Multiphase Flow in the Subsurface
- Flow of a Light Nonaqueous Phase Liquid (LNAPL)

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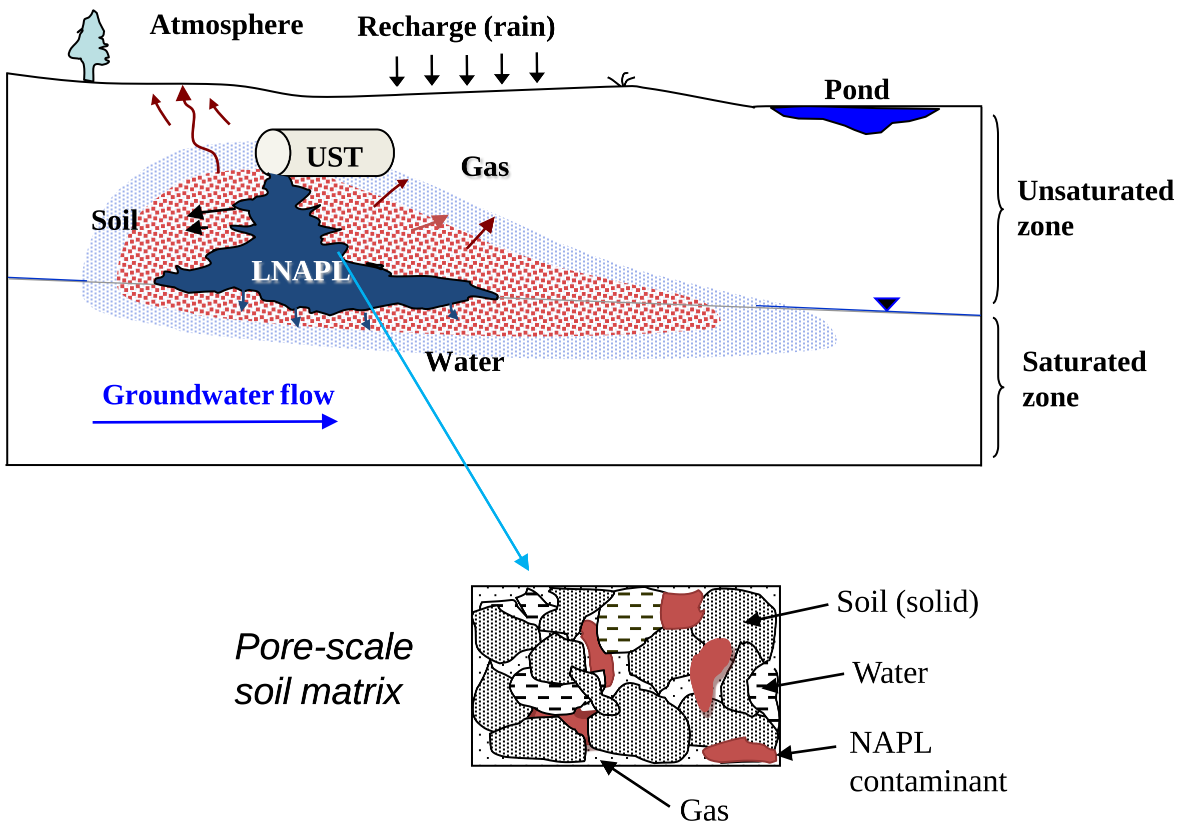
Introduction to Multiphase Flow

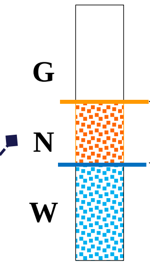
- **Multiphase flow means "the simultaneous movement of multiple phases, such as water, air, non-aqueous phase liquid (NAPL), through porous media."**



Capillary Pressure between Phases

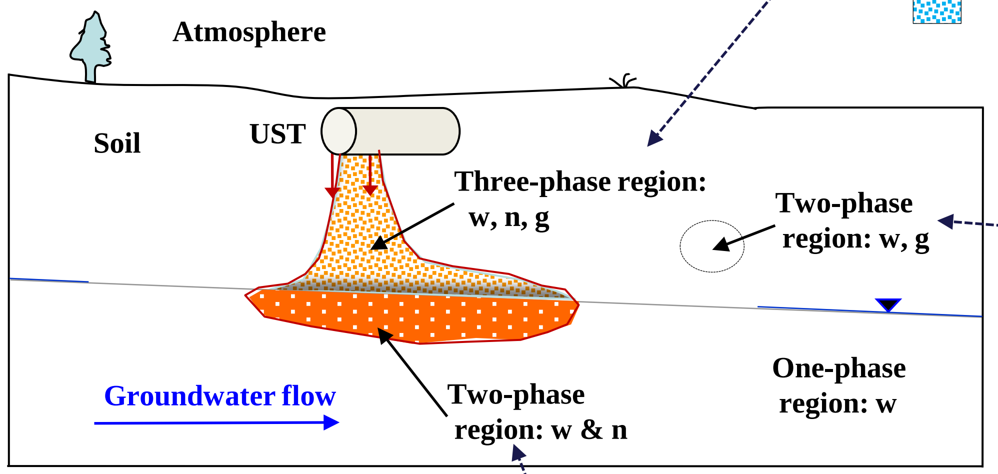
- **Numerical difficulty**
  - Transition between regions.

