^{t}, μmol L^{-1} d^{-1} (μg L^{-1} d^{-1})	k_{obs}, d^{-1}	k_M, L g^{-1} d^{-1}	k_{SA}, L m^{-2} d^{-1}	$t_{0.5}$, d	R^2
Column 2 (ZVI)	1	1	1.6E+01 × C	1.6E+01	3.7E-03	3.9E-04	0.04	0.999
		13	7.2 × C	7.2	1.7E-03	1.8E-04	0.10	0.998
		25	5.1 × C	5.1	1.2E-03	1.2E-04	0.14	0.982
	2	53	1.5 × C	1.5	3.5E-04	3.6E-05	0.47	0.961
Column 3 (BC)	1	1	4.8 × C	4.8	1.0E-02	1.6E-04	0.14	0.999
		13	2.8 × C	2.8	6.0E-03	9.4E-05	0.25	0.999
		25	2.2 × C	2.2	4.8E-03	7.4E-05	0.31	0.996
	2	53	1.0 × C	1.0	2.1E-03	3.3E-05	0.70	0.973
Column 4 (ZVI + BC)	1	1	6.9 × C	6.9	6.0E-03	1.8E-04	0.10	0.996
		13	5.5 × C	5.5	4.8E-03	1.4E-04	0.13	0.989
		25	4.5 × C	4.5	3.9E-03	1.2E-04	0.15	0.973
	2	53	1.7 × C	1.7	1.5E-03	4.5E-05	0.40	0.996

Table 3
First-order removal rate constant (k_{obs}), mass normalized rate constant (k_M), surface area normalized rate constant (k_{SA}, specific reaction rate constant), and half-life ($t_{0.5}$) of pharmaceutical ***sulfamethoxazole*** *in* Column *ZVI*, Column *BC, and* Column *(ZVI + BC)*. k_{obs} is calculated using least-squares regression during two experimental stages. ^{t}C is the sulfamethoxazole concentration. "–" represents not applicable.

Column	Stage	PV	Removal rate^{t}, μmol L^{-1} d^{-1} (μg L^{-1} d^{-1})	k_{obs}, d^{-1}	k_M, L g^{-1} d^{-1}	k_{SA}, L m^{-2} d^{-1}	$t_{0.5}$, d	R^2
Column 1 (Control)	1	25	0.2 × C	0.2	–	–	3.6	0.877
	2	53	0.4 × C	0.4	–	–	1.8	0.984
Column 2 (ZVI)	1	1	4.5E+02 × C	4.5E+02	1.1E-01	1.1E-02	0.002	1.000
		13	4.7E+02 × C	4.7E+02	1.1E-01	1.1E-02	0.001	1.000
		25	4.6E+02 × C	4.6E+02	1.1E-01	1.1E-02	0.001	1.000
	2	53	1.5E+02 × C	1.5E+02	3.5E-02	3.7E-03	0.005	1.000
Column 3 (BC)	1	1	1.6 × C	1.6	3.5E-03	5.4E-05	0.43	0.999
		13	1.2 × C	1.2	2.5E-03	3.8E-05	0.60	0.999
		25	1.1 × C	1.1	2.4E-03	3.8E-05	0.61	0.993
	2	53	0.5 × C	0.5	1.1E-03	1.7E-05	1.4	0.991
Column 4 (ZVI + BC)	1	1	4.5E+02 × C	4.5E+02	4.0E-01	1.2E-02	0.002	1.000
		13	4.7E+02 × C	4.7E+02	4.1E-01	1.2E-02	0.001	1.000
		25	4.6E+02 × C	4.6E+02	4.1E-01	1.2E-02	0.001	1.000
	2	53	1.5E+02 × C	1.5E+02	1.3E-01	3.9E-03	0.005	1.000

Table 4
First-order removal rate constant (k_{obs}), mass normalized rate constant (k_M), surface area normalized rate constant (k_{SA}, specific reaction rate constant), and half-life ($t_{0.5}$) of pharmaceutical ***3,4-methylenedioxyamphetamine (MDA)*** *in* Column *ZVI*, Column *BC, and* Column *(ZVI + BC)*. k_{obs} is calculated using least-squares regression during two experimental stages. ^{t}C is the MDA concentration.

