1	Electronic Supplementary Information (ESI)
2	Removal of Per- and Polyfluoroalkyl Substances (PFASs) from Contaminated
3	Groundwater using Granular Activated Carbon: A Pilot-Scale Study with Breakthrough
4	Modeling
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17	<b>Environmental Science: Water Research and Technology</b>
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#### 61 1.0 Analytical Sample Prep

All samples were collected in 15 mL pre-weighed polypropylene Falcon (Corning, NY) tubes. The following reagents were added: 63.8% water sample, 3.3% Fisher Scientific Optima LCMS grade water (Hampton, NH) mixed with 0.1% of Optima LCMS grade ammonium hydroxide, 13.6% Optima LCMS grade methanol, 9.6% of Optima LCMS grade isopropanol surrogate mixture, and 9.6% of Optima LCMS grade methanol surrogate mixture. All reagents were prepared in the original sampling vial to mitigate transfer losses. Surrogate concentrations were spiked at 74 pg/mL and 1.35 mL of sample was transferred into a 1.5 mL autosampler vial.

69

1mL of sample was injected in a SCIEX X500R QTOF System (Framingham, MA). The 70 analytical column used was Phenomenex Gemini C18, 3mm x 100mm x 5µm (Torrance, CA). 71 Prior to the column, a Phenomenex C18 SecurityGuard<sup>TM</sup> 4mm x 2mm (Torrance, CA) and two 72 Agilent Zorbax 4.6 mm x 12.5 mm x 6 µm DIOL guard columns (Santa Clara, CA) were used. A 73 Phenomenex Luna 5 um C18(2) 100 Ä LC column 30 x 3 mm (Torrance, CA) was used as a 74 delay column to aid in chromatographic separation. The column oven temperature was set to 40C. 75 The eluent mobile phases used were (A) Optima LCMS grade water with 20mM Fisher 76 77 Scientific HPLC grade ammonium acetate (Hampton, NH) and (B) 100% Optima LCMS grade methanol. The autosampler rinse solution was 100% Optima LCMS grade isopropanol. Eluent 78 79 flow rate was held at 0.60 mL/min, and composition was ramped from 90% A to 50% A over the 80 first 0.5 minutes, then to 1.0% A at 8 minutes and held until 13 minutes, then ramped to 90% A at 13.5 minutes and held to 20 minutes. 81

Electrospray ionization in negative mode (ESI-) with SWATH® Data-Independent Acquisition 83 for both TOFMS and MS/MS mode were used. Precursor ion data was collected for m/z 100-84 1200 for 1283 cycles with a total scan time of 842 ms and accumulation time of 20 ms, with ion 85 spray voltage set at - 4500 V and temperature set to 550 °C. The ion source, curtain, and collision 86 (CAD) gas were set to 60 psi, 35 psi, and 10 psi, respectively. For QTOF scanning, the collision 87 energy was set to -5 V and the declustering potential to -20 V, both with no spread. Product ion 88 (MS/MS) scanning was conducted for m/z 50-1200 Da. The accumulation time for each SWATH 89 window is 50 ms and collision energy was -35 V with 30 V spread. The instrument was mass 90 calibrated every 5 injections using SCIEX ESI Negative Calibration Solution. 91

#### 92 2.0 GAC Column Parameters

93

Table S1. GAC column parameters.

GAC Height	45 in
Column Diameter	5.71 in
Flowrate/Column	0.5 gpm
Total Bed Volume	18.88 L
Total Run Time	1841.59 hr
Hydraulic Loading Rate	$2.8 \text{ gpm/ft}^2$
Empty Bed Contact Time	10 min



# 98 3.0 Modeling Input

99

 Table S2. Fixed column model input parameters.

