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Title: Application of a Developed Numerical Model for Surfactant Flushing Combined with Intermittent Air Injection at Field Scale

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S.1 Equation Governing Multiphase Flow

The multiphase system in a porous medium is assumed to be composed of two phases: water and NAPL. For simplicity, we consider only incompressible fluids. The equations describing the flow of two fluid phases in a porous medium are based on conservation of mass (Suk and Yeh, 2007, 2008; Suk et al., 2011):

$$\frac{\partial \phi \rho_i S_i}{\partial t} + \nabla \cdot (\rho_i V_i) = Q_i + \sum_j E_{ij}, \quad i = 1,2 \qquad \text{in } \Omega \tag{S1}$$

$$V_i = -\frac{k_{ri} k}{\mu_i} (\nabla p_i + \rho_i g \nabla z), \quad i = 1,2 \tag{S2}$$

where ρ_i is the density of phase i [M L^{-3}], with the subscript i indicating the phase (1 for water and 2 for NAPL), ϕ is the effective porosity of the porous medium [L^3 L^{-3}], S_i is the saturation of phase i [L^3 L^{-3}], t is time [T], Q_i is the source and sink term for phase i [M L^{-3} T^{-1}], E_{ij} is the rate of mass exchange from phase j to phase i [M L^{-3} T^{-1}], V_i is the Darcy velocity of phase i [L T^{-1}], k_{ri} is the relative permeability of phase i [-], k is the intrinsic permeability tensor [L^2], μ_i is the dynamic viscosity of phase i [M L^{-1} T^{-1}], p_i is the pressure of phase i [M L^{-1} T^{-2}], g is the gravitational constant [L T^{-2}], z is elevation [L], and Ω is an interested bounded area. Initial condition can be expressed as combination of pressures or saturations of each phases:

$$p_i = p_{i,0}, \quad i=1,2 \qquad \text{in } \Omega$$

or

$$S_i = S_{i,0}, \quad i=1,2 \qquad \text{in } \Omega \tag{S3}$$

where $p_{i,0}$ and $S_{i,0}$ are initial pressures [M L^{-1} T^{-2}] and saturations [-] of phase i, respectively, in domain Ω. The boundary conditions for Eq. (S1) are generally given as:

$$p_i = p_{i,D}, \quad i=1,2 \quad \text{on } \Gamma_1$$

$$-n \cdot \left(\frac{k_{ri}k}{\mu_i} \cdot \nabla p_i\right) = q_{i,N}, \quad i=1,2 \quad \text{on } \Gamma_2$$

$$-n \cdot \left[\frac{k_{ri}k}{\mu_i}(\nabla p_i + \rho_i g \nabla z)\right] = n \cdot V_i = q_{i,C}, \quad i=1,2 \quad \text{on } \Gamma_3 \tag{S4}$$

where n is the unit outward vector normal to the boundary Γ, and $p_{i,D}$, $q_{i,N}$, and $q_{i,C}$ are the specified pressure [M L^{-1} T^{-2}] along Γ_1, specified pressure normal gradient [L T^{-1}] on Γ_2, and prescribed flux [L T^{-1}] normal to Γ_3 of phase i, respectively, with $\Gamma = \Gamma_1 + \Gamma_2 + \Gamma_3$ being

the boundary of domain Ω. Relative permeability relationships corresponding to the van Genuchten model are expressed as:

$$k_{r1} = \bar{S}_1^{1/2}\left[1-\left(1-\bar{S}_1^{1/m}\right)^m\right]^2 \tag{S5}$$

$$k_{r2} = \bar{S}_2^{1/2}\left\{\left(1-\bar{S}_1^{1/m}\right)^m - \left[1-(\bar{S}_1+\bar{S}_2)^{1/m}\right]^m\right\}^2 \tag{S6}$$

where m is the curve shape parameter. The capillary pressure-saturation relationship in the water-NAPL phase system follows the model of Parker et al. (1987), as follows:

$$\bar{S_1} = [1+(\alpha_{21}h_{21})^n]^{-m}, \qquad \text{if } h_{21} > 0 \tag{S7}$$