Column	Stage	PV	Removal rate^{t}, μmol L^{-1} d^{-1} (μg L^{-1} d^{-1})	k_{obs}, d^{-1}	k_M, L g^{-1} d^{-1}	k_{SA}, L m^{-2} d^{-1}	$t_{0.5}$, d	R^2
Column 2 (ZVI)	1	1	1.9E+02 × *C*	1.9E+02	4.3E-02	4.6E-03	0.004	1.000
		13	1.3E+01 × *C*	1.3E+01	3.0E-03	3.1E-04	0.06	0.999
		25	7.8 × *C*	7.8	1.8E-03	1.9E-04	0.09	0.998
	2	53	2.4 × *C*	2.4	5.5E-04	5.8E-05	0.29	0.996
Column 3 (BC)	1	1	1.1E+01 × *C*	1.1E+01	2.4E-02	3.7E-04	0.06	0.999
		13	8.1 × *C*	8.1	1.7E-02	2.7E-04	0.09	0.997
		25	5.1 × *C*	5.1	1.1E-02	1.7E-04	0.14	0.998
	2	53	3.2 × *C*	3.2	6.8E-03	1.1E-04	0.22	0.997
Column 4 (ZVI + BC)	1	1	2.0E+01 × *C*	2.0E+01	1.8E-02	5.3E-04	0.03	1.000
		13	1.2E+01 × *C*	1.2E+01	1.0E-02	3.0E-04	0.06	0.999
		25	8.7 × *C*	8.7	7.6E-03	2.3E-04	0.08	0.999
	2	53	3.9 × *C*	3.9	3.4E-03	1.0E-04	0.18	0.999

Table 5
First-order removal rate constant (k_{obs}), mass normalized rate constant (k_M), surface area normalized rate constant (k_{SA}, specific reaction rate constant), and half-life ($t_{0.5}$) of pharmaceutical **3,4-methylenedioxymethamphetamine (MDMA)** *in* Column *ZVI*, Column *BC, and* Column *(ZVI + BC)*. k_{obs} is calculated using least-squares regression during two experimental stages. ^{t}C is the MDMA concentration.

Column	Stage	PV	Removal rate^{t}, μmol L^{-1} d^{-1} (μg L^{-1} d^{-1})	k_{obs}, d^{-1}	k_M, L g^{-1} d^{-1}	k_{SA}, L m^{-2} d^{-1}	$t_{0.5}$, d	R^2
Column 2 (ZVI)	1	1	3.0E+02 × *C*	3.0E+02	6.9E-02	7.3E-03	0.002	1.000
		13	3.5E+02 × *C*	3.5E+02	8.2E-02	8.7E-03	0.002	1.000
		25	1.4E+01 × *C*	1.4E+01	3.2E-03	3.4E-04	0.05	1.000
	2	53	4.0 × *C*	4.0	9.3E-04	9.8E-05	0.17	1.000
Column 3 (BC)	1	1	1.1E+01 × *C*	1.1E+01	2.3E-02	3.6E-04	0.07	0.999
		13	7.7 × *C*	7.7	1.7E-02	2.6E-04	0.09	0.998
		25	5.2 × *C*	5.2	1.1E-02	1.7E-04	0.13	0.997
	2	53	3.1 × *C*	3.1	6.7E-03	1.0E-04	0.22	0.997
Column 4 (ZVI + BC)	1	1	2.5E+01 × *C*	2.5E+01	2.2E-02	6.6E-04	0.03	1.000
		13	1.6E+01 × *C*	1.6E+01	1.4E-02	4.1E-04	0.04	1.000
		25	1.0E+01 × *C*	1.0E+01	9.0E-03	2.7E-04	0.07	0.999
	2	53	4.3 × *C*	4.3	3.8E-03	1.1E-04	0.16	1.000

Table 6
First-order removal rate constant (k_{obs}), mass normalized rate constant (k_M), surface area normalized rate constant (k_{SA}, specific reaction rate constant), and half-life ($t_{0.5}$) of pharmaceutical ***ibuprofen*** *in* Column *ZVI*, Column *BC, and* Column *(ZVI + BC)*. k_{obs} is calculated using least-squares regression during two experimental stages. ^{t}C is the ibuprofen concentration.

