Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Supporting Information

Anion recovery from water by cross-linked cationic surfactant nanoparticles across dialysis membranes

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Table S1. Equations for calculating anion distribution between water and micelles[1]

	Equations[†‡]
Mass balances	$[Cl^-]_{total} = [QASE]_{total} + [Cl^-]_{initial}$ $[Cl^-]_{total} = [Cl^-]_{aq} + [Cl^-]_{mic} * [M]$ $[B_i^-]_{total} = [B_i^-]_{aq} + [B_i^-]_{mic} * [M]$ $[B_j^{2-}]_{total} = [B_j^{2-}]_{aq} + [B_j^{2-}]_{mic} * [M]$ $[M] = [QASE]_{total}$ $[Cl^-]_{mic} + \sum_i [B_i^-]_{mic} + 2\sum_j [B_j^{2-}]_{mic} = 1$
Mass action	$K_{sel_{A^-}}^{B_i^-} = \frac{[Cl^-]_{aq}[B_i^-]_{mic}}{[Cl^-]_{mic}[B_i^-]_{aq}}$ $K_{sel_{A^-}}^{B_j^{2-}} = \frac{[Cl^-]_{\mathrm{aq}}{}^2[B_j^{2-}]_{mic}}{[Cl^-]_{mic}{}^2[B_j^{2-}]_{aq}}$
pH	$pH = -log[H^+]$
Speciation	$K_a = \frac{[H^+][HPO_4^{2-}]}{[H_2PO_4^-]}$

[†] B_i is F^-, Cl^-, $H_2PO_4^-$, NO_2^-, or NO_3^-; B_j is SO_4^{2-} or HPO_4^{2-}. For mass balance of phosphate, $[PO_4^{3-}]_{total} = [H_2PO_4^-]_{aq} + [HPO_4^{2-}]_{aq} + [H_2PO_4^-]_{mic} * [M] + [HPO_4^{2-}]_{mic} * [M]$

[‡] Items and units have been defined in section 2.4 in the paper.