	F400	GAC400	F600	GCN1240
Column Length (m)	1.143	1.143	1.143	1.143
Inner Column Radius (m)	0.073	0.073	0.073	0.073
Total Dry Mass of GAC (kg)	10.1967	9.2525	11.7073	9.6302
Flow Through Column (m <sup>3</sup> /s)	3.15E-05	3.15E-05	3.15E-05	3.15E-05
Dispersion Coefficient (m <sup>2</sup> /s)	9.77E-06	9.85E-06	1.08E-05	8.75E-06
Skeletal Density of GAC (kg/m <sup>3</sup> )	2200	2200	2200	2200
Radius of GAC (m)	0.0065	0.0065	0.0065	0.0065
Intraparticle Porosity	0.59	0.63	0.53	0.61

Table S3.	Compound	specific	model	inputs.
-----------	----------	----------	-------	---------

	Molecular Weight (g/mol)	Avg. Influent Concentration (mM)
PFPeA	264.07	5.62187E-08
PFHxA	314.07	5.60266E-08
PFHpA	364.07	1.46478E-08
PFOA	414.07	5.08504E-08
PFPrS	250.13	1.25937E-08
PFBS	300.13	7.47829E-09
PFPeS	350.13	2.95955E-08
PFHxS	400.13	1.02123E-07
PFHpS	450.13	2.52849E-09
PFOS	500.13	9.89414E-08

# 103 3.1 Dispersion Coefficient Calculation

104 The dispersion coefficient was calculated based on the Chung and Wen equation<sup>1, 2</sup>

$$\frac{D_{disp}\rho_w}{\mu_w} = \frac{Re}{0.2 + 0.011Re^{0.48}} (eq 1)$$

106 where  $D_{disp}$  is the dispersion coefficient (m<sup>2</sup>/s),  $\rho_w$  is the density of water at 14C 999.2 (kg/m<sup>3</sup>),

- 107  $\mu_w$  is the viscosity of water at 14 °C, 0.0010518 (Pa s), and Re is the Reynolds number.
- 108 The Reynolds number was defined as

$$Re = \frac{\rho_w v d_p}{\mu_w} \text{ (eq 2)}$$

- 110 where v is the interstitial velocity (m/s), and  $d_p$  is the particle diameter (m).
- 111 Interstitial velocity was defined as

$$v = \frac{Q}{\pi r_p^2 n} \pmod{(\text{eq 3})}$$

where Q is the flowrate  $(m^3/s)$ , r is the particle radius (r), and n is particle porosity. 113

114

#### **3.2 Intraparticle Porosity Calculation** 115

Intraparticle porosity was defined as 116

$$n = \frac{V_{pores}}{V_{particles} (eq 4)}$$

where n is the porosity,  $V_{pores}$  is the volume of the particle pores, and  $V_{particles}$  is the volume of the 118 particles. V<sub>particles</sub> is the difference between the volume of the bed and the volume of the void. 119 V<sub>pores</sub> is the difference between the volume of the particle and the volume of the skeletal. 120

121

#### **3.3 Instantaneous Sorption Equilibrium Model** 122

123 The column experiments were simulated by considering pollutant transport by advection and dispersion. The pollutant distribution between the mobile column porewater (in between the 124 particles), and the solid matrix of the activated (AC) particles was described by a solid liquid 125 partition coefficient, K<sub>d</sub>. Parameters were expressed in SI units of moles, seconds, kilograms, and 126 meters (Table S4). 127

128

129 Table S4. Independent and dependent column model variables and parameters and their 130 dimensions for the instantaneous sorption equilibrium model.