$$\bar{S_1} = 1, \qquad \text{if } h_{21} \leq 0 \tag{S8}$$

where n [-] and α_{21} [L^{-1}] are the van Genuchten parameters and $h_{21}(= h_2 - h_1)$ is the NAPL-water capillary head [L], h_1 is the pressure head of water phase [L], and h_2 is the pressure head of NAPL phase [L]. $\bar{S_1}$ is water saturation and is defined as follows:

$$\bar{S_1} = \frac{S_1 - S_{1r}}{1-S_{1r}}, \qquad \bar{S}_2 = \frac{S_2 - S_{2r}}{1-S_{2r}} \tag{S9}$$

where S_{1r} is the irreducible saturation of the water phase [-] and S_{2r} is the residual NAPL saturation [-]. The total velocity, V_t [L T^{-1}], given by the sum of the velocities of the two phases, is defined as follows:

$$V_t = V_1 + V_2 \tag{S10}$$

Using Eq. (S2), Eq. (S10) can be rewritten as:

$$V_t = -\sum_{i=1}^{2} \frac{k_{ri}k}{\mu_i}(\nabla p_i + \rho_i g \nabla z) \tag{S11}$$

Based on Eq. (S11), we can define the total mobility, κ [L^3 T M^{-1}], fractional mobility for phase i, κ_i, and mobility-weighted average fluid density [-], $\bar{\rho}$ [M L^{-3}] as follows:

$$\kappa = \sum_{i=1}^{2} \frac{k_{ri}k}{\mu_i} \tag{S12}$$

$$\kappa_i = \frac{\frac{k_{ri}}{\mu_i}}{\sum_{j=1}^{2}\left(\frac{k_{rj}}{\mu_j}\right)}, \quad i=1,2 \tag{S13}$$

$$\bar{\rho} = \kappa_1 \rho_1 + \kappa_2 \rho_2 \tag{S14}$$

Substituting Eqs. (S12)–(S14) into Eq. (S11) results in:

$$V_t = -\kappa\left[\frac{1}{2}\nabla(p_1 + p_2) + \left(\frac{\kappa_1 - \kappa_2}{2}\right)\nabla(p_1 - p_2)\right] - \kappa\bar{\rho} g \nabla z \tag{S15}$$

where $\kappa_1 + \kappa_2 = 1$. If we define the total pressure, P_t [M L^{-1} T^{-2}], of an imaginary variable as follows:

$$P_t = \frac{p_1 + p_2}{2} + \frac{1}{2}\left[\int_0^{p_1 - p_2}(\kappa_1 - \kappa_2)d\eta\right] \tag{S16}$$

Eq. (S15) becomes:

$$V_t = -\kappa \cdot (\nabla P_t + \bar{\rho} g \nabla z) \quad \text{(S17)}$$

The total pressure in the water and NAPL two-phase system is calculated as follows (Suk and Yeh, 2007; Suk and Yeh, 2008; Suk et al., 2011):

$$-\nabla \cdot \kappa \cdot (\nabla P_t + \bar{\rho} g \nabla z) = \frac{Q_1}{\rho_1} + \frac{Q_2}{\rho_2} + \frac{E_n^w}{\rho_1} - \frac{E_n^w}{\rho_2} \quad \text{in } \Omega \quad \text{(S18)}$$

where E_n^w is the mass exchange from the NAPL to the water phase [M L^{-3} T^{-1}]. Initial and boundary conditions of total pressure equation can be transformed from Eqs. (S1)-(S4) according to numerical schemes provided by Suk and Yeh (2008). In Eq. (S18), the total mobility, κ [L^3 T M^{-1}], is an independent parameter of the total pressure, P_t [M L^{-1} T^{-2}], and the equation is linear. The velocities of the water and NAPL phases determined using Eq. (S15) are as follows:

$$V_1 = \kappa_1 V_t - \kappa_1 \kappa \kappa_2 \nabla P_{c12} - \kappa_1 \kappa (\rho_1 - \bar{\rho}) g \nabla z \quad \text{(S19)}$$