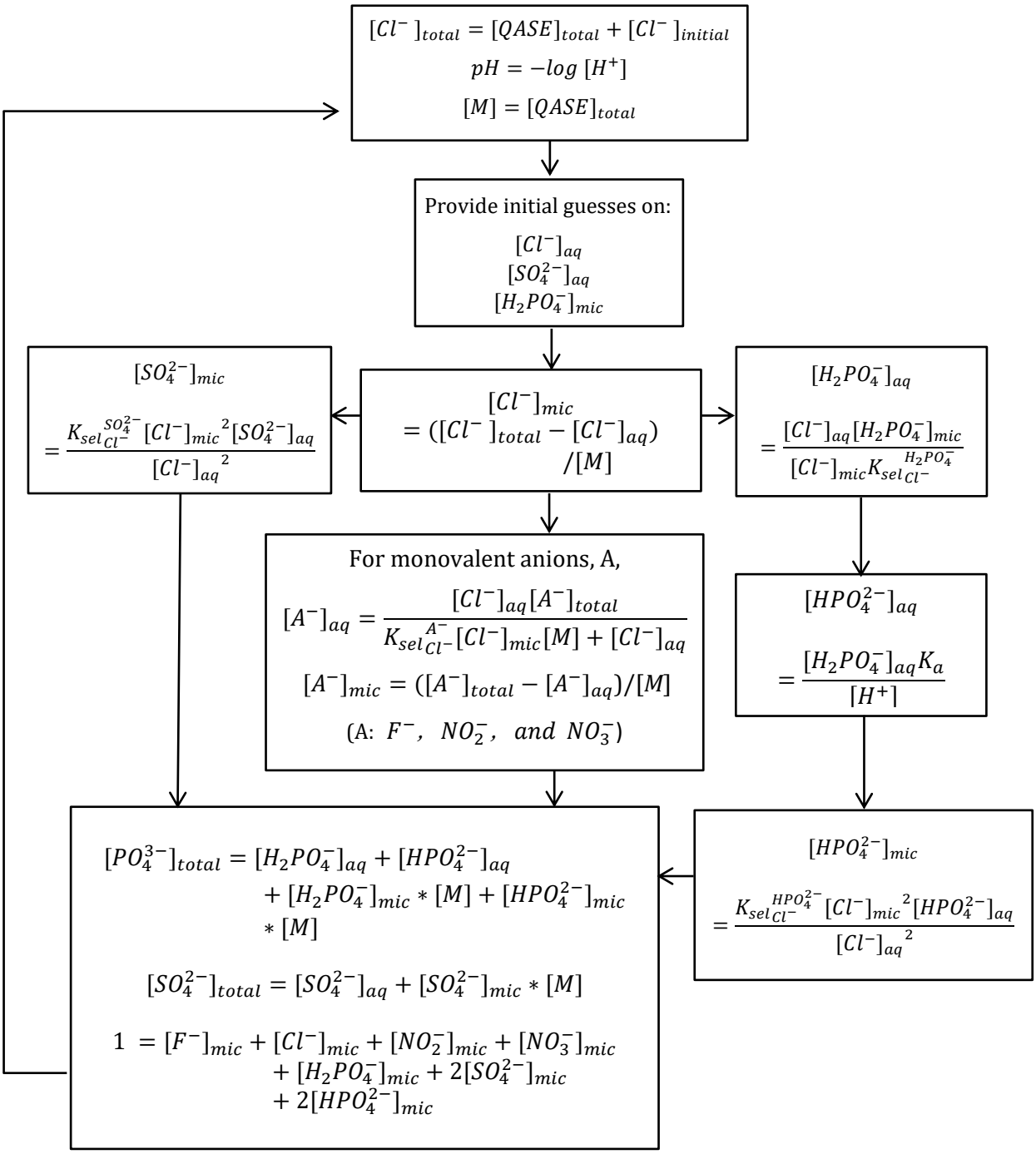

Figure S1. Iterative least squares method used to minimize residuals between the left-hand and right hand sides of the equations in the last box ($[PO_4^{3-}]_{total}$, $[SO_4^{2-}]_{total}$, and the total concentration of micellar phase species {i.e., = 1 mole/mole}), by adjusting the guesses on $[Cl^-]_{aq}$, $[SO_4^{2-}]_{aq}$, and $[H_2PO_4^-]_{mic}$ after each iteration, using Solver in Excel. [1]

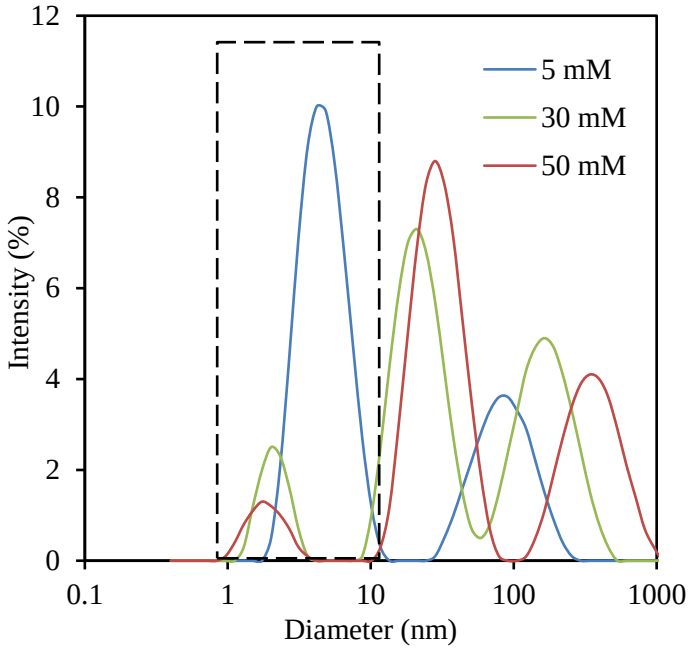

Figure S2. Intensity size distribution of QACLE micelles at different concentrations

The intensity distribution (shown in **Figure S2**) is weighted based on the scattering intensity of each particle fraction, and is more accurate than number and volume distributions; however it is usually influenced by large particles (impurities). Through number distribution and intensity distribution, the average sizes of QACLE micelles were determined to be 4.81 ± 0.21 nm for 5 mM, and 1.86 ± 0.07 nm for 50 mM.

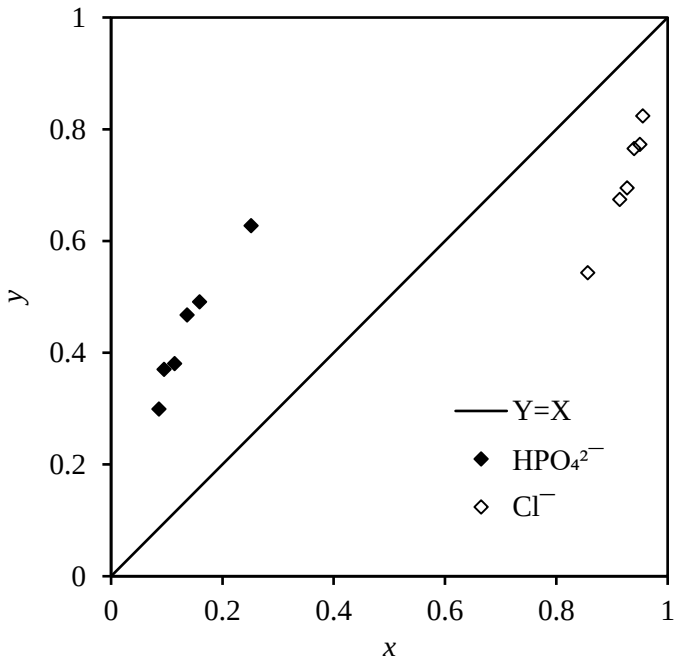

Figure S3. Distribution of HPO_4^{2-} and Cl^- in different phases in binary systems

x: normality fraction of anions in the aqueous phase, $x = \frac{\alpha[A^{\alpha-}]_{aq}}{\alpha[A^{\alpha-}]_{aq}+\beta[B^{\beta-}]_{aq}}$

y: normality fraction of anions in the micellar phase, $y = \frac{\alpha[A^{\alpha-}]_{mic}}{\alpha[A^{\alpha-}]_{mic}+\beta[B^{\beta-}]_{mic}}$