Column	Stage	PV	Removal rate^{t}, μmol L^{-1} d^{-1} (μg L^{-1} d^{-1})	k_{obs}, d^{-1}	k_M, L g^{-1} d^{-1}	k_{SA}, L m^{-2} d^{-1}	$t_{0.5}$, d	R^2
Column 2 (ZVI)	1	1	2.6 × *C*	2.6	6.0E-04	6.3E-05	0.27	0.943
		13	1.2 × *C*	1.2	2.9E-04	3.0E-05	0.56	0.926
		25	0.9 × *C*	0.9	2.2E-04	2.3E-05	0.74	0.932
	2	53	0.2 × *C*	0.2	4.7E-05	4.9E-06	3.5	0.864
Column 3 (BC)	1	1	1.9 × *C*	1.9	4.2E-03	6.5E-05	0.36	0.992
		13	1.2 × *C*	1.2	2.6E-03	4.0E-05	0.57	0.997
		25	1.1 × *C*	1.1	2.4E-03	3.7E-05	0.63	0.996
	2	53	0.4 × *C*	0.4	8.9E-04	1.4E-05	1.7	0.992
Column 4 (ZVI + BC)	1	1	2.9 × *C*	2.9	2.5E-03	7.6E-05	0.24	0.978
		13	1.7 × *C*	1.7	1.5E-03	4.5E-05	0.41	0.958
		25	1.6 × *C*	1.6	1.4E-03	4.1E-05	0.44	0.952
	2	53	0.5 × *C*	0.5	4.0E-04	1.2E-05	1.5	0.941

Table 7
First-order removal rate constant (k_{obs}), mass normalized rate constant (k_M), surface area normalized rate constant (k_{SA}, specific reaction rate constant), and half-life ($t_{0.5}$) of pharmaceutical ***gemfibrozil*** *in* Column *ZVI,* Column *BC, and* Column *(ZVI + BC).* k_{obs} is calculated using least-squares regression during two experimental stages. ^{t}C is the gemfibrozil concentration.

Column	Stage	PV	Removal rate^{t}, μmol L^{-1} d^{-1} (μg L^{-1} d^{-1})	k_{obs}, d^{-1}	k_M, L g^{-1} d^{-1}	k_{SA}, L m^{-2} d^{-1}	$t_{0.5}$, d	R^2
Column 2 (ZVI)	1	1	9.3 × C	9.3	2.2E-03	2.3E-04	0.07	0.999
		13	4.6 × C	4.6	1.1E-03	1.1E-04	0.15	0.969
		25	3.5 × C	3.5	8.2E-04	8.6E-05	0.20	0.954
	2	53	1.0 × C	1.0	2.4E-04	2.5E-05	0.67	0.927
Column 3 (BC)	1	1	4.5 × C	4.5	9.7E-03	1.5E-04	0.15	0.997
		13	2.4 × C	2.4	5.1E-03	8.0E-05	0.29	0.995
		25	1.8 × C	1.8	3.8E-03	5.9E-05	0.39	0.996
	2	53	0.6 × C	0.6	1.4E-03	2.1E-05	1.1	0.981
Column 4 (ZVI + BC)	1	1	5.9 × C	5.9	5.1E-03	1.5E-04	0.12	0.990
		13	3.5 × C	3.5	3.1E-03	9.2E-05	0.20	0.967
		25	2.8 × C	2.8	2.5E-03	7.4E-05	0.24	0.935
	2	53	0.9 × C	0.9	7.6E-04	2.3E-05	0.80	0.989

Table 8
First-order removal rate constant (k_{obs}), mass normalized rate constant (k_M), surface area normalized rate constant (k_{SA}, specific reaction rate constant), and half-life ($t_{0.5}$) of pharmaceutical ***naproxen*** *in* Column *ZVI,* Column *BC, and* Column *(ZVI + BC).* k_{obs} is calculated using least-squares regression during two experimental stages. ^{t}C is the naproxen concentration.

Column	Stage	PV	Removal rate^{t}, μmol L^{-1} d^{-1} (μg L^{-1} d^{-1})	k_{obs}, d^{-1}	k_M, L g^{-1} d^{-1}	k_{SA}, L m^{-2} d^{-1}	$t_{0.5}$, d	R^2
Column 2 (ZVI)	1	1	5.7 × C	5.7	1.3E-03	1.4E-04	0.12	0.988
		13	3.1 × C	3.1	7.2E-04	7.6E-05	0.22	0.908
		25	2.8 × C	2.8	6.4E-04	6.8E-05	0.25	0.949
	2	53	0.6 × C	0.6	1.4E-04	1.5E-05	1.2	0.941
Column 3 (BC)	1	1	3.7 × C	3.7	8.0E-03	1.2E-04	0.19	0.999
		13	2.0 × C	2.0	4.2E-03	6.6E-05	0.35	0.996
		25	1.7 × C	1.7	3.6E-03	5.6E-05	0.41	0.999
	2	53	0.6 × C	0.6	1.4E-03	2.2E-05	1.1	0.985
Column 4 (ZVI + BC)	1	1	4.7 × C	4.7	4.1E-03	1.2E-04	0.15	0.978
		13	3.0 × C	3.0	2.6E-03	7.7E-05	0.23	0.959
		25	2.6 × C	2.6	2.2E-03	6.7E-05	0.27	0.977
	2	53	0.7 × C	0.7	6.5E-04	1.9E-05	0.94	0.980

