Supporting Information for:

Influence of Biochar Thermal Regeneration on Sulfamethoxazole and Dissolved Organic Matter Adsorption

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(Pages 14, Figures 18, Tables 6, Equations 4)

Adsorbent Preparation. Biochar and AC were ground with a mortar and pestle, and wet sieved using RO tap water, with 100 x 200 U.S. standard mesh to target a log-mean particle diameter of 0.11mm. They were decanted in order to remove residual fines, and degassed overnight under a vacuum prior to loading into columns. The semi-oxic heating step was conducted in a Fisherbrand FB-965-D ceramic crucible, with about 30% headspace. See Figure S1 for adsorbent preparation process flow, Tables S1-S2 for mass yields of preparation processes, Table S3 for particle size distribution parameters, Table S4 for BET surface areas, and Table S5 for BET surface area and BJH pore size distribution analyses parameters.

Rapid Small Scale Column Test (RSSCT) Design. The RSSCTs were designed using assumptions of proportional diffusivity in accord with Crittenden et al.[1] They were operated with a target flow rate of 2 mL/min, which corresponds to a small column hydraulic loading rate of 6.7 m/h. The aspect ratio of the columns was 44. Biochar or activated carbon was degassed in RO-produced water overnight prior to loading in 4.76mm Teflon tubing, connected with stainless steel Swagelock components. Influent water was fed to the columns from well-mixed 20L glass carboys through Teflon tubing using a Cole-Parmer PTFE diaphragm pump. A glass wool pre-filter was used between the pump and the adsorbent beds. RSSCTs were operated with 1, 2, or 3 adsorbent beds connected in series, with sampling ports between beds. Each adsorbent bed had a large-column empty bed contact time ($EBCT_{LC}$) of 10 minutes. Sampling ports were controlled with needle valves in order to maintain the target EBCT during sampling. Columns were allowed to operate for at least ten bed volumes after any flowrate change before samples were taken. The exact mass transfer scaling was not considered crucial in this design process, because the goal was to directly compare the performance of the different adsorbents, rather than to predict full scale performance. Breakthrough of TOC, $UVA_{254\ nm}$, and SMX were monitored at the intermediate sample ports between adsorbent beds and at the effluent of each RSSCT. Influent samples were taken concurrently with each effluent sample. See Table S6 for more details

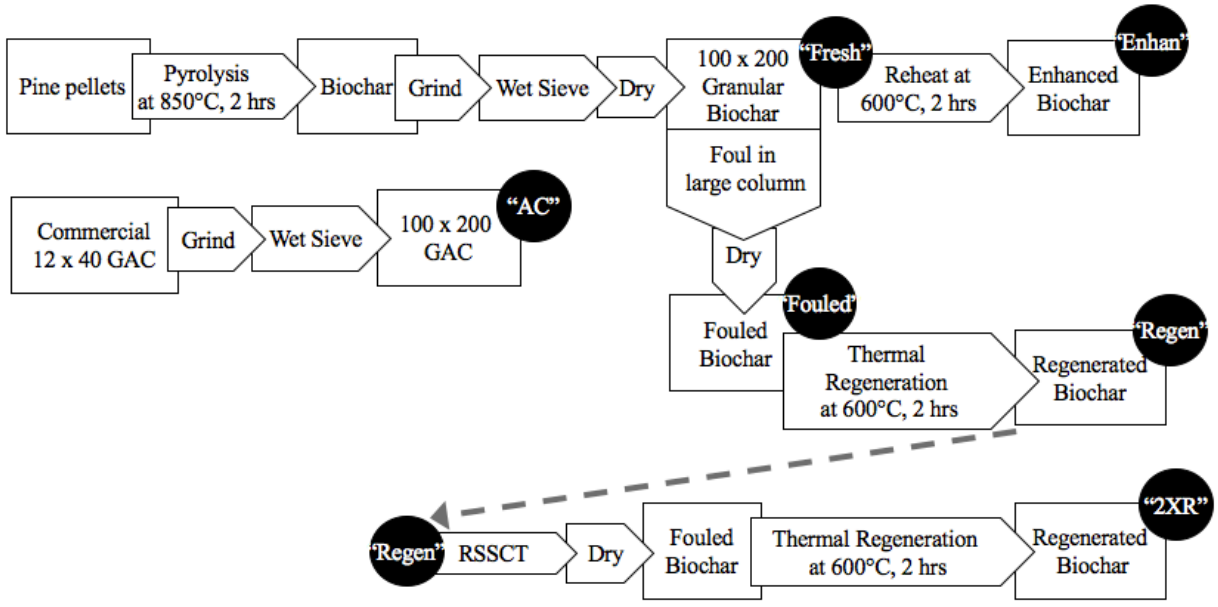

Figure S1: Adsorbent preparation process flow diagram. Black circles designate adsorbents used in RSSCTs.

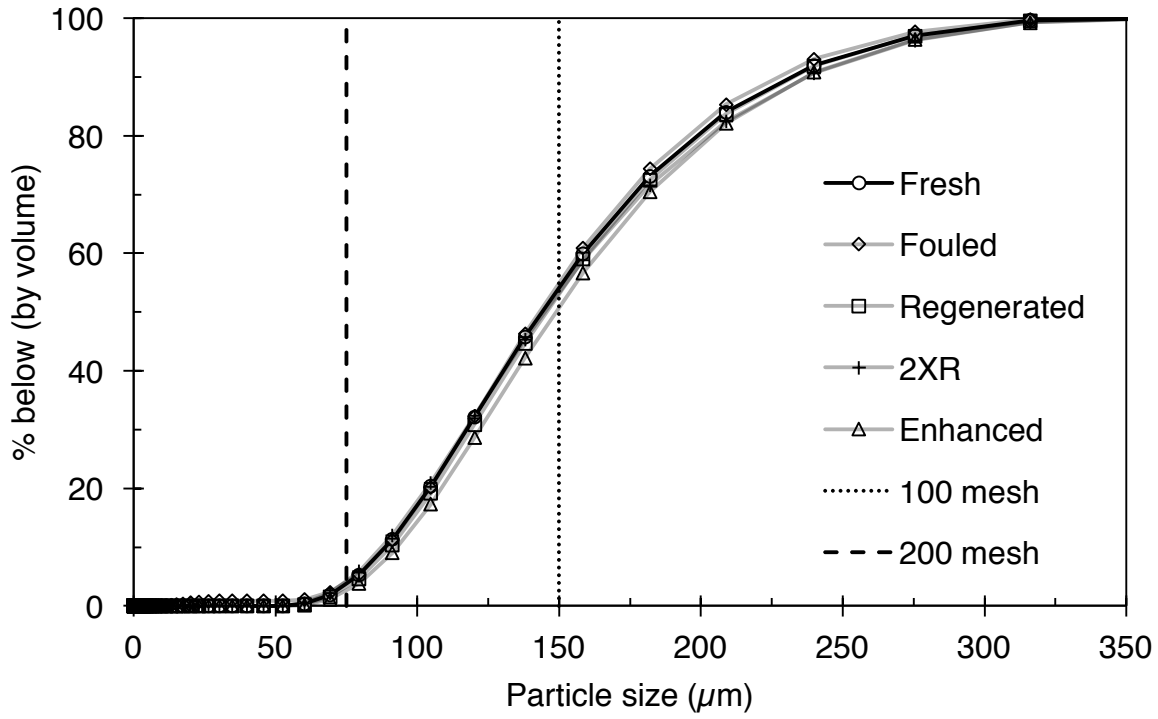

Figure S2: Cumulative distribution function of char particle size. Vertical lines indicate the nominal opening size in the upper (100 mesh) and lower (200 mesh) sieves used to produce the chars. Particle size distributions were collected using a Mastersizer Hydro SM2000(a) instrument.