The experimental conditions of the distribution test were the same as in the experiments to measure selectivity coefficients. It can be seen from the figure, HPO_4^{2-} has a much greater affinity for the micellar phase than Cl^-. For example, when the normality fraction of HPO_4^{2-} in the aqueous phase is 0.2 (x = 0.2), its normality fraction in the micellar phase is about 0.5 (y = 0.5 > x). However, the distribution of Cl^- is below the line of $y = x$, indicating a lower affinity than HPO_4^{2-}.

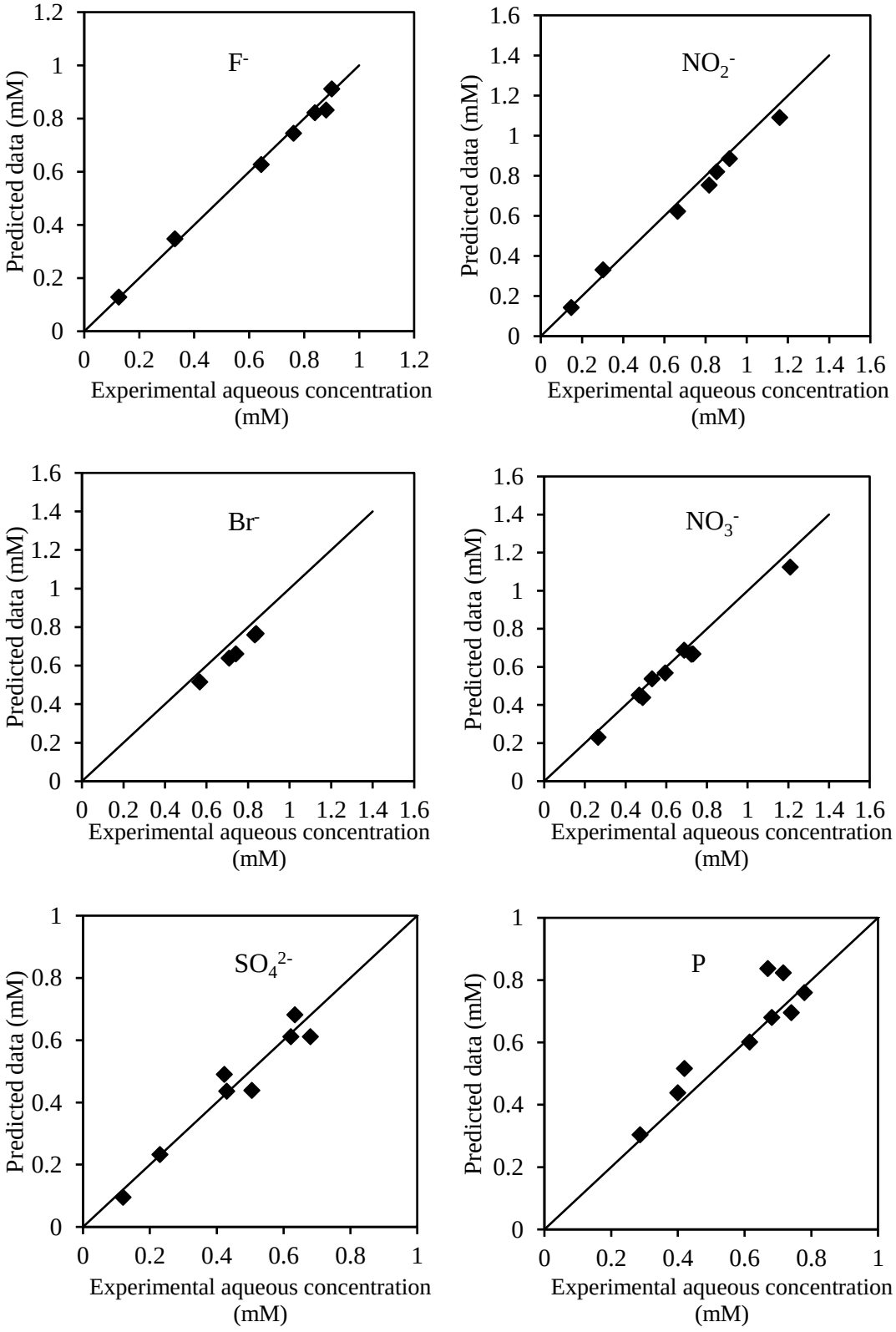

Figure S4. Relationship between measured aqueous concentrations and model predicted values for each anion

Reference:

1. M. Chen and C. T. Jafvert, Anion exchange on cationic surfactant micelles, and a speciation model for estimating anion removal on micelles during ultrafiltration of water, *Langmuir*, 2017, **33**, 6540-6549.