The isotope-labeled standards CBZ-d10, CAF-d3, IBU-d3, GEM-d6, and [^{13}C]-NAP were obtained from Cambridge Isotope Laboratory Inc. (Tewksbury, MA, USA). The native analytes acesulfame-K (ACE-K), sucralose (SCL), and the isotope-labeled standards SMX-d4, CYC-d11, SAC-^{13}C6, ACE-K-d4, and SCL-d6 were obtained from Toronto Research Chemicals Inc. (Toronto, ON, Canada). The native analytes 3,4-methylenedioxyamphetamine (MDA), 3,4-methylenedioxymethamphetamine (MDMA), and isotope-labeled MDA-d5 and MDMA-d5 were obtained from Cerilliant Corporation (Round Rock, TX, USA). The native analytes perfluorooctanoic acid (PFOA), perfluorooctane sulfonic acid (PFOS), and their isotope-labeled standards [^{13}C]-PFOA and [^{13}C]-PFOS were obtained from Wellington Laboratories Inc. (Guelph, ON, Canada). The analytes PFOA and PFOS as dry powder for preparation of the input stock solution were obtained from Sigma-Aldrich, Canada. The silica sand (SS; 0.6–0.8 mm) was obtained from US Silica Company Inc. (Ottawa, IL, USA). The granular zero-valent iron (ZVI; 0.25–1.19 mm) was obtained from Connelly-GPM Inc. (Chicago, IL, USA). The biochar (BC; oak hard wood; 0.50–2.36 mm) was obtained from Cowboy Charcoal Co. (Brentwood, TN, USA).

2.2. Column experimental design

Four acrylic columns were used, each column was 30 cm in length and 5 cm inner diameter. Influent and effluent ports were installed on the bottom and top of each column, respectively, for introducing

Table 9
Zero- or first-order removal rate constant (k_{obs}), mass normalized rate constant (k_M), surface area normalized rate constant (k_{SA}, specific reaction rate constant), and half-life ($t_{0.5}$) of artificial sweetener ***acesulfame-K*** *in* Column *ZVI,* Column *BC, and* Column *(ZVI + BC)*. Removal rate constant k_{obs} is calculated using least-squares regression during two experimental stages. [i]C is the acesulfame-K concentration. "—" represents no removal of acesulfame-K was observed.

Column	Stage	PV	Removal rate[i], μmol L^{-1} d^{-1} (μg L^{-1} d^{-1})	k_{obs}	k_M	k_{SA}	$t_{0.5}$,	R^2
Column 2 (ZVI)	1	1	2.3E-01 × C[a]	2.3E-01[a]	5.3E-05[a]	5.6E-06[a]	3.1	0.749
		13	1.0E-01 × C[a]	1.0E-01[a]	2.4E-05[a]	2.6E-06[a]	6.6	0.906
		25	9.8E-02 × C[a]	9.8E-02[a]	2.3E-05[a]	2.4E-06[a]	7.0	0.874
	2	53	1.1E-01 × C[a]	1.1E-01[a]	2.7E-05[a]	2.8E-06[a]	6.1	0.870
Column 3 (BC)	1	1	1.6 E+01[b]	1.6 E+01[b]	3.4E-02[b]	5.3E-04[b]	3.2	0.864
		13	–	–	–	–	–	–
		25	–	–	–	–	–	–
	2	53	–	–	–	–	–	–
Column 4 (ZVI + BC)	1	1	5.9[b]	5.8[b]	5.1E-03[b]	1.5E-04[b]	8.3	0.976
		13	4.2[b]	4.2[b]	3.7E-03[b]	1.1E-04[b]	12	0.634
		25	4.9[b]	4.9[b]	4.3E-03[b]	1.3E-04[b]	10	0.835
	2	53	3.2[b]	3.2[b]	2.8E-03[b]	8.3E-05[b]	17	0.866

[a] Removal of acesulfame-K followed a first-order reaction rate, unit of k_{obs} is d^{-1}, unit of k_M is L g^{-1} d^{-1}, unit of k_{SA} is L m^{-2} d^{-1}.
[b] Removal of acesulfame-K followed a zero-order reaction rate, unit of k_{obs} is μmol acesulfame-K L^{-1} d^{-1} (μg acesulfame-K L^{-1} d^{-1}), unit of k_M is μmol acesulfame-K d^{-1} g^{-1} (μg acesulfame-K d^{-1} g^{-1}), unit of k_{SA} is μmol acesulfame-K d^{-1} m^{-2} (μg acesulfame-K d^{-1} m^{-2}).

input solution and discharging effluent. Seven sampling ports were installed along the length of each column at 3.75-cm intervals for profile sampling. Column *Control* was packed with 100% SS. Column *ZVI* and Column *BC* were packed with 50% (vol%) of ZVI and BC, respectively, and balanced with SS. Column *(ZVI + BC)* was packed with 10% (vol%) of ZVI, 40% (vol%) of BC, and balanced with SS.