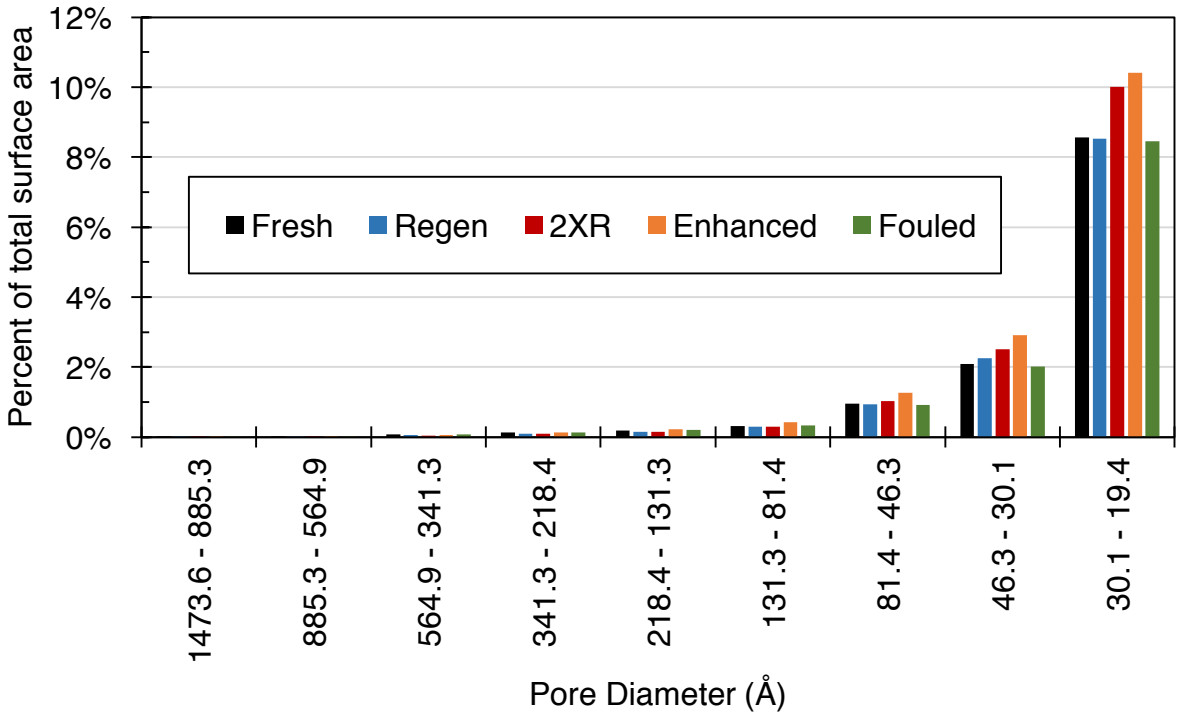

Figure S3: Pore size distribution of char internal surface area

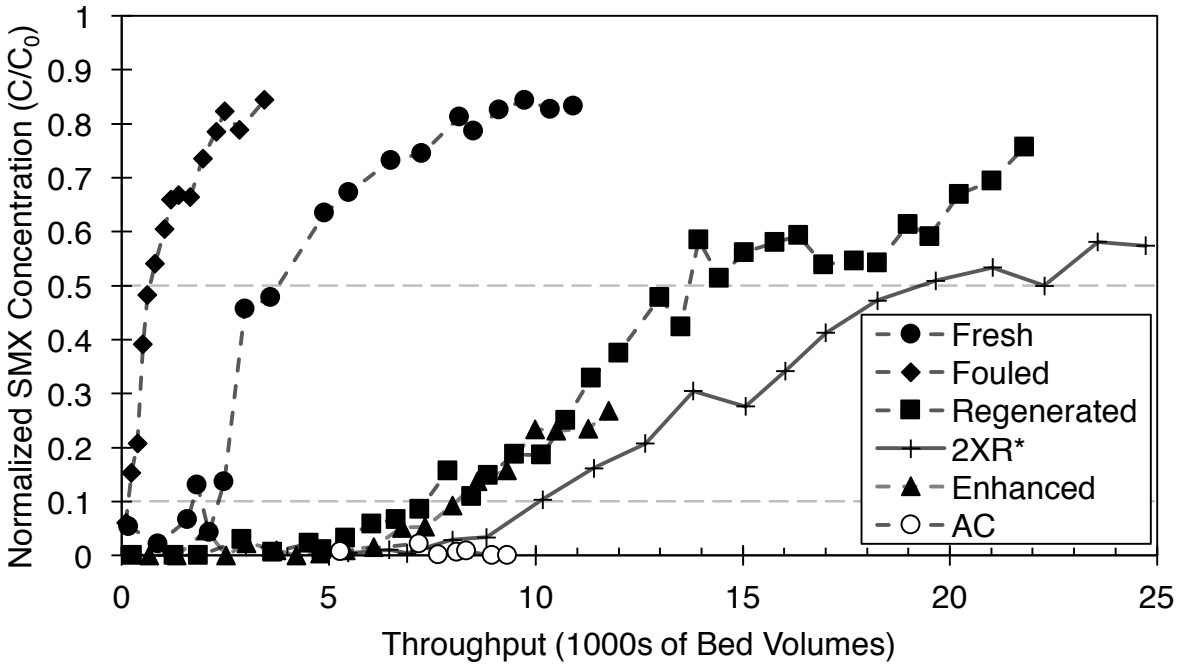

Figure S4: Breakthrough of sulfamethoxazole (SMX) for various adsorbents for large column empty bed contact time of 20 minutes ($EBCT_{LC}$).
*Twice-regenerated biochar (2XR) is shown for $EBCT_{LC}$ of 10 minutes.