t(s)	Time
x (m)	Distance from the column inlet

C <sub>w</sub> (moles nm <sup>-3</sup> )	Pollutant concentration in mobile water in between the AC				
	particles				
$K_d(m^3 kg^{-1})$	Reversible, linear AC solid-water partitioning coefficient for				
	the pollutant				
$L_{C}(m)$	Length of the column				
$R_{C}(m)$	Radius of the column				
C <sub>in</sub> (moles m <sup>-3</sup> )	Pollutant concentration in the influent				
v <sub>x</sub> (m s <sup>-1</sup> )	Interstitial velocity of the mobile water in between the AC				
	particles in the x direction				
$D_{disp}$ (m <sup>2</sup> s <sup>-1</sup> )	Dispersion coefficient for pollutants in the water in between				
	the AC particles in the x direction				
M <sub>AC</sub> (kg)	Total dry AC mass of particles (of all sizes) in the column				
$\Theta_{\mathrm{AC,w}}$ (-)	Water-filled AC intraparticle porosity				
d <sub>AC</sub> (kg m <sup>-3</sup> )	Solid density of the AC skeleton				

## 132 3.3.1 Calculated Column Properties

133 The volume fraction of the column filled with AC particles,  $\theta_{AC}$ , is defined as

$$\theta_{AC} = \frac{M_{AC}}{(1 - \theta_{AC,w})d_{AC}L_C\pi R_C^2} (\text{eq 5})$$

135 where  $M_{AC}$  is the total dry mass of AC particles in the column,  $\theta_{AC,w}$  is the water-filled 136 intraparticle AC porosity,  $d_{AC}$  is the skeletal solid density of the AC,  $L_C$  is the length of the 137 column, and  $R_C$  is the radius of the column.

139 The volume fraction of the space in the column in between the AC particles, which is assumed to 140 be entirely filled with mobile water,  $\theta_w$ , is defined as

$$\theta_w = 1 - \theta_{AC} \text{ (eq 6)}$$

142

#### 143 3.3.2 Differential Equation

144 Pollutant transport in mobile water moving in between the AC particles:

145 The following partial differential equation is assumed to govern the pollutant concentration in146 the mobile water phase moving in between the AC particles

$$(\theta_{w} + \theta_{AC} \cdot (\theta_{AC,w} + (1 - \theta_{AC,w})d_{AC}K_{d})) \cdot \frac{d}{dt}C_{w} = \theta_{w}D_{disp}\frac{\partial^{2}}{\partial x^{2}}C_{w} - \theta_{w}v_{x}\frac{\partial}{\partial x}C_{w}$$

148 (eq 7)

where  $\theta_w$  is the fraction of the column volume in between the AC particles, which is assumed to be fully water saturated, K<sub>d</sub> is the linear AC solid-water partitioning coefficient of the pollutant, D<sub>disp</sub> is the dispersion coefficient of pollutants in mobile water, and v<sub>x</sub> is the interstitial velocity of this water, both in the x direction.

153 Boundary conditions for the column:

154 The pollutant concentration at the column inlet is equal to the concentration in the column 155 influent,  $C_{in}$ ,

156 
$$C_w|_{x=0} = C_{in \text{ (eq 8)}}$$

157 And a zero concentration gradient boundary condition is enforced at the column outlet

$$\frac{\partial}{\partial x} C_w \Big|_{x=L} = 0 \quad (\text{eq } 9)$$

### 160 3.4 Intraparticle Diffusion Model

161 The column experiments were simulated by considering pollutant transport by advection and 162 dispersion in the mobile water moving in between the AC particles in addition to sorption-163 retarded intraparticle diffusion into AC particles. The pollutant distribution between water and 164 the solid matrix of the AC particles was described by a linear sorption coefficient  $K_d$ . Parameters 165 were expressed in SI units of moles, seconds, kilograms, and meters (Table S5).

