Supplementary material

Behavior of weakly adsorbing impurities in flow-through ion-exchange chromatography

Chase E. Herman, Xuankuo Xu, Steven J. Traylor, Sanchayita Ghose,
Zheng Jian Li, and Abraham M. Lenhoff

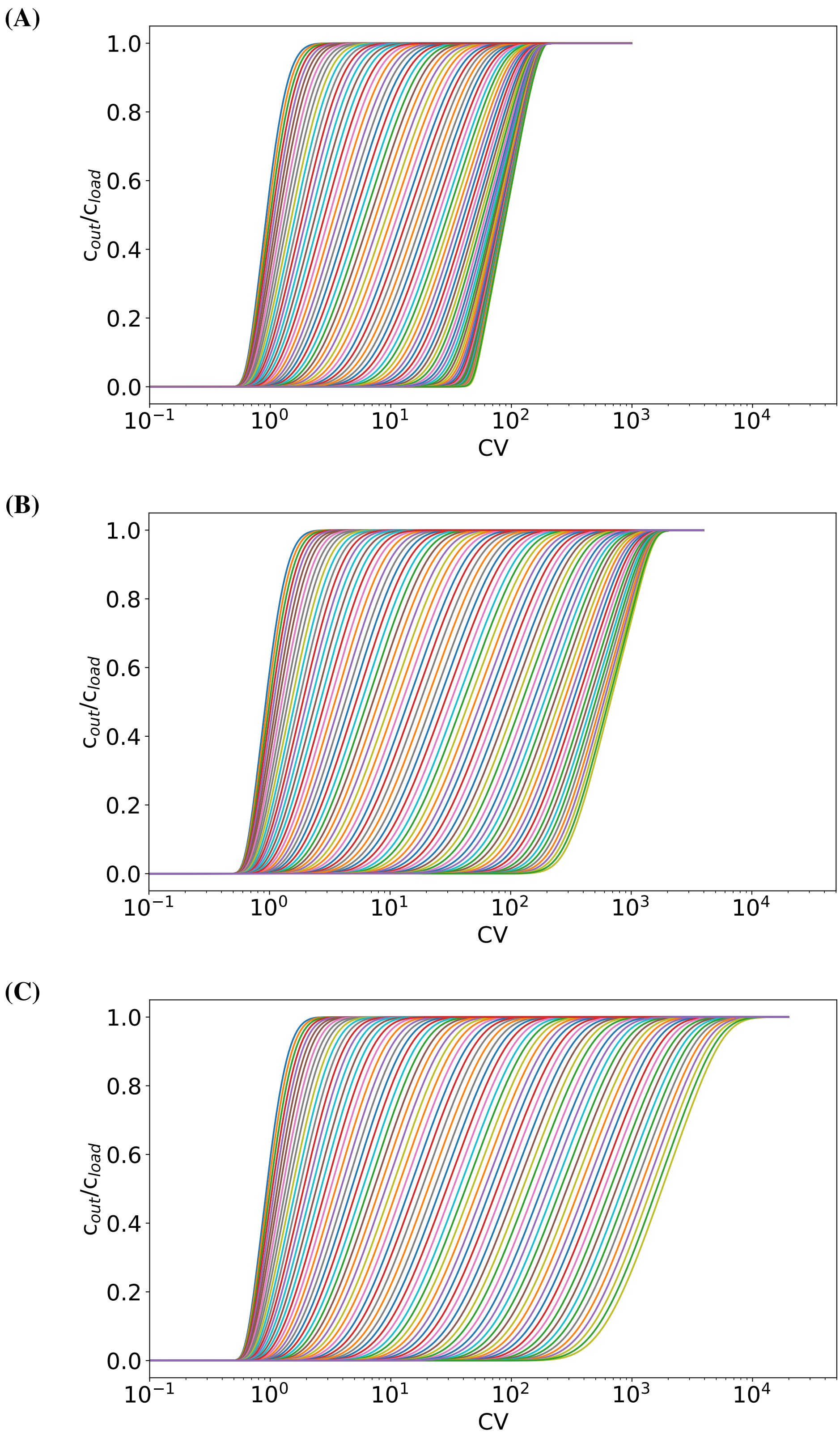

Figure S1: Breakthrough profiles from a simulation of solute loading at (A) 1 mg/ml, (B) 100 μg/ml, and (C) 10 μg/ml. Lines correspond to simulations with different K_{eq}, which increases by 4 orders of magnitude from left to right. Note that q_{max} was fixed at 100 mg/ml of packed column for all simulations, and the abscissa is on a logarithmic scale.