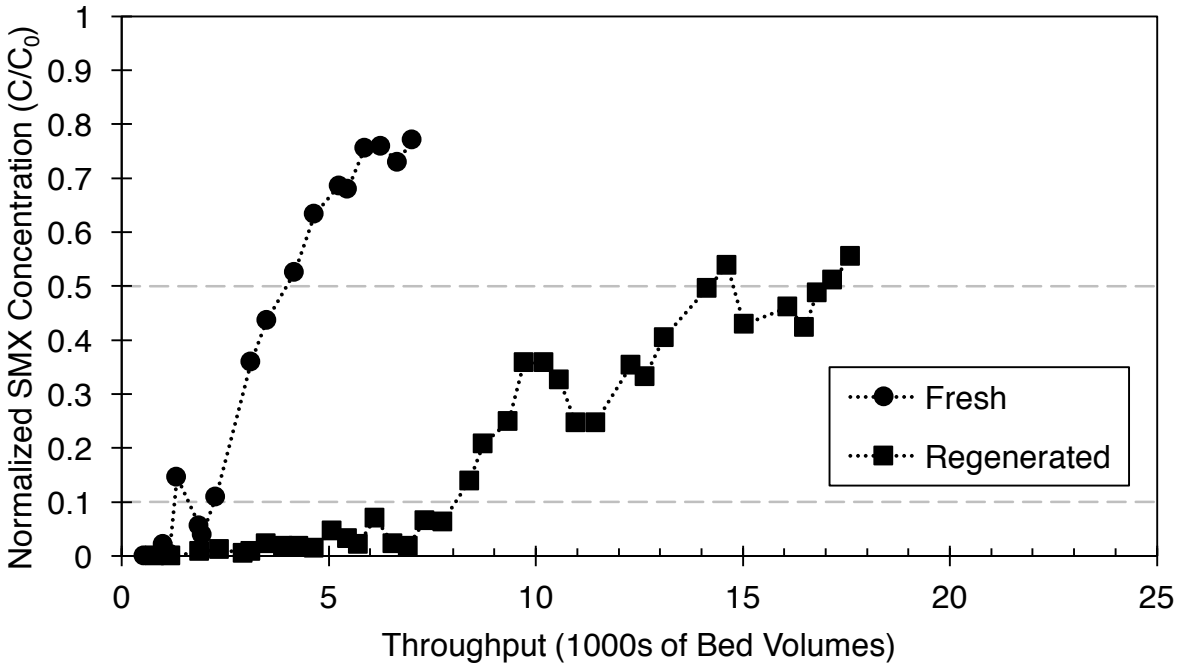

Figure S5: Breakthrough of sulfamethoxazole (SMX) for fresh and regenerated biochar with a large column empty bed contact time ($EBCT_{LC}$) of 30 minutes.

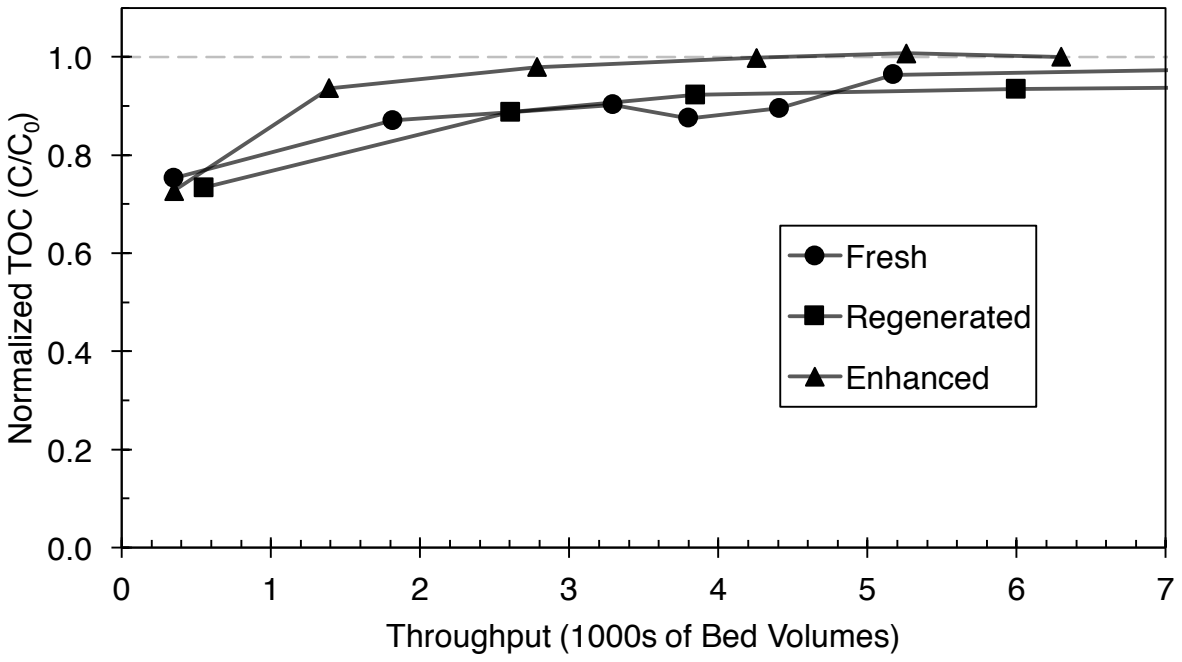

Figure S6: TOC breakthrough for various biochars with empty bed contact times ($EBCT_{LC}$) of 10 minutes

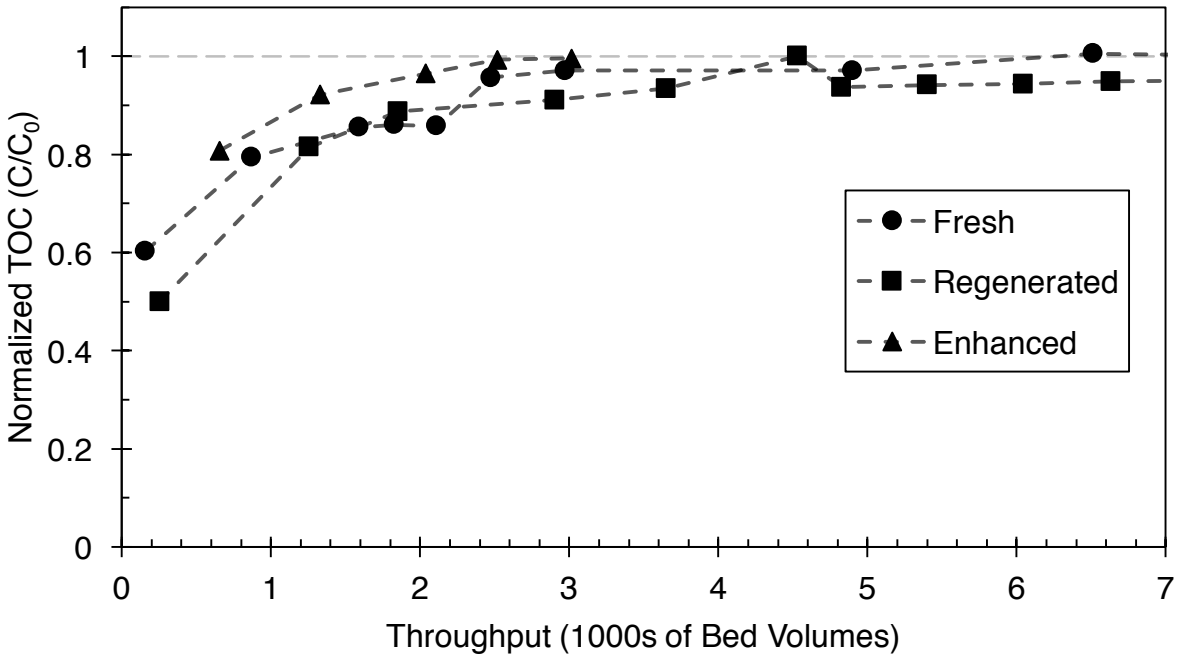

Figure S7: TOC breakthrough for various biochars with empty bed contact times ($EBCT_{LC}$) of 20 minutes

