Supplementary information

for

Transport and attenuation of an artificial sweetener and six pharmaceutical compounds in a sequenced wetland-steel slag wastewater treatment system

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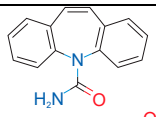
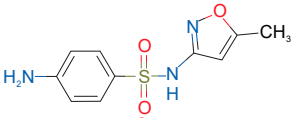
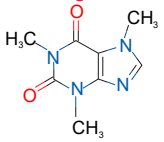
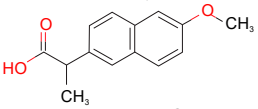
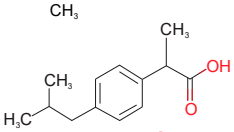
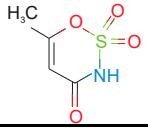
Table S1. Chemical properties and structures of target pharmaceutically active compounds and artificial sweetener acesulfame**.**

Name	Drug Class	Chemical Structure	log K_{ow}	pK_a
Carbamazepine Carbamazepine-d10	Anticonvulsant, antidepressant		2.45	13.9
Sulfamethoxazole Sulfamethoxazole-d4	Antibiotic		0.89	1.7, 5.6
Caffeine Caffeine-d3	Stimulant		-0.07	10.4
Naproxen Naproxen-13C	Non-steroidal anti-inflammatory		3.18	4.15
Ibuprofen Ibuprofen-d3	Non-steroidal anti-inflammatory		3.97	4.91
Acesulfame Acesulfame-d4	Artificial sweetener		-1.33	2.0

Note: pK_a and log K_{ow} of target compounds were obtained from Chemicalize.org by ChemAxon (http://www.chemicalize.org).

Table S2. Quality control samples and preparation blanks, continuing calibration verification, and continuing calibration blanks. Target contaminants included artificial sweetener acesulfame (ACE), carbamazepine (CBZ), caffeine (CAF), sulfamethoxazole (SMX), ibuprofen (IBU), and naproxen (NAP).

	ACE	**CBZ**	**CAF**	**SMX**	**IBU**	**GEM**	**NAP**
LOD (ng L^{-1}) Limit of detection	50	0.1	3	3	10	3	30
LOQ (ng L^{-1}) Limit of quantification	70	9	30	10	80	10	250
Internal Standard Recovery %	ACE	CBZ	CAF	SMX	IBU	GEM	NAP
Samples	33	119	101	104	113	119	81
Trip Blank	59	97	104	84	88	90	80
Field Blank	50	96	73	108	95	78	93
Preparation Blank (PRB)	12	90	98	102	122	113	74
Quality control samples (QCS)	20	95	98	98	118	94	72
Continuing calibration verification (CCV)	20	113	97	116	120	125	90
Analyte Recovery %	ACE	CBZ	CAF	SMX	IBU	GEM	NAP
Quality control samples (QCS)	105	106	127	118	105	105	72
Continuing calibration verification (CCV)	85	97	102	103	98	91	87
Continuing calibration blank (CCB)	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Recovery sample different dilutions %	115	117	110	200	127	111	105
Standards Range (ng L^{-1})	1000-100000	20-2000	50-2000	50-2000	100-40000	10-40000	50-40000
Correlation coefficient %	0.9998	0.9999	0.9993	0.9998	0.9997	0.9993	0.9991

Quality control samples and preparation blank samples were prepared with every set of samples. Continuing calibration verification and continuing calibration blank samples were analyzed every 5 or 10 samples. SPE factor (30) and the dilution factor (10) were considered on the calculation of LOD and LOQ.

Table S3. P-values obtained from t-Test, two-sample assuming unequal variances, for Cells 1-2, 2-3, 3-4, 1-3, 1-4, and 2-4 for the selected contaminants, including caffeine (CAF), carbamazepine (CBZ), sulfamethoxazole (SMX), ibuprofen (IBU), naproxen (NAP), and an artificial sweetener, acesulfame (ACE).

P(T<=t) two-tail	**Cell 1-2**	**Cell 1-3**	**Cell 1-4**	**Cell 2-3**	**Cell 2-4**	**Cell 3-4**
CAF	0.73	0.11	0.08	0.13	0.09	0.29
CBZ	0.93	0.82	0.86	0.88	0.92	0.95
SMX	0.46	0.40	0.32	0.87	0.75	0.89
IBU	0.59	0.05	0.03	0.03	0.01	0.50
NAP	0.45	0.75	0.19	0.33	0.05	0.40
ACE	0.47	0.25	0.12	0.56	0.25	0.45

Table S4. Physical and chemical properties of the BOFS materials used in the experiments.