$$V_2 = \kappa_2 V_t - \kappa_2 \kappa \kappa_1 \nabla P_{c21} - \kappa_2 \kappa (\rho_2 - \bar{\rho}) g \nabla z \quad \text{(S20)}$$

where $P_{c12}(P_{c21})$ [M L^{-1} T^{-2}] is the capillary pressure of water (NAPL) and NAPL (water). Assuming incompressible flow and continuity of the total flux, Eq. (S19) can be substituted into the water-phase mass conservation equation (S1), resulting in the following water saturation equation:

$$\frac{\partial \phi S_1}{\partial t} + V_t \cdot \frac{d\kappa_1}{dS_1} \nabla S_1 = \nabla \cdot \kappa_1 \kappa \kappa_2 \frac{\partial P_{c12}}{\partial S_1} \cdot \nabla S_1 - \kappa_1 \nabla \cdot V_t$$

$$+\nabla \cdot \kappa_1 \kappa \cdot (\rho_1 - \bar{\rho}) g \nabla z + \frac{Q_1}{\rho_1} + \frac{E_n^w}{\rho_1} \quad \text{(S21)}$$

Initial and boundary conditions of water saturation equation can be obtained from Eqs. (S1)-(S4) according to numerical schemes provided by Suk and Yeh (2008).

S.2 Transport Equations for Dissolved NAPL Species and Surfactant

The transport behavior of a dissolved contaminant can be described based on adsorption and surfactant-enhanced dissolution from the NAPL to aqueous phase, as follows:

$$\frac{\partial \theta_1 C_o}{\partial t} + \rho_b \frac{\partial S_o}{\partial t} + \nabla \cdot (V_1 C_o) - \nabla \cdot (\theta_1 D \cdot \nabla C_o) = E_n^w$$

Initial conditions

$C_o = C_{o,0}$ in Ω

Boundary conditions

$C_o = C_{o,D}$ on Γ_D

$-n \cdot (\theta_1 D \cdot \nabla C_o) = f_{o,N}$ on Γ_N

$n \cdot (V_1 C_0 - \theta_1 D \cdot \nabla C_o) = f_{o,C}$ on Γ_C (S22)

where C_o is the concentration of the dissolved contaminant [M L^{-3}], ρ_b is the bulk density [M L^{-3}], S_o is the contaminant mass adsorbed into the soil mass [M M^{-1}], θ_1 is the water content [L^3 L^{-3}], $C_{o,0}$ is initial concentration of the dissolved contaminant [M L^{-3}] in domain Ω, and $C_{o,D}$, $f_{o,N}$, and $f_{o,C}$ are the specified concentration [M L^{-3}] along Dirichlet boundary Γ_D, specified gradient concentration [M L^{-2} T^{-1}] normal to Neumann boundary Γ_N, and prescribed flux [M L^{-2} T^{-1}] normal to Cauchy boundary Γ_C of the dissolved contaminant, respectively. $\theta_1 D$ is the dispersion coefficient [L^2 T^{-1}], which is defined as follows:

$$\theta_1 D = \alpha_T |V_1| \delta + (\alpha_L - \alpha_T) \frac{V_1 V_1}{|V_1|} + \theta_1 a_m \tau \delta \quad \text{(S23)}$$

where $|V_1|$ is the magnitude of V_1 [L T^{-1}], δ is the Kronecker delta tensor, α_L and α_T are the longitudinal and transverse dispersivities [L], respectively, a_m is the molecular diffusion coefficient [L^2 T^{-1}], and τ is the tortuosity [-]. Considering linear adsorption:

$$S_o = K_{d,o} C_o \quad \text{(S24)}$$

where $K_{d,o}$ is the distribution coefficient between adsorbed and aqueous NAPL species [L^3 M^{-1}]. Eq. (S22) can be rewritten using Eq. (S24), as follows:

$$\theta_1 \frac{\partial C_o}{\partial t} + C_o \frac{\partial \theta_1}{\partial t} + \rho_b K_{d,o} \frac{\partial C_o}{\partial t} + V_1 \nabla \cdot (C_o) + C_o \nabla \cdot (V_1) - \nabla \cdot (\theta_1 D \cdot \nabla C_o) = E_n^w \quad \text{(S25)}$$