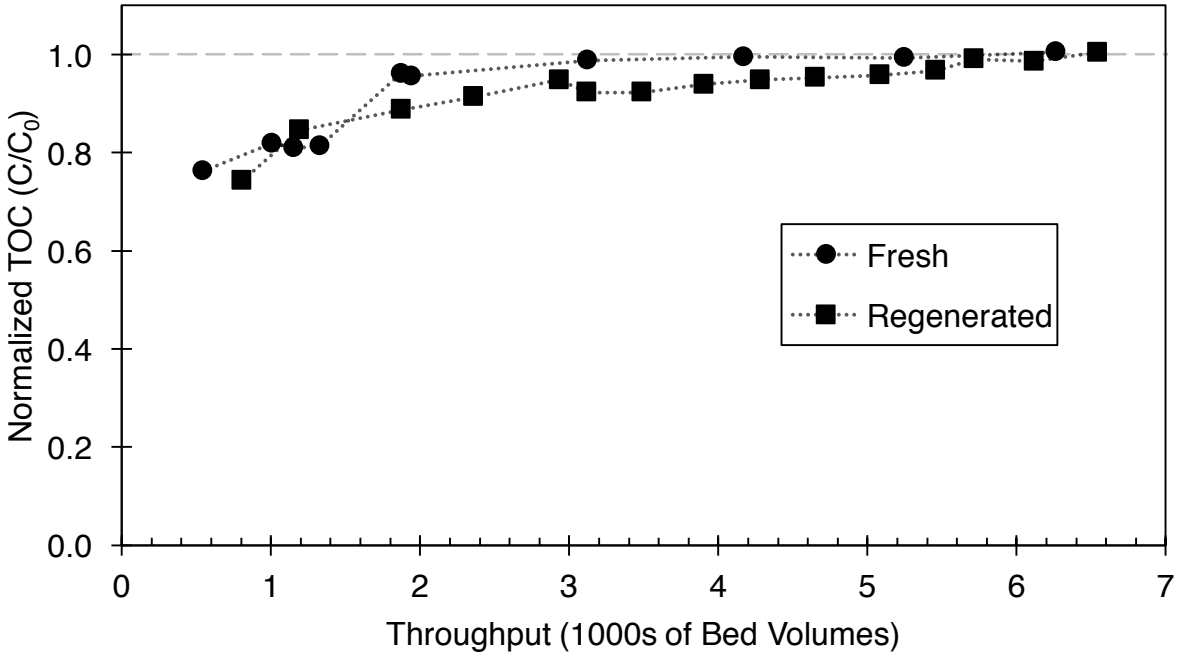

Figure S8: TOC breakthrough for various biochars with empty bed contact times ($EBCT_{LC}$) of 30 minutes

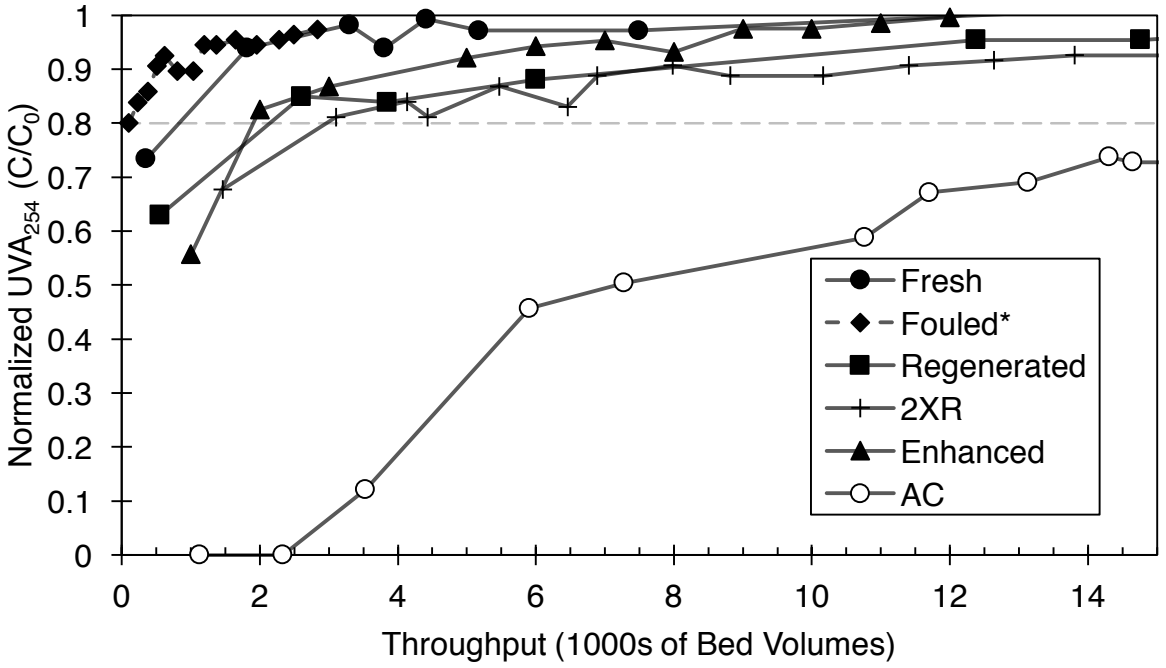

Figure S9: UVA_{254} breakthrough for various adsorbents with empty bed contact time ($EBCT_{LC}$) of 10 minutes, only showing part of the dataset for AC.
*Fouled biochar shown for $EBCT_{LC}$ of 20 minutes.