BOFS **Source:** Stelco Hamilton	
Physical properties	
Particle size (mm)	Surface area (m^2g^{-1})
4-2	6.05
2-1	8.98
1-0.5	11.5
<0.5	13.9
Particle size (mm)	Mass weighted surface area (m^2g^{-1})
4-2	154
2-1	196
1-0.5	250
<0.5	429
Density (g cm^{-3}):	3.49
Chemical properties	
Chemical composition	wt. %
CaO	33.8
Fe_2O_3	24.3
SiO_2	11.3
MgO	9.62
MnO	4.08
Al_2O_3	7.43
P_2O_5	-
TiO_2	0.38
K_2O	0.03
Na_2O	0.07
Cr_2O_3	-
Loss on ignition	8.96

Table S5. Physical and chemical properties of the ZVI materials used in the experiments.

ZVI **Source:** Connelly GPM Inc., Chicago, Illinois, USA	
Physical properties	
Particle size (mm)	Surface area (m^2g^{-1})
0.297-2.38	4.4
Density (g cm^{-3}):	3.49
Chemical properties	
Chemical composition	wt. %
Iron/Iron Oxide	Balance
Total Carbon	2.48
Manganese	0.93
Sulphur	0.12
Phosphorous	ND
Silicon	0.35
Nickel	>0.01
Chromium	>0.01
Vanadium	ND
Molybdenum	0.33
Copper	0.10
Aluminum	>0.01
Magnesium	0.01
Boron	0.01
Zinc	0.01
Zirconium	0.01

ND= Not Detectable

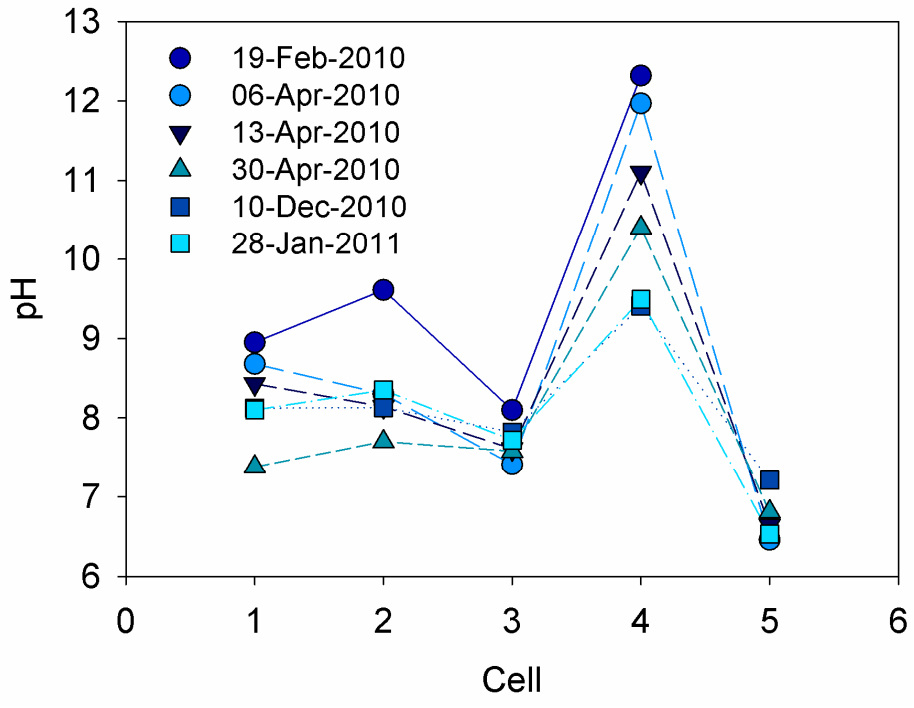


Figure S1. pH versus distance (Cells 1-5) along the treatment flow path.

