

Supplementary material

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

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

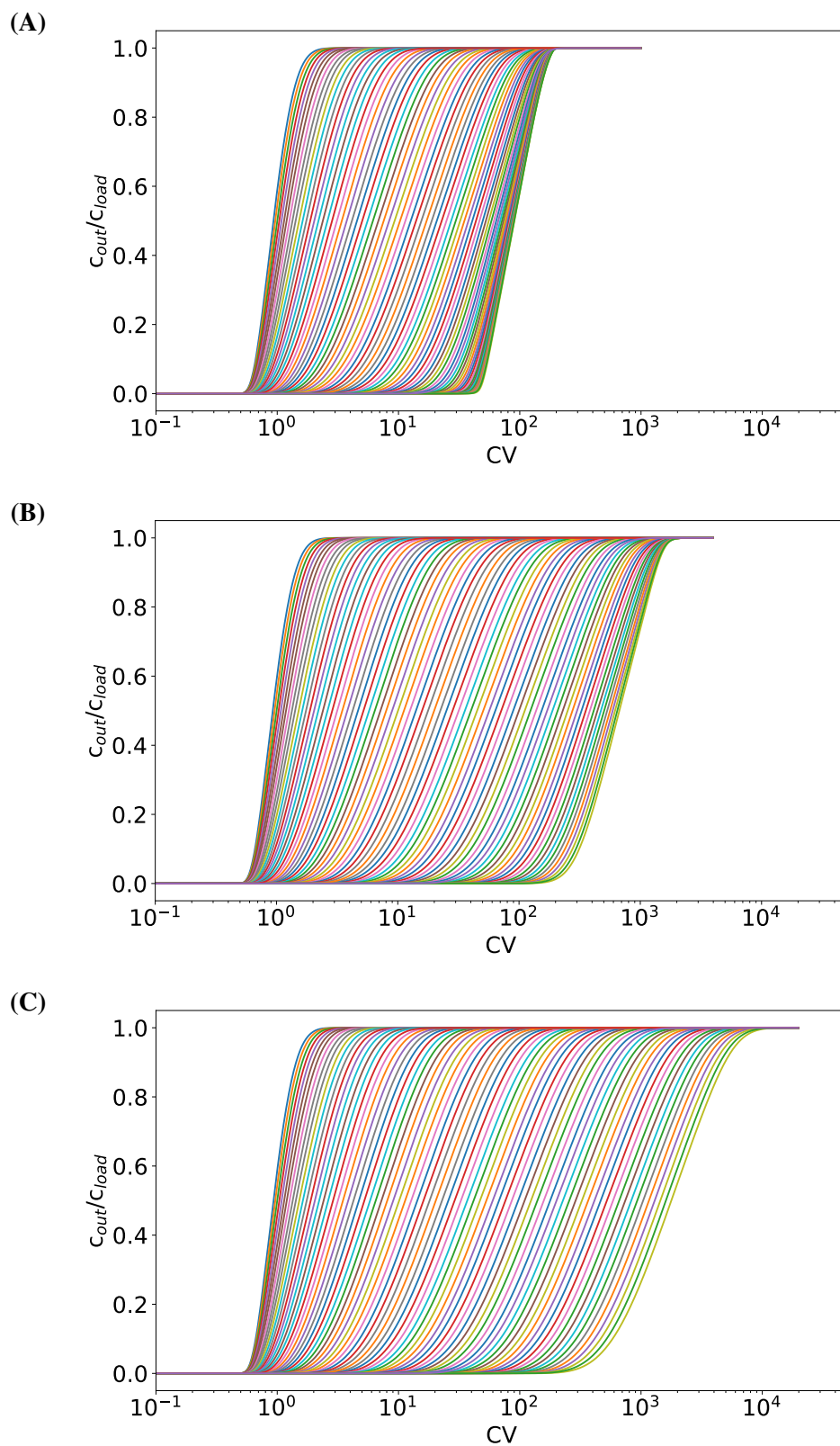


Figure S1: Breakthrough profiles from a simulation of solute loading at (A) 1 mg/ml, (B) 100 $\mu\text{g/ml}$, and (C) 10 $\mu\text{g/ml}$. Lines correspond to simulations with different K_{eq} , which increases by 4 orders of magnitude from left to right. Note that q_{max} was fixed at 100 mg/ml of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