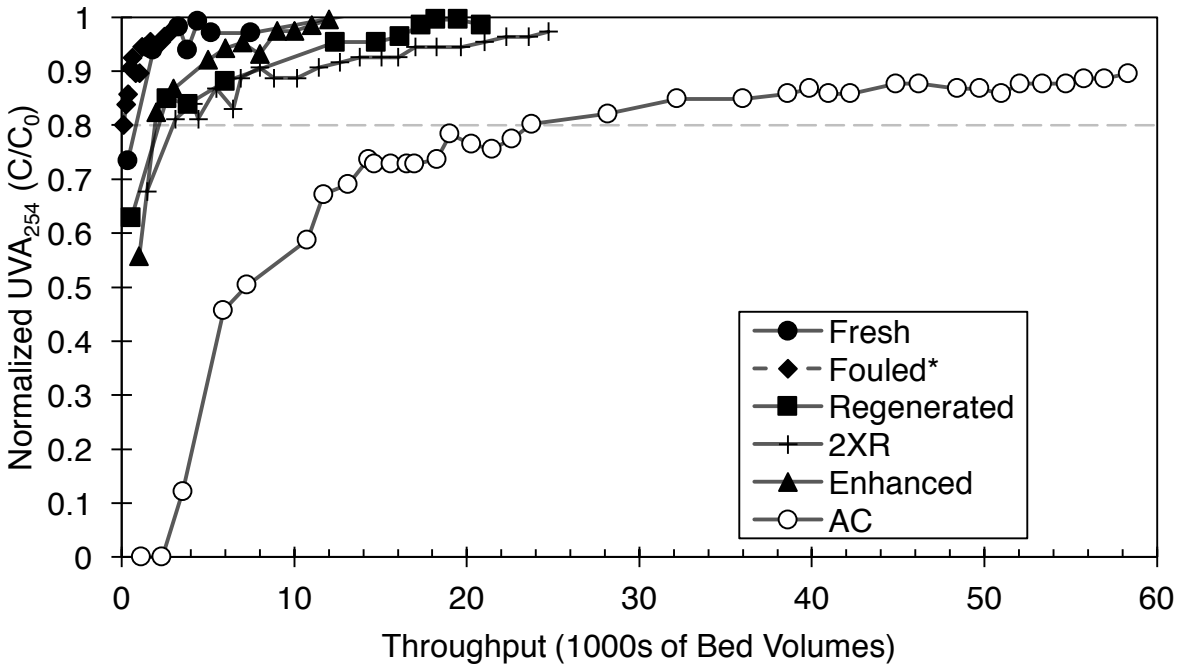

Figure S10: UVA_{254} breakthrough for various adsorbents with empty bed contact time ($EBCT_{LC}$) of 10 minutes, showing the full dataset for AC.
*Fouled biochar shown for $EBCT_{LC}$ of 20 minutes.

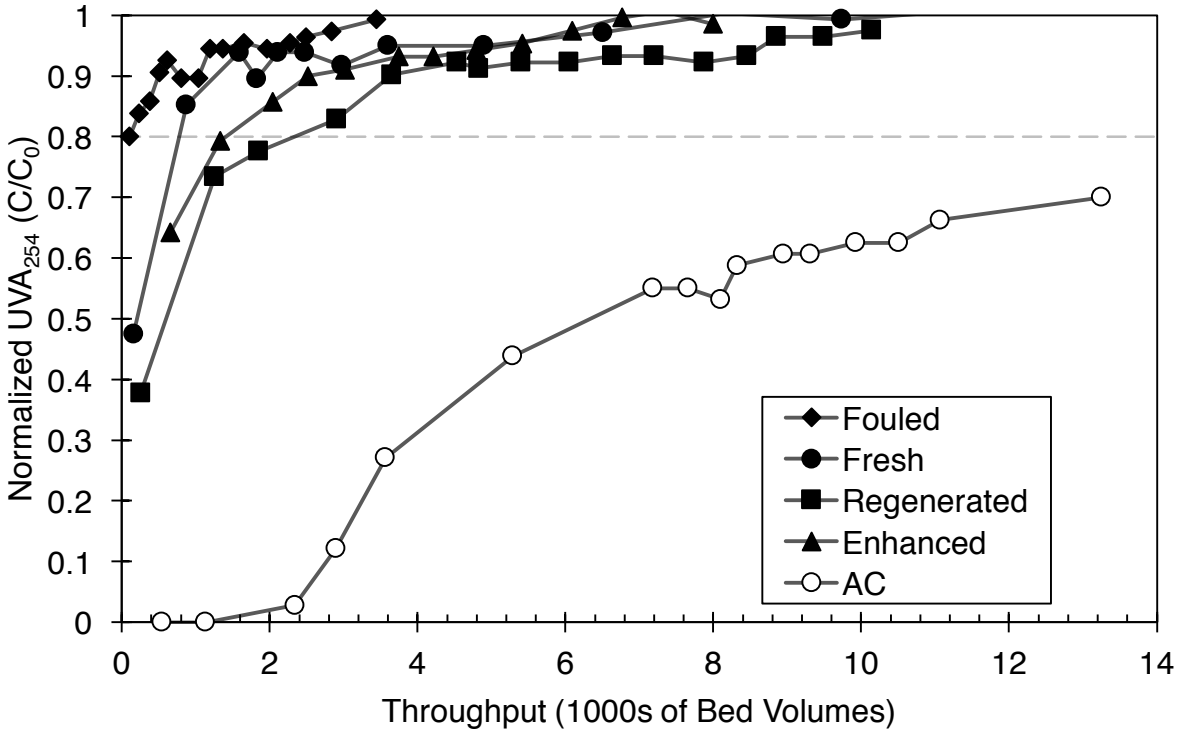

Figure S11: UVA_{254} breakthrough for various adsorbents with empty bed contact time ($EBCT_{LC}$) of 20 minutes.

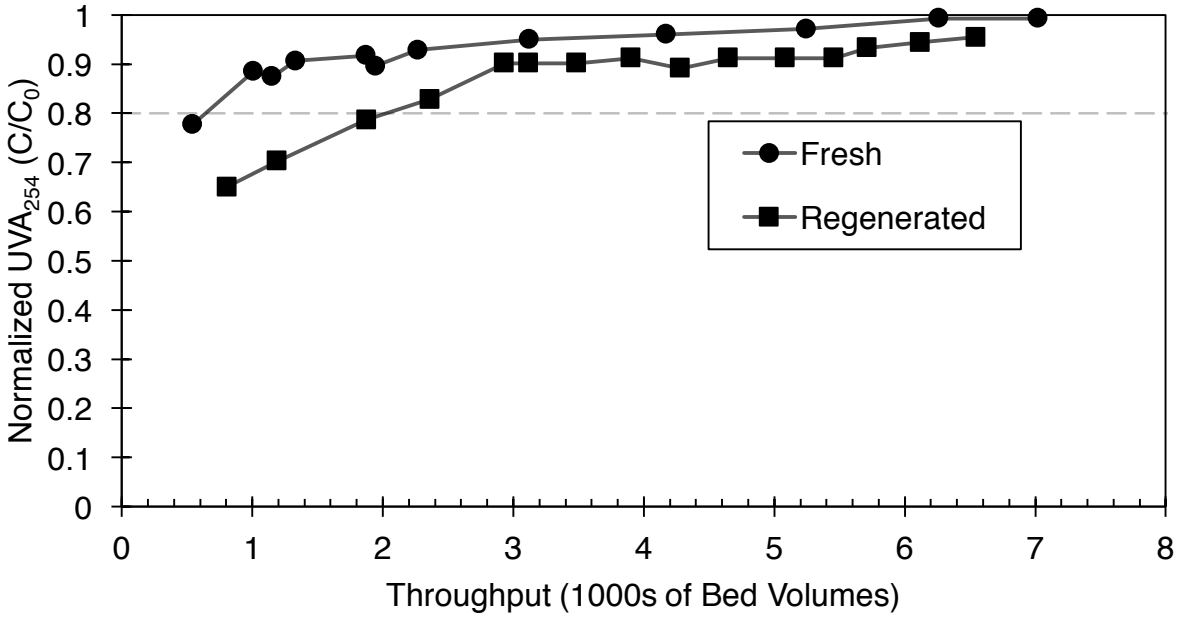

Figure S12: UVA_{254} breakthrough for various adsorbents with empty bed contact time ($EBCT_{LC}$) of 30 minutes.