167	Table S5. Independent and dependent column model variables and parameters and their
168	dimensions for the intraparticle diffusion model.

t (s)	Time				
x (m)	Distance from the column inlet				
r (m)	Radial distance from the AC particle centre				
C <sub>w</sub> (moles m <sup>-3</sup> )	Pollutant concentration in mobile water in between the AC				
	particles				
C <sub>AC</sub> (moles m <sup>-3</sup> )	Pollutant concentration in the AC intraparticle porewater				
$K_{d}(m^{3}kg^{-1})$	Reversible, linear AC solid-water partitioning coefficient for				
	the pollutant				
$L_{C}(m)$	Length of the column				
$R_{C}(m)$	Radius of the column				
C <sub>in</sub> (moles m <sup>-3</sup> )	Pollutant concentration in the influent				
v <sub>x</sub> (m s <sup>-1</sup> )	Interstitial velocity of the mobile water in between the AC				
	particles in the x direction				
$D_{disp}$ (m <sup>2</sup> s <sup>-1</sup> )	Dispersion coefficient for pollutants in the mobile water in				

	between the AC particles in the x direction
M <sub>AC</sub> (kg)	Dry AC mass of particles
$R_{AC}(m)$	AC particle radius
$\Theta_{\mathrm{AC,w}}$ (-)	Water-filled AC intraparticle porosity
d <sub>AC</sub> (kg m <sup>-3</sup> )	Solid density of the AC skeleton
τ(-)	AC pore network tortuosity factor
$D_{aq} (m^2 s^{-1})$	The molecular diffusion coefficient of the pollutant in water

170

### 171 3.4.1 Calculated Column Properties

172 The volume fraction of the column filled with AC particles  $\theta_{AC}$ , is defined as

$$\theta_{AC} = \frac{M_{AC}}{(1 - \theta_{AC,w})d_{AC}L_C\pi R_C^2} \quad (\text{eq 10})$$

where  $M_{AC}$  is the dry mass of AC particles,  $\theta_{AC,w}$  is the water-filled intraparticle AC porosity, d<sub>AC</sub> is the skeletal solid density of the AC, L<sub>C</sub> is the length of the column, and R<sub>C</sub> is the radius of the column.

177 The volume fraction of the column in between the AC particles, which is assumed to be entirely

178 filled with mobile water,  $\theta_w$ , is defined as

$$\theta_w = 1 - \theta_{AC} \text{ (eq 11)}$$

180

# 181 3.4.2 Differential Equations

182 Pollutant diffusion in intraparticle pore water:

183 The following partial differential equation is assumed to govern the pollutant concentration in 184 the AC intraparticle pore water,  $C_{AC,ippw}$ 

$$(\theta_{AC,w} + (1 - \theta_{AC,w})d_{AC}K_d)^d / dt^{C_{AC,ippw}} = D_{eff,AC} \frac{1}{r^2} \cdot \frac{\partial}{\partial r} r^{2\partial} / \frac{\partial}{\partial r} C_{AC,ippw}$$
(eq 12)

186 where r is the radial distance from the AC particle center, and t is the time.

187 The effective diffusion coefficient of the pollutant in the AC pore network is defined as

$$D_{eff,AC} = \frac{\theta_{AC,w} D_{aq}}{\tau} (eq \ 13)$$

189 where  $\tau$  is the AC pore network tortuosity factor, and  $D_{aq}$  is the molecular diffusion coefficient of

- 190 the pollutant in water.
- 191 Boundary conditions for the AC particles:
- 192 A no net diffusion flux boundary condition is enforced at r=0 in the AC particle cores

$$\frac{\partial}{\partial r} C_{AC,ippw} \Big|_{r=0} = 0 \quad (\text{eq } 14)$$

The pollutant concentration in AC intraparticle pore water at the mobile water-AC interface is assumed to be equal to the pollutant concentration in the mobile water in between the soil and AC particles (i.e. no external aqueous film mass transfer resistance)

197 
$$C_{AC,ippw}|_{r=R_{BC}} = C_w \text{ (eq 15)}$$

- 198 where  $R_{BC}$  is the particle radius.
- 199 Pollutant transport in mobile water in between the AC particles:

200 The following partial differential equation is assumed to govern the pollutant concentration in201 the mobile water phase in between the AC particles:

$$\theta_{w} \cdot \frac{d}{dt} C_{w} = \theta_{w} D_{disp} \frac{\partial^{2}}{\partial x^{2}} C_{w} - \theta_{w} v_{x} \frac{\partial}{\partial x} C_{w} + r_{ippwd,out}$$
(eq 16)

where  $\theta_w$  is the fraction of the column volume in between the AC particles, which is assumed to be fully water saturated,  $D_{disp}$  is the dispersion coefficient for pollutants in mobile water in the x direction, and  $v_x$  is the interstitial velocity also in the x direction.