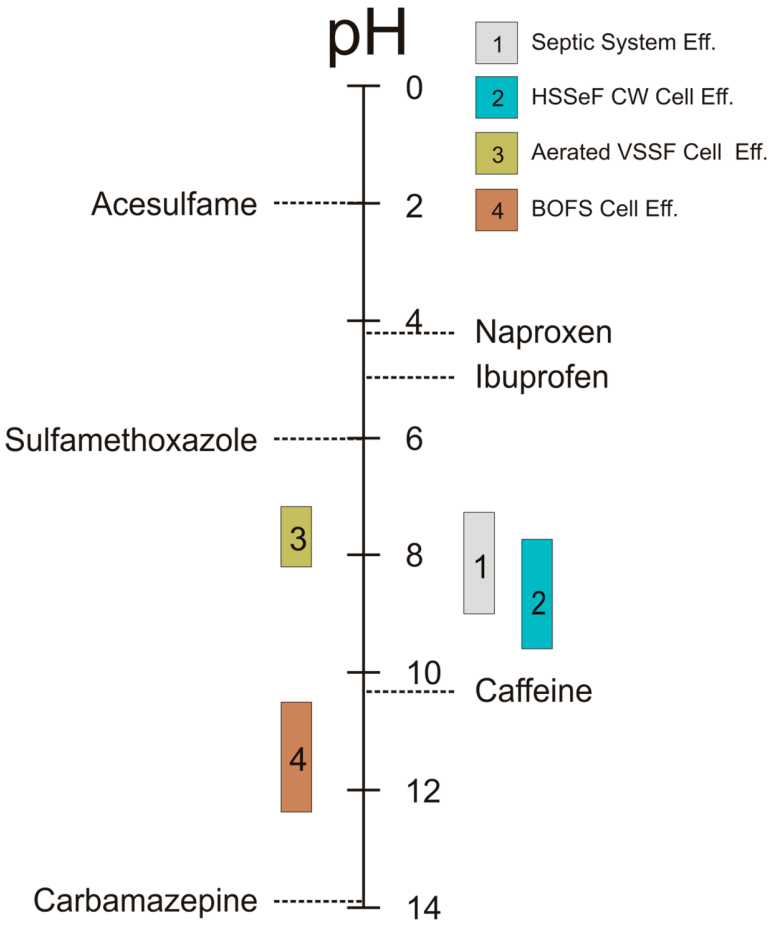


Figure S2. pK_a of each pharmaceutical of interest plotted on the pH scale with dotted lines and the pH range of the treatment cells (Cells 1-4) shown with vertical bars.

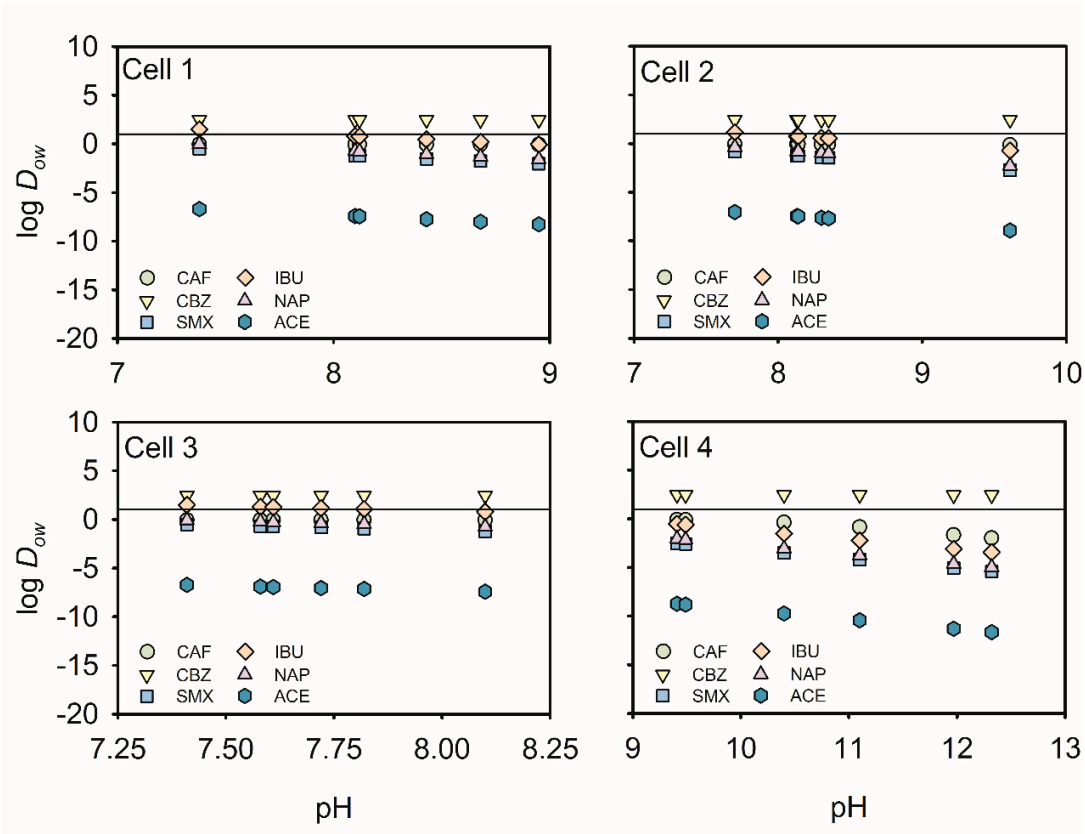


Figure S3. Calculated values of log D_{ow} versus pH in the influent (Cell 1 effluent) and three other treatment cells (Cells 2, 3, and 4).