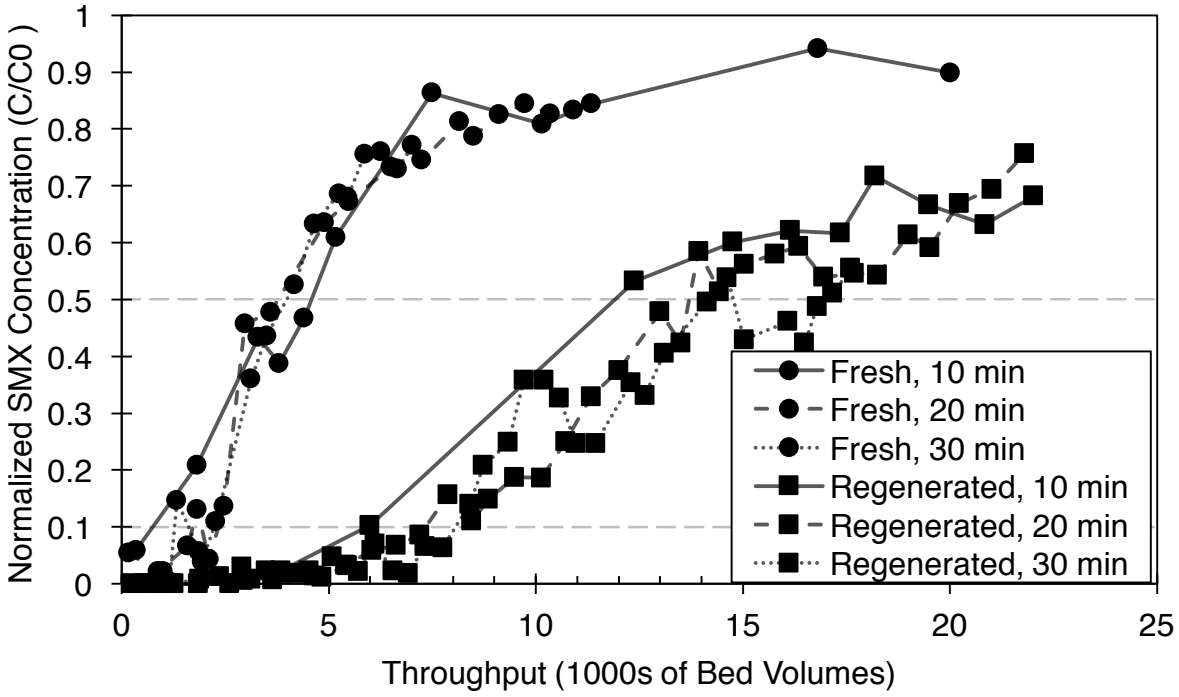

Figure S13: Effect of empty bed contact time ($EBCT_{LC}$) on SMX breakthrough for fresh and regenerated biochar.

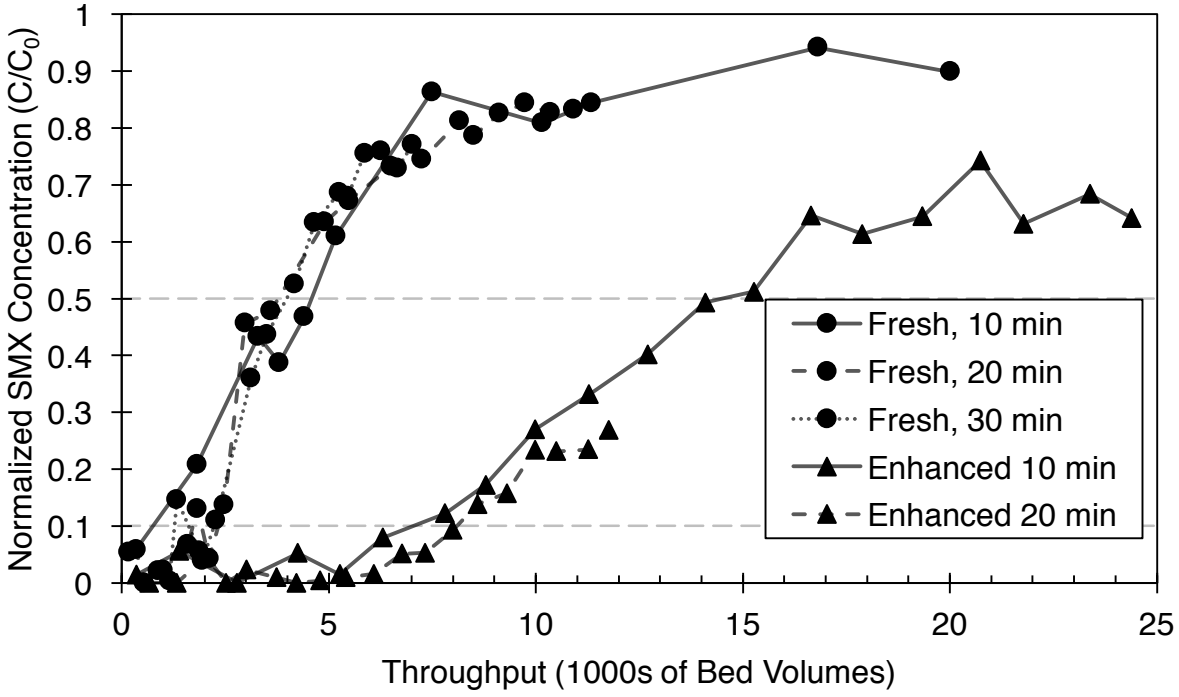

Figure S14: Effect of empty bed contact time ($EBCT_{LC}$) on SMX breakthrough for fresh and enhanced biochar.

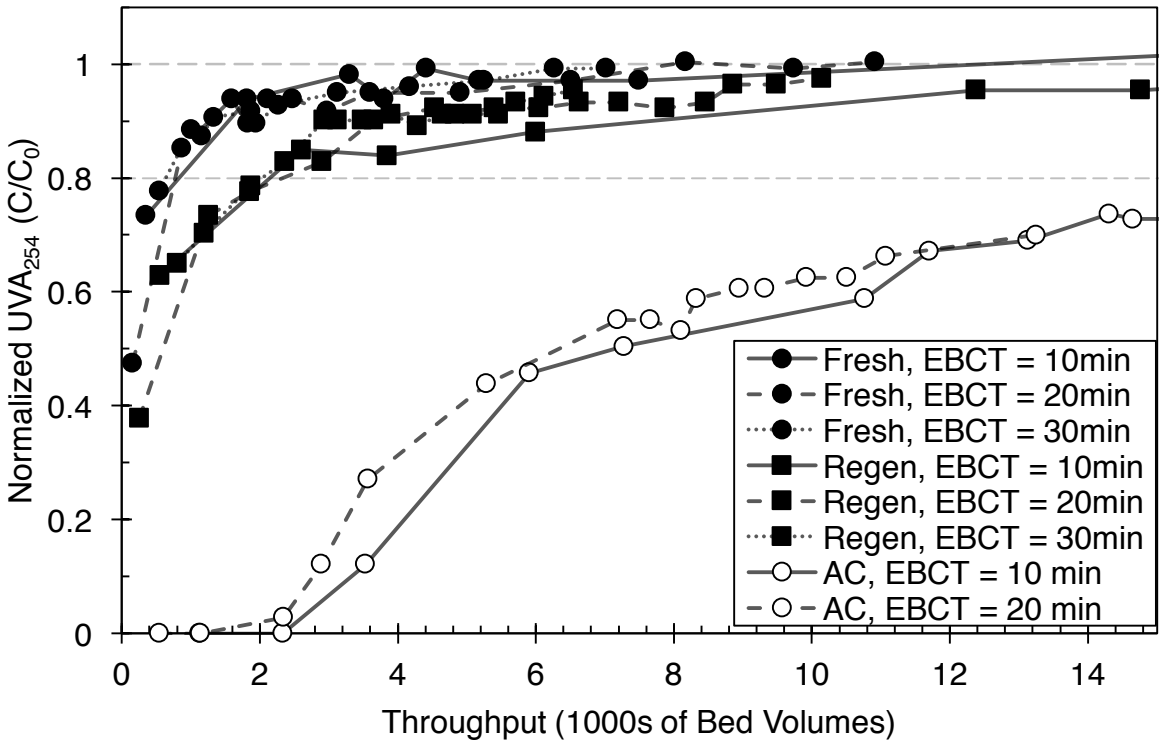

Figure S15: UVA_{254} breakthrough for various adsorbents with different empty bed contact times ($EBCT_{LC}$).