Input solution contained 10 μg L^{-1} of pharmaceuticals CBZ, CAF, SMX, MDA, MDMA, IBU, GEM, and NAP; 100 μg L^{-1} of artificial sweeteners ACE-K, CYC, SAC, and SCL; and 50 μg L^{-1} of PFOA and 20–100 μg L^{-1} of PFOS. The input solution was pumped through four columns from bottom to top at a flow rate of 0.3 pore volume (PV) d^{-1} before 50 PV during the first stage of the experiment; the flow rate was decreased to 0.1 PV d^{-1} after 50 PV during the second stage of the experiment. Three profile samplings (along the length of the columns) were performed during the first stage of the experiment after 1, 13, and 25 PV of flow through the columns; one profile sampling was conducted during the second stage of the experiment after 53 PV of flow.

All the emerging contaminant samples were spiked with isotopically-labeled internal standards before analysis. The pharmaceutical, PFOA, and PFOS samples were then concentrated through a solid phase extraction (SPE) process; their concentrations were determined using liquid chromatography (LC) followed by tandem mass spectrometry (MS). The concentrations of artificial sweeteners were directly analyzed by ion chromatography (IC) followed by MS without SPE. Detailed information on column experimental setup and analytical procedures for target emerging contaminants are summarized by Liu et al. [1].

*2.3. Removal kinetics of target emerging contaminants by ZVI, BC, and (*ZVI + BC*)*

The removal rates (k_{obs}) for target emerging contaminants during two experimental stages were calculated using least-squares regression in SigmaPlot. The removal of target pharmaceuticals within Columns *ZVI*, *BC*, and *(ZVI+BC)* followed a first-order rate model reported by Liu et al. [1] that can be described by equation (1). k_M and k_{SA} were calculated according to equations (2) and (3) which are defined by Johnson et al. [2]. The half-life ($t_{0.5}$) of the first-order rate for target pharmaceuticals was calculated following equation (4).

$$-\frac{dC}{dt} = k_{obs}\, C \tag{1}$$

Table 10
Zero-order removal rate constant (k_{obs}), mass normalized rate constant (k_M), surface area normalized rate constant (k_{SA}, specific reaction rate constant), and half-life ($t_{0.5}$) of artificial sweetener ***cyclamate*** *in* Column *ZVI*, Column *BC, and* Column *(ZVI + BC)*. Removal rate constant k_{obs} is calculated using least-squares regression during two experimental stages. "–" represents no removal of cyclamate was observed.

Column	Stage	PV	Removal rate, μmol L^{-1} d^{-1} (μg L^{-1} d^{-1})	k_{obs}, μmol L^{-1} d^{-1} (μg L^{-1} d^{-1})	k_M, μmol g^{-1} d^{-1} (μg g^{-1} d^{-1})	k_{SA}, μmol m^{-2} d^{-1} (μg m^{-2} d^{-1})	$t_{0.5}$, d	R^2
Column 2 (ZVI)	1	1	1.5E+01	1.5E+01	3.6E-03	3.8E-04	3.3	0.697
		13	–	–	–	–	–	–
		25	–	–	–	–	–	–
	2	53	–	–	–	–	–	–
Column 3 (BC)	1	1	8.4	8.4	1.8E-02	2.8E-04	5.8	0.839
		13	–	–	–	–	–	–
		25	–	–	–	–	–	–
	2	53	–	–	–	–	–	–
Column 4 (ZVI + BC)	1	1	2.0	2.0	1.8E-03	5.2E-05	23	0.624
		13	–	–	–	–	–	–
		25	–	–	–	–	–	–
	2	53	–	–	–	–	–	–

Note: The poor R^2 values at 1 PV in this table are likely due to little removal of cyclamate in the three treatment columns.