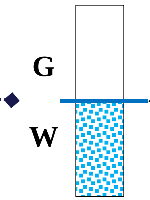
- Three flow equations
  for water, gas and NAPL phases



$$\psi_{cgn} = \psi_g - \psi_n$$

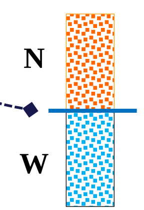
$$\psi_{cnw} = \psi_n - \psi_w$$





$$\psi_{cgw} = \psi_g - \psi_w$$

- Two flow equations
  for water and gas phases



$$\psi_{cnw} = \psi_n - \psi_w$$

- Two flow equations
  for water and NAPL phases

W, w = water
G, g = gas
N, n = NAPL

Mathematical Approach for Multiphase Flow

- **Governing equations: Groundwater, gas, and NAPL**

$$\frac{\partial(\phi s_f \rho_f)}{\partial t} + \nabla \cdot (\rho_f \boldsymbol{q}_f) = I_f + Q_f$$

$$\boldsymbol{q}_f = -\frac{\mathbf{k}\, k_{rf}}{\mu_f} \rho_{rw} g \cdot \left(\nabla \psi_f - \left(\frac{\rho_f}{\rho_{rw}} \right) e_z \right)$$

$$\psi_f = P_f / \rho_{RW}\, g$$

ρ_{RW} = the reference water density

$f = w\ (water), g\ (gas), and\ n\ (NAPL).$

Capillary pressure

$$\psi_{cgw} = \psi_g - \psi_w,$$

$$\psi_{cnw} = \psi_n - \psi_w,$$

$$\psi_{cgn} = \psi_g - \psi_n$$

- C. Pressure (ψ_c)-Saturation (s_f)-R. Permeability (k_{rf}) Relations

→ Nonlinear and very complicated to solve the equations.

C. Pressure-Saturation-R. Permeability (1)

- **cP-S-kr relationships**
  - Brooks-Corey law (1964)

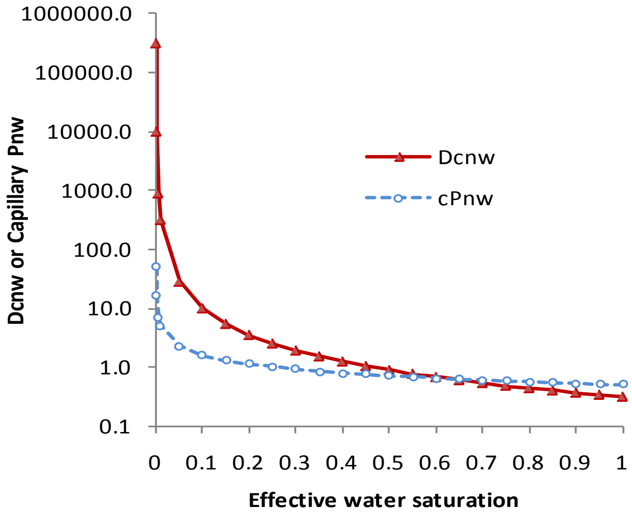
$$s_{we} = \frac{1 - s_n - s_{wr}}{1 - s_{nr} - s_{wr}} = \left(\frac{\psi_d}{\psi_{cnw}}\right)^{\lambda}, \quad \psi_d > \psi_{cnw}$$

$$k_{rw} = s_{we}^{\frac{2+3\lambda}{\lambda}}$$

$$k_{ro} = (s_{te} - s_{we})^2 \left(s_{te}^{\frac{2-\lambda}{\lambda}} - s_{w}^{\frac{2-\lambda}{\lambda}}\right)$$

- ψ_d is the air-entry pressure head of the air-water system.
- λ is the pore size distribution.

Brooks-Corey law	
Size index	2
Entry Pr. (Pd)	0.5099
Residual Sw	0.1
Residual Sn	0.1



$$\nabla\psi_{cnw} = \frac{d\psi_{cnw}}{ds_n}\nabla s_n = D_{cnw}\nabla s_n$$

C. Pressure-Saturation-R. Permeability (2)

- **cP-S-kr relationships**
  - van Genuchten law (1980)

$$s_{we} = [1 + (\alpha\beta_{nw}\psi_{nw})^n]^{-m} \qquad \psi_{nw} > 0$$

$$s_{we} = 1 \qquad \psi_{nw} \leq 0$$

$$s_{te} = \left[1 + \left(\alpha\beta_{gn}\psi_{gn}\right)^n\right]^{-m} \qquad \psi_{gn} > 0$$

$$s_t = s_w + s_n$$

s_t=Total liquid saturation

$$s_{te} = 1 \qquad \psi_{gn} \leq 0$$

$$m = 1 - 1/n$$

- α (L^{-1}) and n (dimensionless) are empirical parameters describing soil media
- β_{gn} and β_{nw} are the scaling factors