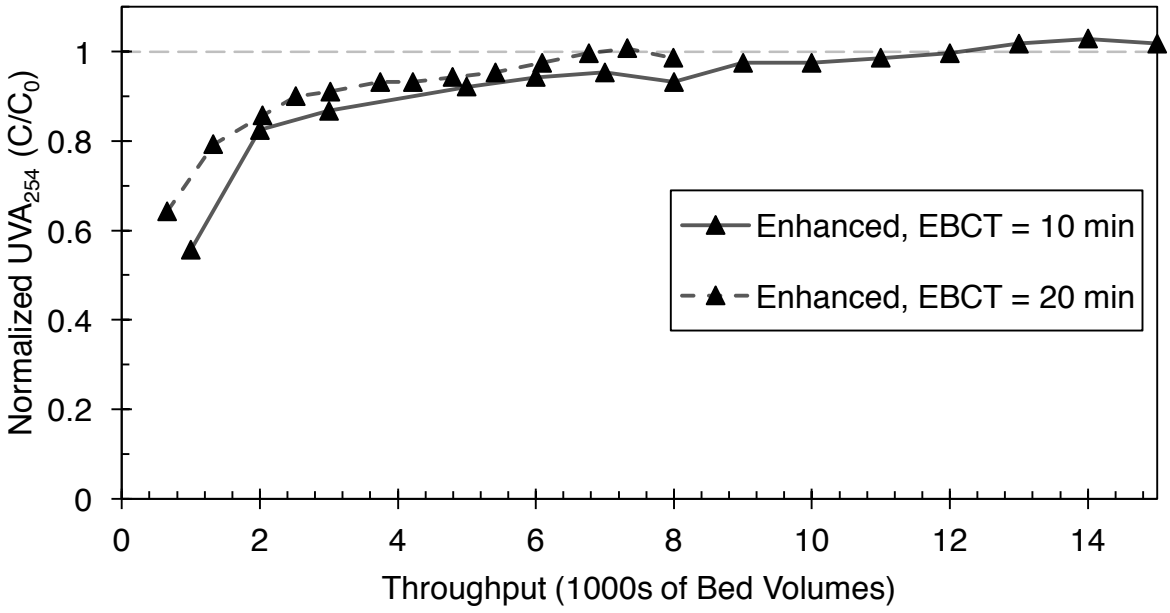

Figure S16: UVA_{254} breakthrough for enhanced biochar with two different empty bed contact times ($EBCT_{LC}$).

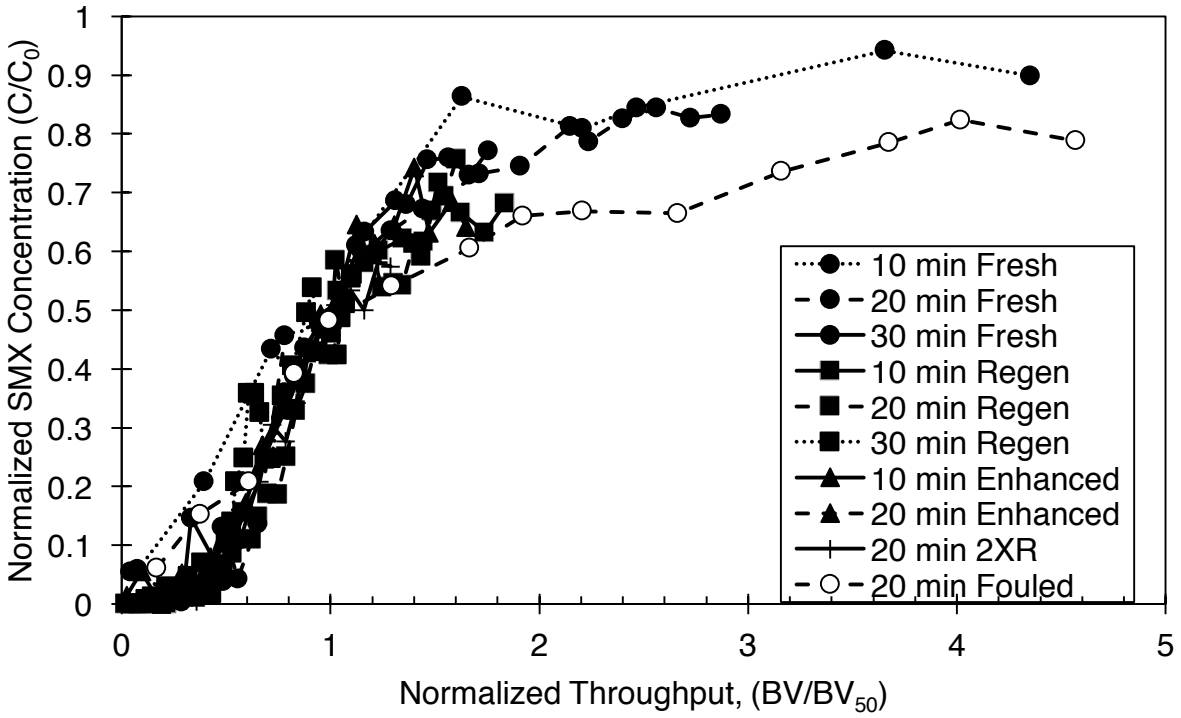

Figure S17: SMX breakthrough with throughput normalized to $BV_{50,SMX}$.