The mass conservation equation of a dissolved contaminant can be expressed as follows:

$$\frac{\partial \rho_1 \theta_1}{\partial t} = -\nabla \cdot (\rho_1 V_1) + Q_1 \quad \text{(S26)}$$

where Q_1 is the source and sink term for water [M L^{-3} T^{-1}]. Eq. (S25) can be rewritten using Eq. (S26), as follows:

$$\left(\theta_1 + \rho_b K_{d,o}\right) \frac{\partial C_o}{\partial t} + V_1 \cdot \nabla C_o - \nabla \cdot (\theta_1 D \cdot \nabla C_o) + \frac{Q_1}{\rho_1} C_o = E_n^w \quad \text{(S27)}$$

To solve this equation using Lagrangian-Eulerian methods, Eq. (S27) can be expressed in the advective form:

$$\left(\theta_1 + \rho_b K_{d,o}\right)\frac{D_{V_{d,o}}C_o}{Dt} - \nabla \cdot (\theta_1 D \cdot \nabla C_o) + \frac{Q_1}{\rho_1}C_o = E_n^w \tag{S28}$$

where

$$V_{d,o} = \frac{V_1}{\theta_1 + \rho_b K_{d,o}} \tag{S29}$$

The mass exchange rate from the NAPL phase to the water phase can be determined as follows Zhong et al. (2003):

$$E_n^w = C_n^w\left(\overline{\rho_n^w} - C_o\right) \tag{S30}$$

$$C_n^w = \frac{a_m}{(d_p)^2}Sh, \quad Sh = \beta_0(R_e)^{\beta_1}(\theta_2)^{\beta_2}, \; R_e = \frac{d_p v_1 \rho_1}{\mu_1} \tag{S31}$$

$$\overline{\rho_n^w} = \overline{\rho_{n,pure}^w} + \gamma C_s \tag{S32}$$

where C_n^w is the rate coefficient, which regulates the rate at which equilibrium is reached [T^{-1}], a_m is the molecular diffusion coefficient [$L^2\ T^{-1}$], d_p is the mean particle diameter [L], Sh is the Sherwood number [-], R_e is the Reynolds number [-], v_1 is the seepage velocity [$L\ T^{-1}$], ρ_1 is the water density [$M\ L^{-3}$], μ_1 is the dynamic viscosity of water [$M\ L^{-1}\ T^{-1}$], θ_2 is the NAPL phase volumetric content [-], $\overline{\rho_n^w}$ is the equilibrium concentration of NAPL species in the water phase (solubility limit) [$M\ L^{-3}$], β_0, β_1 and β_2 are dimensionless fitting parameters [-], $\overline{\rho_{n,pure}^w}$ is the equilibrium concentration of NAPL species in the pure water phase [$M\ L^{-3}$], γ is an empirical parameter [-], and C_s is the concentration of surfactant [M

L^{-3}]. Eq. (S32) was formulated by Pennell et al. (1994). Equilibrium solubility is linearly related to surfactant concentration over the CMC, as shown in Eq. (S32). Finally, the multiphase flow and solute transport equations can be obtained by substituting the mass exchange rate in Eq. (S30) into Eqs. (S18), (S21), and (S28). Because the solute transport equation for the surfactant is not related to mass exchange, its governing equation can be expressed as follows:

$$\left(\theta_1 + \rho_b K_{d,s}\right)\frac{D_{V_{d,s}} C_s}{Dt} - \nabla \cdot (\theta_1 D \cdot \nabla C_s) + \frac{Q_1}{\rho_1} C_s = 0$$