Table 11
Zero- or first-order removal constant (k_{obs}), mass normalized rate constant (k_M), surface area normalized rate constant (k_{SA}, specific reaction rate constant), and half-life ($t_{0.5}$) of artificial sweetener ***saccharin*** *in* Column *ZVI*, Column *BC*, *and* Column *(ZVI + BC)*. Removal rate constant k_{obs} is calculated using least-squares regression during two experimental stages. ^{t}C is the saccharin concentration. "–" represents no removal of saccharin was observed.

Column	Stage	PV	Removal rate[t], μmol L^{-1} d^{-1} (μg L^{-1} d^{-1})	k_{obs}	k_M	k_{SA}	$t_{0.5}$, d	R^2
Column 2 (ZVI)	1	1	3.5E+01[b]	3.5E+01[b]	8.1E-03[b]	8.6E-04[b]	1.5	0.898
		13	4.7[b]	4.7[b]	1.1E-03[b]	1.2E-04[b]	9.3	0.804
		25	–	–	–	–	–	–
	2	53	1.7[b]	1.7[b]	3.9E-04[b]	4.1E-05[b]	32	0.583
Column 3 (BC)	1	1	1.0 × C[a]	1.0[a]	2.2E-03[a]	3.4E-05[a]	0.7	0.978
		13	0.5 × C[a]	0.5[a]	9.8E-04[a]	1.5E-05[a]	1.5	0.981
		25	2.4E+01[b]	2.4E+01[b]	5.2E-02[b]	8.0E-04[b]	2.2	0.983
	2	53	2.6[b]	2.6[b]	5.6E-03[b]	8.6E-05[b]	21	0.828
Column 4 (ZVI + BC)	1	1	3.4E+01[b]	3.4E+01[b]	3.0E-02[b]	8.9E-04[b]	1.3	0.969
		13	1.4E+01[b]	1.4E+01[b]	1.2E-02[b]	3.6E-04[b]	3.1	0.960
		25	1.1E+01[b]	1.1E+01[b]	9.4E-03[b]	2.8E-04[b]	4.9	0.845
	2	53	2.1[b]	2.1[b]	1.9E-03[b]	5.6E-05[b]	25	0.701

[a] Removal of saccharin followed a first-order reaction rate, unit of k_{obs} is d^{-1}, unit of k_M is L g^{-1} d^{-1}, unit of k_{SA} is L m^{-2} d^{-1}.
[b] Removal of saccharin followed a zero-order reaction rate, unit of k_{obs} is μmol saccharin L^{-1} d^{-1} (μg saccharin L^{-1} d^{-1}), unit of k_M is μmol saccharin d^{-1} g^{-1} (μg saccharin d^{-1} g^{-1}), unit of k_{SA} is μmol saccharin d^{-1} m^{-2} (μg saccharin d^{-1} m^{-2}).

Table 12
Zero- or first-order removal constant (k_{obs}), mass normalized rate constant (k_M), surface area normalized rate constant (k_{SA}, specific reaction rate constant), and half-life ($t_{0.5}$) of artificial sweetener ***sucralose*** *in* Column *ZVI*, Column *BC*, *and* Column *(ZVI + BC)*. Removal rate constant k_{obs} is calculated using least-squares regression during two experimental stages. ^{t}C is the sucralose concentration.

Column	Stage	PV	Removal rate[t], μmol L^{-1} d^{-1} (μg L^{-1} d^{-1})	k_{obs}	k_M	k_{SA}	$t_{0.5}$, d	R^2
Column 2 (ZVI)	1	1	2.1 × C[a]	2.1[a]	4.8E-04[a]	5.1E-05[a]	0.3	0.922
		13	1.0 × C[a]	1.0[a]	2.4E-04[a]	2.5E-05[a]	0.7	0.927
		25	4.4E+01[b]	4.4E+01[b]	1.0E-02[b]	1.1E-03[b]	1.4	0.963
	2	53	1.2E+01[b]	1.2E+01[b]	2.8E-03[b]	2.9E-04[b]	4.9	0.995
Column 3 (BC)	1	1	1.3 × C[a]	1.3[a]	2.7E-03[a]	4.2E-05[a]	0.5	0.999
		13	0.9 × C[a]	0.9[a]	1.9E-03[a]	2.9E-05[a]	0.8	0.983
		25	0.7 × C[a]	0.7[a]	1.4E-03[a]	2.2E-05[a]	1.1	0.983
	2	53	0.2 × C[a]	0.2[a]	4.3E-04[a]	6.6E-06[a]	3.5	0.981
Column 4 (ZVI + BC)	1	1	1.6 × C[a]	1.6[a]	1.4E-03[a]	4.2E-05[a]	0.4	0.948
		13	0.9 × C[a]	0.9[a]	8.1E-04[a]	2.4E-05[a]	0.8	0.961
		25	0.7 × C[a]	0.7[a]	6.4E-04[a]	1.9E-05[a]	1.0	0.942
	2	53	0.2 × C[a]	0.2[a]	1.6E-04[a]	4.7E-06[a]	3.9	0.995

