**Supplementary Material**

**Release of Colloids in Saturated Porous Media under Transient Hydro-Chemical Conditions: A Pore-Scale Study**

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**S1. DLVO interaction energy calculations**

The interaction energies when the colloid approach another colloid or collector surface are calculated using DLVO theory as the sum of electrostatic double layer, van der Waals, and Born repulsion energies. The total interaction energies (φtot) are evaluated as a function of separation distance (D) for each interaction.

[1]

where φvdW, φDL andφB are the van der Waals, electrostatic, and Born energies, respectively. The values of φtot, φvdW, φDL and φhyd are made dimensionless by dividing by the product of Boltzmann’s constant and absolute temperature.

The van der Waals interaction exists between colloids and the charged surfaces in the medium due to the presence of intermolecular forces during the polarization of molecules into dipoles. The retarded van der Waals interaction energy for a sphere-sphere interaction is given by [1].

 [2]

where D is the separation distance; λ is the characteristic wavelength that is often taken as 100 nm [1]; H123 is the complex Hamaker constant for solids 1 and 3 (i.e., colloid and collector) in medium 2 (i.e., water) given by:

 [3]

where H11, H22 and H33 are the Hamaker constants for each medium. The Hamaker constants of polystyrene latex, glass and water are reported to be 6.6 x 10-20, 6.34 x 10-20 and 3.7 x 10-20, respectively [2].

The van der Waals potential energy for colloid-colloid interaction can be calculated using Eq. [2] and for the colloid-collector surface can be calculated using Eq. [4] considering sphere-plate interaction.

 [4]

The electrostatic double-layer interaction forces of charged bodies in ionic solutions was approximated from the Poisson-Boltzmann equation using the constant surface potential interaction by Hogg et al. (1966) for a sphere-sphere interaction as

 [5]

where ε is the dielectric constant of the medium; ε0 is the permittivity of free space; r1 and r2 are the radii of the two colloids; κ is the inverse Debye-Huckel length calculated from the following equation [2].

 or  [6]

where the constants are listed in Table S1 and I is the ionic strength of the solution given by

 [7]

where c is the molar concentration of the electrolyte (mol L-1) and z is the valence of the electrolyte.

**Table S1:** Values of constants used for DLVO energy calculations

|  |  |
| --- | --- |
| Parameter | Value |
| Dielectric constant of water, ε | 80.4 |
| Permittivity of free space, ε0, (C2J-1m-1) | 8.85 x 10-12 |
| Electronic charge, e, (C) | -1.602 x 10-19 |
| Avogadro Number, NA, (mol-1) | 6.022 x 1023 |
| Boltzmann’s constant, kB, (JK-1) | 1.381 x 10-23 |
| Absolute temperature, T, (K) | 298 |

ψc and ψs are the surface potentials of the colloid and the other sphere interacting with the colloid. For colloid-colloid interactions, ψs will be ψc and for colloid-collector surface interaction, ψs can be taken as the surface potential for collector surface. Measured zeta potentials are used in place of surface potentials for the colloids (ψc) and are listed in Table 1 for the colloids used in this study. ψs for clean glass is reported to be -10 to -85 mV [4]. The calculations presented in this paper uses a value of -60 mV for glass.

The sphere-plate interaction for collector surfaces can be calculated using Eq. 5 by taking the quantity (r1r2)/(r1+r2) as the colloid radius r.

Born repulsion energy can be calculated as [5]

[8]

where σ is the collision diameter and is taken as 0.5 nm [6].

**References**

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