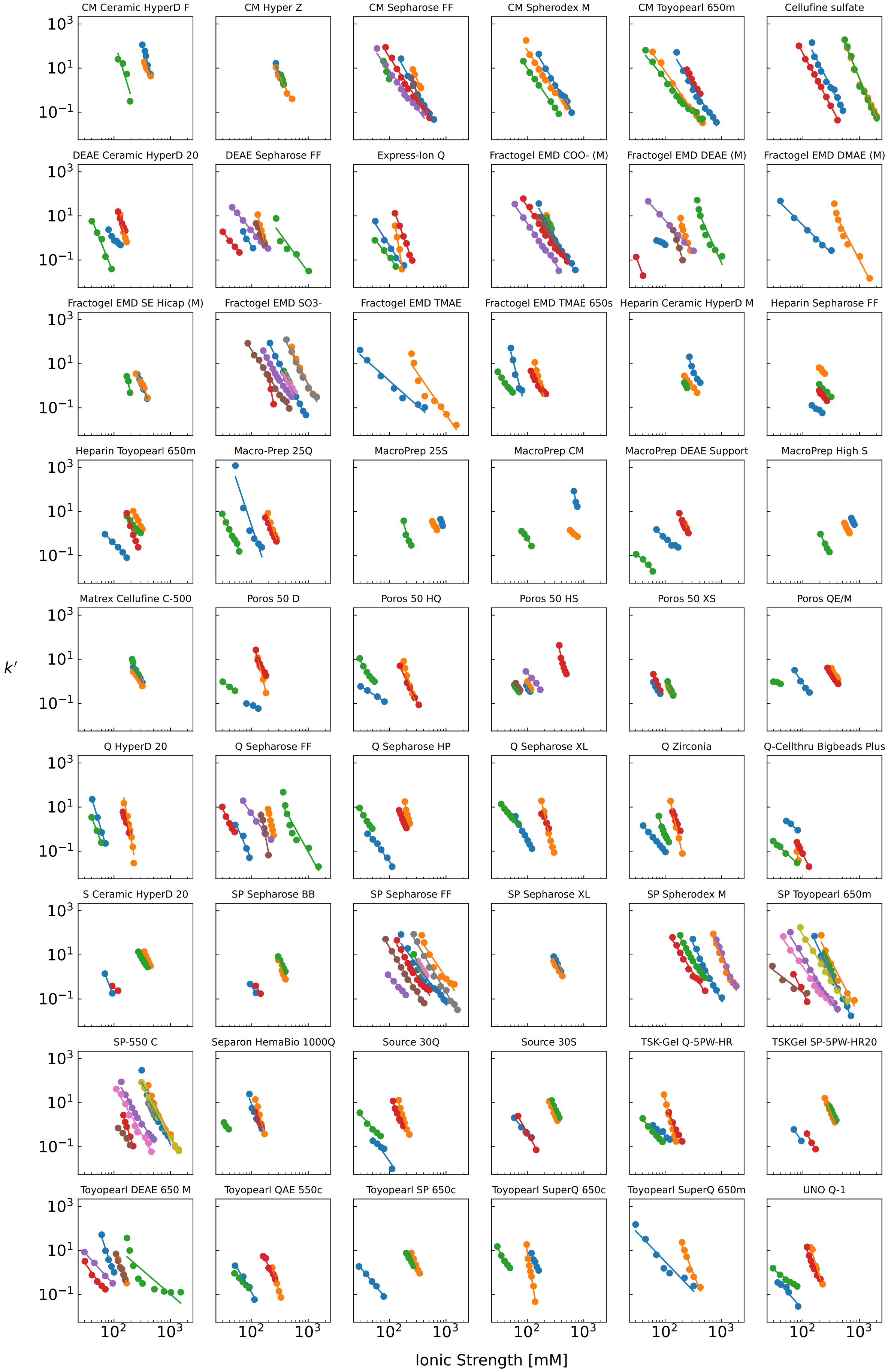

Figure S2: Isocratic k' data that were consolidated from the literature. Each series represents a unique protein-pH-resin combination, and lines represent quasi-SDM fits to the data. These data, which are available in the `Supplementary_table_S2.xlsx` file, were acquired by digitizing plots (using the Engauge Digitizer software), which may introduce some error into the precise k' values.

Table S1: Simulation parameters.

Variable	Figures 1, 2, and S1	Figure 3
L_{col} [cm]	4.2	5.0 – 20.0
r_p [μm]	25.0	2.5 – 100.0
ε_c [-]	0.49	0.49
ε_p [-]	0.40	0.40
u, superficial velocity [cm/h]	300	100 – 200
D_{ax} [m^2/s]	1.25×10^{-7}	Function of u
k_{film} [m/s]	1.0×10^{-3}	1.0×10^{-3}
D_p [m^2/s]	1.0×10^{-11}	5.0×10^{-12} – 4.0×10^{-11}
a [m^2/s] (in $D_s = aK_{eq}^b$)	7.76×10^{-12}	1.66×10^{-12}
b [-] (in $D_s = aK_{eq}^b$)	-1.54	-0.24
K_{eq} [-]	1.0 – 1.0×10^4	1.0 – 1.0×10^4
q_{max} [mg/ml column]	100	100
c_{load} [mg/ml]	1.0×10^{-3} – 1.0×10^1	1.0×10^{-3}