[a] Removal of sucralose followed a first-order reaction rate, unit of k_{obs} is d^{-1}, unit of k_M is L g^{-1} d^{-1}, unit of k_{SA} is L m^{-2} d^{-1}.
[b] Removal of sucralose followed a zero-order reaction rate, unit of k_{obs} is μmol sucralose L^{-1} d^{-1} (μg sucralose L^{-1} d^{-1}), unit of k_M is μmol sucralose d^{-1} g^{-1} (μg sucralose d^{-1} g^{-1}), unit of k_{SA} is μmol sucralose d^{-1} m^{-2} (μg sucralose d^{-1} m^{-2}).

$$k_M = \frac{k_{obs}}{\rho_m} \tag{2}$$

$$k_{SA} = \frac{k_{obs}}{\rho_a} = \frac{k_M}{a_s} \tag{3}$$

$$t_{0.5} = \frac{0.693}{k_{obs}} \tag{4}$$

Table 13
Zero- or first-order removal constant (k_{obs}), mass normalized rate constant (k_M), surface area normalized rate constant (k_{SA}, specific reaction rate constant), and half-life ($t_{0.5}$) of **perfluorooctanoic acid (PFOA)** *in* Column *ZVI,* Column *BC, and* Column *(ZVI + BC)*. Removal rate constant k_{obs} is calculated using least-squares regression during two experimental stages. ^{t}C is the PFOA concentration. "—" represents no removal of PFOA was observed.

Column	Stage	PV	Removal rate^{t}, μmol L^{-1} d^{-1} (μg L^{-1} d^{-1})	k_{obs}	k_M	k_{SA}	$t_{0.5}$, d	R^2
Column 2 (ZVI)	1	1	2.2E+01[b]	2.2E+01[b]	5.2E-03[b]	5.5E-04[b]	1.3	0.821
		13	–	–	–	–	–	–
		25	–	–	–	–	–	–
	2	53	–	–	–	–	–	–
Column 3 (BC)	1	1	1.0 × C[a]	1.0[a]	2.1E-03[a]	3.3E-05[a]	0.7	0.980
		13	0.5 × C[a]	0.5[a]	1.1E-03[a]	1.8E-05[a]	1.3	0.987
		25	1.2E+01[b]	1.2E+01[b]	2.5E-02[b]	3.9E-04[b]	2.3	0.956
	2	53	0.9[b]	0.9[b]	1.9E-03[b]	3.0E-05[b]	25	0.780
Column 4 (ZVI + BC)	1	1	2.0E+01[b]	2.0E+01[b]	1.8E-02[b]	5.3E-04[b]	1.3	0.935
		13	7.7[b]	7.7[b]	6.7E-03[b]	2.0E-04[b]	3.3	0.933
		25	2.0[b]	2.0[b]	1.7E-03[b]	5.1E-05[b]	13	0.725
	2	53	–	–	–	–	–	–

[a] Removal of PFOA followed a first-order reaction rate, unit of k_{obs} is d^{-1}, unit of k_M is L g^{-1} d^{-1}, unit of k_{SA} is L m^{-2} d^{-1}.
[b] Removal of PFOA followed a zero-order reaction rate, unit of k_{obs} is μmol PFOA L^{-1} d^{-1} (μg PFOA L^{-1} d^{-1}), unit of k_M is μmol PFOA d^{-1} g^{-1} (μg PFOA d^{-1} g^{-1}), unit of k_{SA} is μmol PFOA d^{-1} m^{-2} (μg PFOA d^{-1} m^{-2}).

Table 14
Zero- or first-order removal constant (k_{obs}), mass normalized rate constant (k_M), surface area normalized rate constant (k_{SA}, specific reaction rate constant), and half-life ($t_{0.5}$) of **perfluorooctane sulfonic acid (PFOS)** *in* Column *ZVI,* Column *BC, and* Column *(ZVI + BC)*. Removal rate constant k_{obs} is calculated using least-squares regression during two experimental stages. ^{t}C is the PFOS concentration.