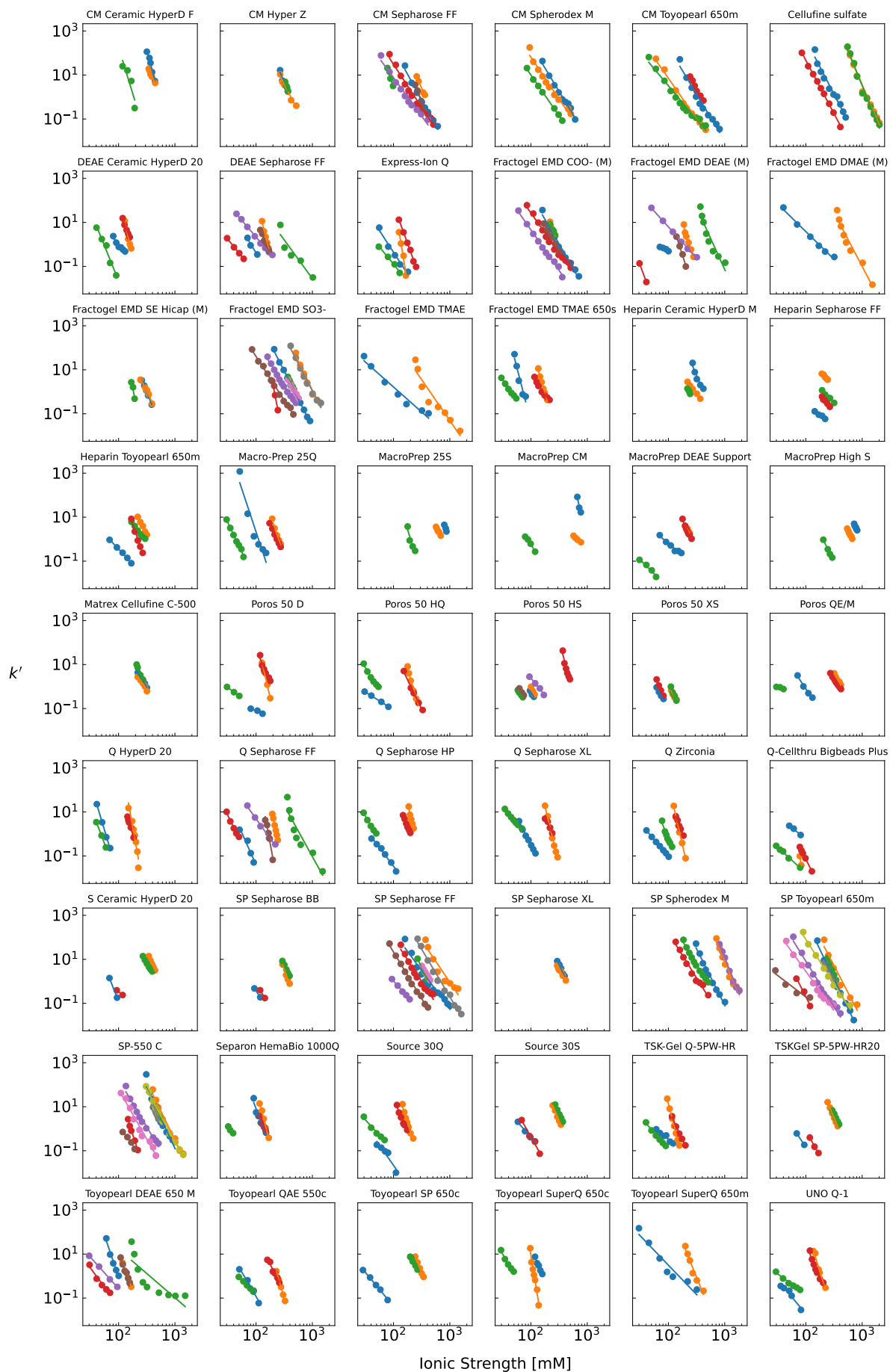


Figure S2: Isocratic k' data that were consolidated from the literature. Each series represents a unique protein-pH-resin combination, and lines represent quasi-SDM fits to the data. [These data, which are available in the Supplementary table_S2.xlsx file, were acquired by digitizing plots \(using the Engauge Digitizer software\), which may introduce some error into the precise \$k'\$ values.](#)

Table S1: Simulation parameters.

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