Initial conditions

$C_s = C_{s,0}$ in Ω

Boundary conditions

$C_s = C_{s,D}$ on Γ_D

$-n \cdot (\theta_1 D \cdot \nabla C_s) = f_{s,N}$ on Γ_N

$$n \cdot (V_1 C_s - \theta_1 D \cdot \nabla C_s) = f_{s,C} \quad \text{on } \Gamma_C \tag{S33}$$

where C_s is the surfactant concentration [M L^{-3}], $C_{s,0}$ is initial concentration of the surfactant [M L^{-3}] in domain Ω, and $C_{s,D}$, $f_{s,N}$, and $f_{s,C}$ are the specified concentration [M L^{-3}] along Dirichlet boundary Γ_D, specified gradient concentration [M L^{-2} T^{-1}] normal to Neumann boundary Γ_N, and prescribed flux [M L^{-2} T^{-1}] normal to Cauchy boundary Γ_C of the surfactant, respectively. $K_{d,s}$ is the distribution coefficient [L^3 M^{-1}] between adsorbed and aqueous surfactant, and

$$V_{d,s} = \frac{V_1}{\theta_1 + \rho_b K_{d,s}} \tag{S34}$$

S.3 Numerical Formulations of Water-NAPL Phase Flow and Multispecies Transport

The total pressure equation (S18) can be solved using the standard Galerkin finite element method to obtain the total pressure at every node, as follows:

$$\sum_{e\in M_e}\int_{R^e} N_i^e\left[\nabla\cdot\kappa\cdot(\nabla P_t+\bar{\rho}g\nabla z)+\frac{Q_1}{\rho_1}+\frac{Q_2}{\rho_2}+\frac{E_n^w}{\rho_1}-\frac{E_n^w}{\rho_2}\right]dR=0,\quad i\in\{1,2,\cdots,N\} \tag{S35}$$

where e is the element number, M_e is the total number of elements, R^e is the domain occupied by element e, N_i^e is the Galerkin weighting function for node i of the eth element, i is the node number, and N is the total number of nodes. Eq. (S35) can be expressed in matrix form as follows:

$$[M]\{P_t\}=\{G\}+\{B\}+\{Q\}+\{E\} \tag{S36}$$

where

$$[M]_{i,j}=\sum_{e\in M_e}\int_{R^e}\nabla N_i^e\cdot\kappa\cdot\nabla N_j^e dR,\qquad i,j\in\{1,2,\cdots,N\} \tag{S37}$$

$$\{G\}_i=-\sum_{e\in M_e}\int_{R^e}\nabla N_i^e\cdot\kappa\cdot\bar{\rho}\mathrm{g}\nabla\mathrm{z}dR,\qquad i\in\{1,2,\cdots,N\} \tag{S38}$$

$$\{B\}_i=\sum_{e\in M_e}\int_{B^e}N_i^e\hat{n}\cdot\kappa\cdot(\nabla P_t+\bar{\rho}\mathrm{g}\nabla\mathrm{z})dB=-\sum_{e\in M_e}\int_{B^e}N_i^e\hat{n}\cdot V_t dB,$$

$$i\in\{1,2,\cdots,N\} \tag{S39}$$

$$\{Q\}_i=\sum_{e\in M_e}\int_{R^e}N_i^e\left[\frac{Q_1}{\rho_1}+\frac{Q_2}{\rho_2}\right]dR,\qquad i\in\{1,2,\cdots,N\} \tag{S40}$$

$$\{E\}_i=\sum_{e\in M_e}\int_{R^e}N_i^e\left[\frac{E_n^w}{\rho_1}-\frac{E_n^w}{\rho_2}\right]dR,\qquad i\in\{1,2,\cdots,N\} \tag{S41}$$

where B^e represents the boundary of element e, and $\hat{n}$ is the unit vector normal to the boundary of element e. The water saturation equation (S21) can be discretized using the finite element method, as follows:

$$[C_1]\left\{\frac{\partial S_1}{\partial t}\right\} + [ADW_1 + DD_1 + WW_1]\{S_1\} = \{f_1\} \tag{S42}$$

where

$$[C_1]_{i,j} = \int_\Omega N_i \phi N_j dR, \quad i,j \in \{1,2,\cdots,N\} \tag{S43}$$