Column	Stage	PV	Removal rate^{t}, μmol L^{-1} d^{-1} (μg L^{-1} d^{-1})	k_{obs}	k_M	k_{SA}	$t_{0.5}$, d	R^2
Column 2 (ZVI)	1	1	2.0 × C[a]	2.0[a]	4.6E-04[a]	4.9E-05[a]	0.4	0.911
		13	0.9 × C[a]	0.9[a]	2.1E-04[a]	2.3E-05[a]	0.8	0.834
		25	2.2E+01[b]	2.2E+01[b]	5.1E-03[b]	5.4E-04[b]	1.5	0.929
	2	53	2.6[b]	2.6[b]	6.2E-04[b]	6.5E-05[b]	16	0.734
Column 3 (BC)	1	1	1.8 × C[a]	1.8[a]	3.9E-03[a]	6.0E-05[a]	0.4	0.989
		13	0.5 × C[a]	0.5[a]	1.2E-03[a]	1.8E-05[a]	1.3	0.511
		25	0.9 × C[a]	0.9[a]	1.8E-03[a]	2.8E-05[a]	0.8	0.961
	2	53	0.2 × C[a]	0.2[a]	4.6E-04[a]	7.2E-06[a]	3.2	0.967
Column 4 (ZVI + BC)	1	1	2.2 × C[a]	2.2[a]	1.9E-03[a]	5.7E-05[a]	0.3	0.974
		13	0.7 × C[a]	0.7[a]	5.8E-04[a]	1.7E-05[a]	1.1	0.881
		25	1.1 × C[a]	1.1[a]	9.6E-04[a]	2.9E-05[a]	0.6	0.962
	2	53	7.0[b]	7.0E+01[b]	6.1E-03[b]	1.8E-04[b]	5.9	0.966

[a] Removal of PFOS followed a first-order reaction rate, unit of k_{obs} is d^{-1}, unit of k_M is L g^{-1} d^{-1}, unit of k_{SA} is L m^{-2} d^{-1}.
[b] Removal of PFOS followed a zero-order reaction rate, unit of k_{obs} is μmol PFOS L^{-1} d^{-1} (μg PFOS L^{-1} d^{-1}), unit of k_M is μmol PFOS d^{-1} g^{-1} (μg PFOS d^{-1} g^{-1}), unit of k_{SA} is μmol PFOS d^{-1} m^{-2} (μg PFOS d^{-1} m^{-2}).

where C is the contaminant concentration (μmol L^{-1} or μg L^{-1}), k_{obs} is the first-order removal rate constant (d^{-1}), k_M is the mass normalized first-order rate constant (L g^{-1} d^{-1}), k_{SA} is the specific first-order reaction rate constant or surface area normalized first-order rate constant (L m^{-2} d^{-1}), ρ_m is the mass concentration of reactive media (g L^{-1} of solution), ρ_a is the surface area concentration of reactive media (m^2 L^{-1} of solution), a_s is the specific surface area of reactive media (m^2 g^{-1}), and $t_{0.5}$ is the half-life of contaminant (d). The specific surface areas of the reactive media ZVI, BC, and (ZVI + BC) used are 9.5, 64.5, and 33.6 m^2 g^{-1} which are reported previously [3,4].

The removal of artificial sweeteners, PFOA, and PFOS within three treatment columns followed a first- or zero-order rate model or followed a first-order rate in the early stage of the experiment followed by a zero-order rate in the late stage of the experiment [1]. The k_{obs}, k_M, k_{SA}, and $t_{0.5}$ for the first-order rate of artificial sweeteners, PFOA, and PFOS were calculated following the equations (1)–(4). The

zero-order rate model can be described by equation (5). k_M and k_{SA} for the zero-order reaction can also be calculated according to equations (2) and (3). However, the half-life ($t_{0.5}$) of the zero-order reaction for target artificial sweeteners, PFOA, and PFOS was calculated following equation (6).

$$-\frac{dC}{dt} = k_{obs} \tag{5}$$

$$t_{0.5} = \frac{C_0}{2\,k_{obs}} \tag{6}$$

where C_0 is the initial contaminant concentration (μmol L^{-1} or μg L^{-1}). The units of k_{obs}, k_M, and k_{SA} for the zero-order rate were different from that for the first order rate. For the zero-order rate, the unit of k_{obs} is μmol contaminant L^{-1} d^{-1} (μg contaminant L^{-1} d^{-1}), the unit of k_M is μmol contaminant d^{-1} g^{-1} (μg contaminant d^{-1} g^{-1}), and the unit of k_{SA} is μmol contaminant d^{-1} m^{-2} (μg contaminant d^{-1} m^{-2}).

Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this article.

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