206 The AC particles to mobile water mass transfer rate, r<sub>ippwd,out</sub>, is described by

$$= -\frac{\theta_{AC}}{\frac{4}{3}\pi R_{AC}^{3}} \cdot 4\pi R_{AC}^{2} \cdot D_{eff,AC} \cdot \frac{\partial}{\partial r} C_{AC,ippw} \Big|_{r=R_{AC}} = -3\frac{\theta_{AC}}{R_{AC}} \cdot D_{eff_{AC}} \cdot \frac{\partial}{\partial r} C_{AC,ippw} \Big|_{r=R_{AC}}$$

207 208 (eq 17)

- 209 Boundary conditions for the column:
- 210 The pollutant concentration at the column inlet is equal to the concentration in the column
- 211 influent, Cin,
- 212  $C_w|_{x=0} = C_{in} (eq 18)$
- 213 And a zero-concentration gradient boundary condition is enforced at the column outlet

$$\frac{\partial}{\partial x} C_w \Big|_{x=L} = 0 \quad (\text{eq 19})$$

# 216 3.5 Influent Concentration



218 Figure S2. Influent concentration over time.

219

217

# 220 3.6 Modeling Output Results

#### 221

# **Table S6.** Equilibrium model derived K<sub>d</sub> and SSR values.

		PFPeA	PFHxA	PFHpA	PFOA	PFPrS	PFBS	PFPeS	PFHxS	PFHpS	PFOS
F400	Log Kd (L/kg)	4.40	4.56	4.88	4.80	4.46	4.62	4.74	4.82	4.87	4.86
	SSR	0.170	0.079	0.001	0.013	0.082	0.136	0.334	0.021	0.003	0.001
GAC400	Log Kd (L/kg)	4.45	4.56	4.92	4.80	4.47	4.63	4.74	4.85	4.89	4.89
	SSR	0.130	0.053	0.000	0.075	0.044	0.159	0.367	0.030	0.010	0.018
F600	Log Kd (L/kg)	4.34	4.47	4.80	4.61	4.42	4.55	4.64	4.68	4.70	4.66
	SSR	0.248	0.253	0.007	0.387	0.241	0.397	0.402	0.241	0.066	0.245
GCN1240	Log Kd (L/kg)	4.41	4.45	4.86	4.59	4.43	4.49	4.54	4.64	4.76	4.70
	SSR	0.282	0.191	0.038	0.156	0.202	0.052	0.177	0.170	0.355	0.267

		PFPeA	PFHxA	PFHpA	PFOA	PFPrS	PFBS	PFPeS	PFHxS	PFHpS	PFOS
F400	Log Kd (L/kg)	4.49	4.71	5.58	5.32	4.54	4.82	5.02	5.35	5.61	5.60
	SSR	1.710	1.022	0.002	0.018	1.385	0.434	0.105	0.011	0.007	0.005
GAC400	Log Kd (L/kg)	4.52	4.69	5.58	5.18	4.54	4.79	4.99	5.32	5.54	5.49
	SSR	1.164	1.113	0.002	0.054	1.299	0.501	0.197	0.008	0.020	0.008
F600	Log Kd (L/kg)	4.44	4.62	5.43	4.89	4.54	4.77	4.90	5.01	5.17	5.07
	SSR	1.735	0.652	0.001	0.167	0.607	0.265	0.076	0.055	0.084	0.139
GCN1240	Log Kd (L/kg)	4.47	4.52	5.36	4.77	4.50	4.59	4.68	4.85	5.09	5.02
	SSR	0.773	1.132	0.008	0.651	0.939	1.166	0.689	0.393	0.110	0.266

**Table S7.** Intraparticle diffusion model derived  $K_d$  and SSR values at  $\tau = 1$ .



Figure S3. Effect of the tortuosity on the best fit K<sub>d</sub> for the intraparticle diffusion model using
GCN1240 breakthrough results for four different compounds, PFPeA, PFOA, PFPeS, and PFOS.

