Supplementary material

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

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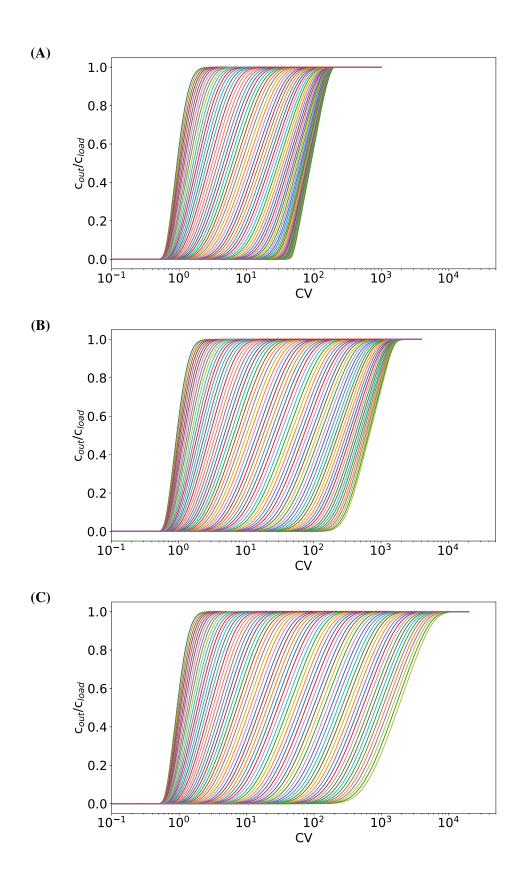


Figure S1: Breakthrough profiles from a simulation of solute loading at (A) 1 mg/ml, (B) 100 μ g/ml, and (C) 10 μ g/ml. Lines correspond to simulations with different K_{eq} , which increases by 4 orders of magnitude from left to right. Note that q_{max} was fixed at 100 mg/ml of packed column for all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

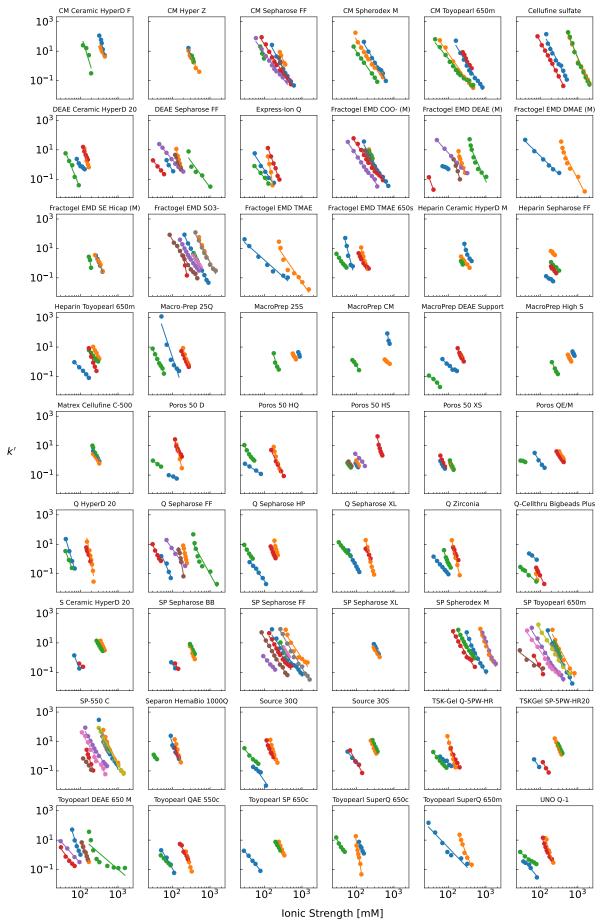


Figure S2: Isocratic k' data that were consolidated from the literature. Each series represents a unique protein-pH-resin combination, and lines represent quasi-SDM fits to the data. These data, which are available in the Supplementary_table_S2.xlsx file, were acquired by digitizing plots (using the 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
Lcol [cm]	4.2	5.0 – 20.0
$r_p[\mu m]$	25.0	2.5 – 100.0
$\varepsilon_{\rm c}$ [-]	0.49	0.49
$arepsilon_p$ [z]	0.40	0.40
u, superficial velocity [cm/h]	300	100 – 200
D_{ax} [m ² /s]	1.25×10^{-7}	Function of u
$\underline{k}_{film}[\underline{m}/\underline{s}]$	1.0×10^{-3}	1.0×10^{-3}
$\mathcal{D}_{p}[\underline{\mathbf{m}^{2}/\mathbf{s}}]$	1.0×10^{-11}	$5.0 \times 10^{-12} - 4.0 \times 10^{-11}$
$\underbrace{a [\text{m}^2/\text{s}] (\text{in} D_s = a K_{eq}^b)}_{}$	7.76×10^{-12}	1.66×10^{-12}
$b \left[-\right] \left(in D_{s} = aK_{eq}^{b} \right)$	_1.54	0.24
$\underbrace{K_{eq}}[-]$	$1.0 - 1.0 \times 10^4$	$1.0 - 1.0 \times 10^4$
q_{max} [mg/ml column]	100	100
c_{load} [mg/ml]	$1.0 \times 10^{-3} - 1.0 \times 10^{1}$	1.0×10^{-3}