$$[ADW_1]_{i,j} = \int_\Omega W_i \frac{d\kappa_1}{dS_1} V_t \cdot \nabla N_j dR - \int_\Omega W_i \frac{d\kappa_1 \kappa g(\rho_1 - \bar{\rho})}{dS_1} \nabla z \cdot \nabla N_j \, dR,$$

$$i,j \in \{1,2,\cdots,N\} \tag{S44}$$

$$[DD_1]_{i,j} = \int_\Omega \kappa_1 \kappa (1-\kappa_1) \frac{dP_{c12}}{dS_1} \nabla N_i \cdot \nabla N_j dR, \quad i,j \in \{1,2,\cdots,N\} \tag{S45}$$

$$[WW_1]_{i,j} = \int_\Omega N_i \left(\frac{\kappa_1 \nabla \cdot V_t - Q_1/\rho_1 - E_n^W/\rho_1}{S_1}\right) N_j dR, \quad i,j \in \{1,2,\cdots,N\} \tag{S46}$$

$$\{f_1\}_i = \int_B N_i \kappa_1 V_t \cdot \hat{n} dB - \int_B N_i V_1 \cdot \hat{n} dB - \int_B N_i \kappa_1 \kappa (\rho_1 - \bar{\rho}) g \nabla z \cdot \hat{n} dB,$$

$$i \in \{1,2,\cdots,N\} \tag{S47}$$

The time derivative term in Eq. (S42) can be numerically expressed as follows:

$$\frac{[C_1]}{\Delta t}\{S_1\}^{n+1} + w[ADW_1 + DD_1 + WW_1]\{S_1\}^{n+1} =$$

$$\frac{[C_1]}{\Delta t}\{S_1\}^{n} + (w-1)[ADW_1 + DD_1 + WW_1]\{S_1\}^{n} + \{f_1\} \tag{S48}$$

where the superscripts n and $n+1$ indicate the old and new time levels, respectively. Eq. (S48) can be solved in an explicit form at $w = 0$, in a Crank-Nicholson central difference form at $w = 0.5$, and in an implicit form at $w = 1$. Similarly, the equations governing dissolved

contaminant concentration (S28) and surfactant concentration (S33) can be solved using the Galerkin finite element method, as follows:

$$[M_k]\left\{\frac{D_{V_{d,k}}C_k}{Dt}\right\} + [D + K_k]\{C_k\} = \{B_k\} + \{R_k\}, \qquad k = o, s \tag{S49}$$

where k indicates the solute species $(k = o)$ or surfactant $(k = s)$.

$$[M_k]_{i,j} = \int_\Omega N_i(\theta_1 + \rho_b K_{d,k})N_j dR, \quad i,j \in \{1,2,\cdots,N\},\ k = o, s \tag{S50}$$

$$[D]_{i,j} = \int_\Omega \nabla N_i \cdot \theta_1 D \cdot \nabla N_j dR, \quad i,j \in \{1,2,\cdots,N\},\ k = o, s \tag{S51}$$

$$[K_k]_{i,j} = \int_\Omega N_i \left[\frac{Q_1}{\rho_1} + C_n^w\right] N_j dR, \quad i,j \in \{1,2,\cdots,N\},\ k = \mathrm{o} \tag{S52}$$

$$[K_k]_{i,j} = \int_\Omega N_i \frac{Q_1}{\rho_1} N_j dR, \quad i,j \in \{1,2,\cdots,N\}, \quad k = \mathrm{s} \tag{S53}$$

$$\{B_k\}_i = \int_\mathrm{B} N_i \hat{n} \cdot (\theta_1 D \cdot \nabla C_k) dB, \quad i \in \{1,2,\cdots,N\}, \quad k = \mathrm{o}, \mathrm{s} \tag{S54}$$

$$\{R_k\}_i = \int_\mathrm{B} N_i\left(C_n^w \overline{\rho_n^w}\right) dR, \quad i \in \{1,2,\cdots,N\}, \quad k = \mathrm{o} \tag{S55}$$