**Table S8.** SSR at different tortuosity values for selected compounds in GCN1240 pilot data.

	$\tau = 1$	$\tau = 3$	$\tau = 6$	
PFPeA	0.773	1.549	1.851	
PFOA	0.651	0.976	1.113	
PFPeS	0.689	1.104	1.259	
PFOS	0.266	0.370	0.460	





239

# 240 3.7 Linear Regressions from Model Outputs

Table S7 and S8 show linear regression fits from the model output  $K_d$  fits. The x variable is PFAS chain length and the y variable is log  $K_d$  (L/kg). The intraparticle diffusion model outputs are performed with a tortuosity = 1.

244

245

246

Equilibrium Model							
		Carboxylates	Sulfonates				
F400	Regression	y = 0.153x + 3.66	y = 0.081x + 4.28				
	R2	0.8	0.89				
GAC400	Regression	y = 0.139x + 3.78	y = 0.085x + 4.27				
	R2	0.72	0.89				
F600	Regression	y = 0.114x + 3.81	y = 0.049x + 4.34				
	R2	0.55	0.74				
GCN1240	Regression	y = 0.094x + 3.97	y = 0.064x + 4.24				
	R2	0.35	0.89				

**Table S10.** Intraparticle diffusion model linear regression fits at  $\tau = 1$ .

Intraparticle Diffusion Model								
		Carboxylates	Sulfonates					
F400	Regression	y = 0.337x + 2.83	y = 0.228x + 3.90					
	R2	0.72	0.96					
GAC400	Regression	y = 0.286x + 3.13	y = 0.210x + 3.96					
	R2	0.59	0.94					
F600	Regression	y = 0.216x + 3.44	y = 0.113x + 4.289					
	R2	0.42	0.86					
GCN1240	Regression	y = 0.176x + 3.64	y = 0.122x + 4.115					
	R2	0.31	0.93					

	PFPeA	PFHxA	PFHpA	PFOA	PFPrS	PFBS	PFPeS	PFHxS	PFHpS	PFOS
Xiao et al. Batch K <sub>d</sub>	4.29	4.18	4.49	5.25	3.83	4.69	4.64	5.28	5.79	5.95
F400 EQ	4.40	4.56	4.88	4.80	4.46	4.62	4.74	4.82	4.87	4.86
GAC400 EQ	4.45	4.56	4.92	4.80	4.47	4.63	4.74	4.85	4.89	4.89
F600 EQ	4.34	4.47	4.80	4.61	4.42	4.55	4.64	4.68	4.70	4.66
GCN1240 EQ	4.41	4.45	4.86	4.59	4.43	4.49	4.54	4.64	4.76	4.70
F400 Intraparticle Diffusion	4.49	4.71	5.58	5.32	4.54	4.82	5.02	5.35	5.61	5.60
GAC400 Intraparticle Diffusion	4.52	4.69	5.58	5.18	4.54	4.79	4.99	5.32	5.54	5.49
F600 Intraparticle Diffusion	4.44	4.62	5.43	4.89	4.54	4.77	4.90	5.01	5.17	5.07
GCN1240 Intraparticle Diffusion	4.47	4.52	5.36	4.77	4.50	4.59	4.68	4.85	5.09	5.02

# **Table S11.** K<sub>d</sub> value comparison between Xiao et al. 2017<sup>3</sup> and EQ model predictions.

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