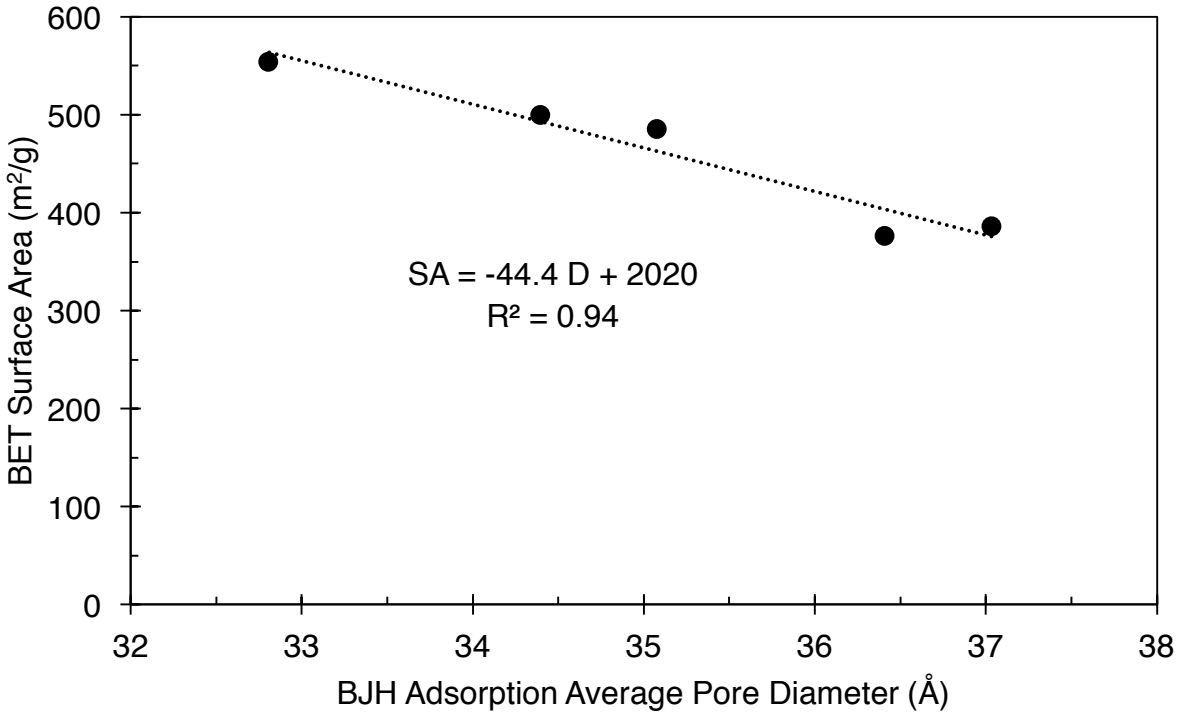

Figure S18: Relationship between BET surface area and BJH adsorption average pore diameter

Table S1: Mass yields for char and GAC grinding and wet sieving handling.

Process	Mass Yield	Used in RSSCT
Char Grind/Sieve	48.1%	Fouled, Regenerated, 2XR
Char Grind/Sieve	38.6%	Fresh, Enhanced
GAC Grind/Sieve	33.2%	AC

Table S2: Char yield of pyrolysis, first and second regeneration cycles, and enhancement reheat cycle.

Process	Temperature (°C)	Mass Yield	Used in RSSCT
Pyrolysis	850	21.5%	All
Regeneration	600	85.4%	Regenerated, 2XR
Regeneration	700	78.3%	-
Regeneration	850	70.1%	-
2nd Regeneration	600	75.0%	2XR
Enhancement Reheat	600	80.2%	Enhanced

Table S3: Particle Size Distribution Parameters. See equations S1-S4 for span, D_x, uniformity, and C_U definitions.

	Span	D [4, 3], Volume weighted mean	Uniformity	D_{10}	D_{50}	D_{90}	D_{60}*	C_U, Coefficient of Uniformity
Sample	[μm]	[μm]	[unitless]		[μm]			[unitless]
Fresh	0.99	153	0.30	89	144	231	159	1.78
Fouled	0.96	151	0.30	89	143	226	157	1.76
Regenerated	0.97	154	0.30	91	145	231	160	1.77
2XR	1.03	155	0.32	88	145	237	161	1.84
Enhanced	0.96	158	0.30	93	149	236	164	1.76

*D_{60} interpolated from Figure S2 data.

Table S4: Measured and reported BET surface area of adsorbents

Sample	BET Surface Area (m^2/g)
Fresh	376 ± 9
Fouled	385 ± 9
Regenerated	500 ± 12
2XR	554 ± 12
Enhanced	485 ± 11
Norit 1240 GAC	1062 ± 21

Table S5: BET Surface Area and BJH Pore Size Distribution Analyses Parameters

Sample	BET Surface Area (m^2/g)	BET SA Standard Deviation (m^2/g)	Langmuir Surface Area (m^2/g)	BJH Adsorption cumulative surface area of pores between 17.000 Å and 3000.000 Å diameter (m^2/g)	BJH Desorption cumulative surface area of pores between 17.000 Å and 3000.000 Å diameter (m^2/g)	Adsorption average pore width (4V/A by BET) (Å)	Desorption average pore width (4V/A by BET) (Å)	BJH Adsorption average pore diameter (4V/A) (Å)	BJH Desorption average pore diameter (4V/A) (Å)
Fresh	375.7499	8.6432	496.3021	46.307	37.8783	20.5046	20.6246	36.41	32.097
Fouled	385.383	8.9069	509.1899	46.814	37.8509	20.5289	20.6634	37.037	31.448
Regenerated	499.3928	11.5132	658.3282	61.597	67.3522	20.3781	20.3981	34.397	32.056
2XR	553.5491	12.4668	730.672	78.141	86.5718	20.4042	20.4249	32.809	30.883
Enhanced	484.8114	10.6968	640.2248	74.799	82.7565	20.9425	20.9857	35.078	32.615

Table S6: Proportional Diffusivity RSSCT selected design parameters.

Design Parameter	Value	
Upper Sieve Size (Small Scale)	100	
Lower Sieve Size (Small Scale)	200	
$d_{p,SC}$	0.11	mm
RSSCT column diameter	4.76	mm
Target Flow Rate	2.00	mL/min
HLR_{SC}	6.7	m/hr
Aspect Ratio	44	
Bed length	13.2	cm
$EBCT_{LC}$	10	min

Equation S1: D_X

$$D_X = diameter\ for\ which\ X\%\ (by\ volume) of\ sample\ is\ composed\ of\ smaller\ particles$$

Equation S2: Span[2]

$$Span = \frac{D_{90} - D_{10}}{D_{50}}$$

Equation S3: Coefficient of Uniformity[3]

$$C_u = \frac{D_{60}}{D_{10}}$$

Equation S4: Uniformity[2]

$$U = \frac{\Sigma v_i |d(v,0.5) - d_i|}{d(v,0.5)\Sigma v_i}$$

where $d(v,0.5)$ is the median size of the distribution in terms of volume, and d_i and v_i are respectively the mean diameter of, and result in, size class i.

Equation S1: Volume weighted mean [2]

$$D[m,n] = \left[\frac{\Sigma V_i {d_i}^{m-3}}{\Sigma V_i {d_i}^{n-3}}\right]^{\frac{1}{m-n}}$$

where $m = 4$ and $n = 3$.

References

(1) Crittenden, J.C., Reddy, P.S., Arora, H., Trynoski, J., Hand, D.W., Perram, D.L. and Summers, R.S.: "Predicting GAC Performance With Rapid Small Scale Column Tests," *J. Amer. Water Works Assoc.*, 83(1)(1991):77-87.

(2) Mastersizer 2000 User Manual. Malvern Instruments March 2007.

(3) Sontheimer, H.; Crittenden, J. C.; Summers, R. S. *Activated Carbon for Water Treatment*, 2nd Edition.; DVGW-Forschungsstelle: Karlsruhe, Germany, 1988.