$$\{R_k\}_i = 0, \quad i \in \{1,2,\cdots,N\},\ k = \mathrm{s} \tag{S56}$$

with C_n^w and $\overline{\rho_n^w}$ in Eqs. (S52) and (S55) representing parameters related to the dissolution process described by Eq. (S30). The numerical procedure is in detail presented in Fig. S1. First of all, the numerical simulation conducts to the total pressure P_t using Eq. (S36) at step II, and solves the total velocity V_t using Eq. (S17) at step III. After then, using the total pressure and total velocity, the water saturation S_1 is solved in Eq. (S42) at step IV. Since the water saturation equation is a nonlinear, the iterative process is needed to get the conserved solution at step V. After getting the conserved solution of the water saturation, NAPL saturation is obtained using $S_2 = 1 - S_1$ and water phase Darcy velocity V_1 is calculated in Eq. (S19). The concentration of the dissolved contaminant C_o in Eq. (S28) and the concentration of surfactant C_s in Eq. (S33) care calculated by using Eq. (S49) at step VIII.

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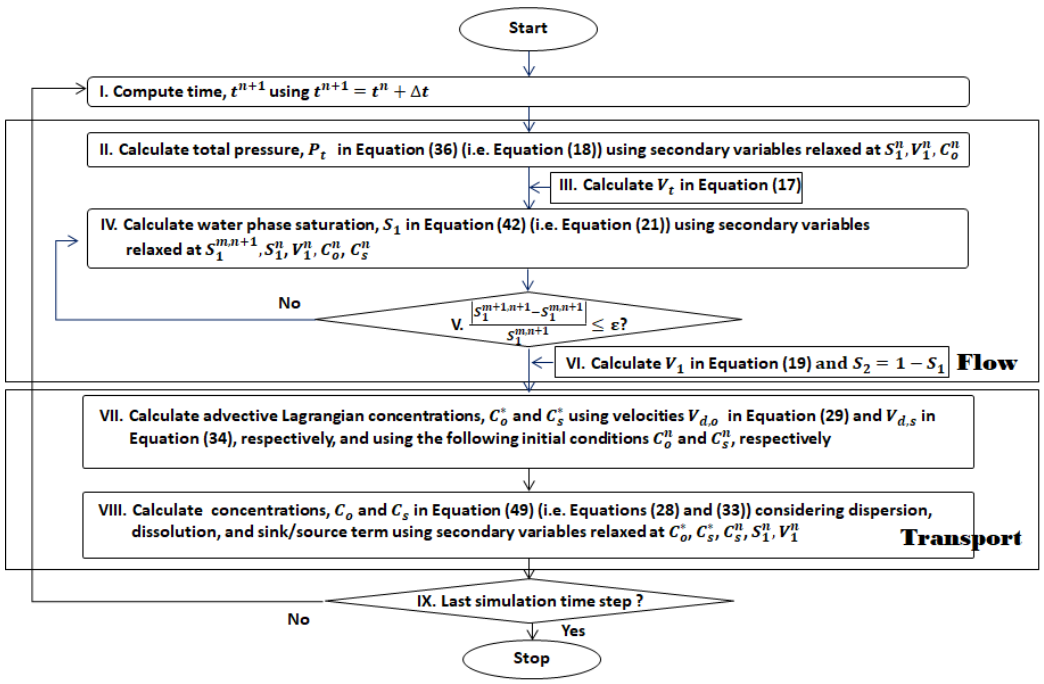

Figure S1. Flow chart for proposed numerical method. t^{n+1} and t^n are new and old time levels, respectively, Δt is time step, P_t is the total pressure, S_1 and S_2 are the water phase and NAPL phase saturations, respectively, V_t is the total velocity, V_1 is the Darcy velocity of water, C_o and C_s are the concentrations of dissolved contaminant and surfactant, respectively, $V_{d,o}$ and $V_{d,s}$ are the particle tracking velocities for dissolved contaminant and surfactant, respectively, superscripts $n+1$ and n indicate the new and old time levels, respectively, superscript m is the nonlinear iteration level, and superscript $*$ indicates the results of particle tracking.