Three-Phase Systems in the Shallow Aquifer

- **Mobile phases: Water and NAPL**
- **Constant pressure head: Gas**
  - The soil gas in the unsaturated zone is connected to the atmosphere.
  - The gas movement has negligible impacts on the movement of water and NAPL.

$$\frac{\partial\left(\phi\rho_w(1-s_n-s_g)\right)}{\partial t}=\nabla\left(\frac{k\rho_w k_{rw}}{\mu_w}\rho_{RW}g\left(\nabla\psi_w+\frac{\rho_w}{\rho_{RW}}\mathrm{e_z}\right)\right)+Q_w$$

$$\frac{\partial(\phi\rho_n s_n)}{\partial t}=\nabla\left(\frac{k\rho_n k_{rn}}{\mu_n}\rho_{RW}g\left(\nabla(\psi_w+\psi_{cnw})+\frac{\rho_n}{\rho_{RW}}\mathrm{e_z}\right)\right)+I_n+Q_w$$

$$s_w+s_g+s_n=1.$$

$$\psi_n=\psi_w+\psi_{cnw}$$

- Primary variables: ψ_w *and* s_n
- Secondary variables: ψ_n, s_w, s_g

Water-NAPL Two-Phase System

- **Mobile phases: Water and NAPL**
- **No gas phase**
- **Example: CO_2 injection in deep geological systems**

$$s_w + s_n = 1.$$

$$\frac{\partial(\phi\rho_w s_n)}{\partial t} = \nabla\left(\frac{k\rho_w k_{rw}}{\mu_w}\rho_{RW}\, g\left(\nabla\psi_w + \frac{\rho_w}{\rho_{RW}}\mathrm{e_z}\right)\right) + Q_w$$

$$\frac{\partial(\phi\rho_n s_n)}{\partial t} = \nabla\left(\frac{k\rho_n k_{rn}}{\mu_n}\rho_{RW}\, g\left(\nabla(\psi_w + \psi_{cnw}) + \frac{\rho_n}{\rho_{RW}}\mathrm{e_z}\right)\right) + I_n + Q_w$$

$$\nabla\psi_{cnw} = \frac{\mathrm{d}\psi_{cnw}}{ds_n}\nabla s_n = D_{cnw}\nabla s_n$$

Numerical Techniques

- **Global implicit scheme**
  - Solves multiphase flow equations simultaneously.
  - Generates a non-symmetric global matrix.

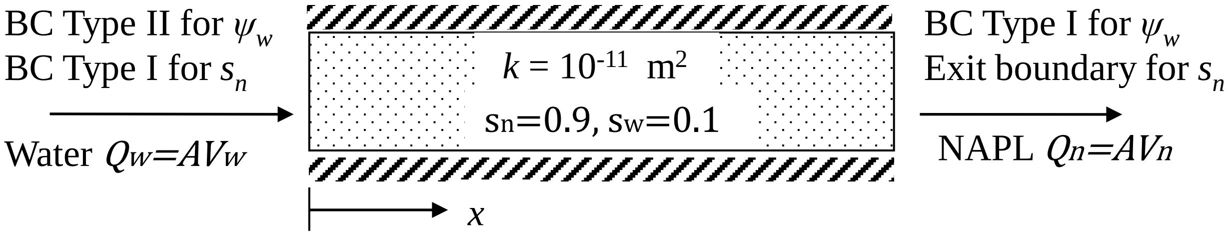
$$\begin{bmatrix} \psi_w & \cdots & s_n \\ \vdots & \ddots & \vdots \\ \psi_w & \cdots & s_n \end{bmatrix} \begin{bmatrix} \psi \\ s \end{bmatrix} = \begin{bmatrix} \psi_0 \\ s_0 \end{bmatrix}$$

- **Upstream weighting scheme (Upwind scheme)**
  - Relative permeability is evaluated based on a flow direction.

- **Sparse matrix solvers**
  - Iterative matrix solver: IML++
    - <u>Failed</u> when the global implicit scheme is used.
  - Direct matrix solver: Pardiso solver
    - <u>Works good</u> with the global implicit scheme.

Buckley-Leverett Problem

- **Buckley-Leverett problem represents a linear water-flood of a petroleum reservoir in a one-dimensional, horizontal domain.**
  - The pore spaces of the domain is initially filled with a NAPL, i.e., liquid oil.



Properties	Values
Boundary condition	
Water influx at x=0 m Water pressure at x=300 m NAPL saturation at x=0 m (Sw at x=0 m)	v_w = 0.01 m/s, BC Type II p_w = 2.9 m H_2O, BC Type I s_n = 0.1, BC Type I (s_w = 0.9, BC Type I)
Initial condition	
Water saturation NAPL saturation	s_w = 0.1 s_n = 0.9

Darcy velocity = 0.01 m/s

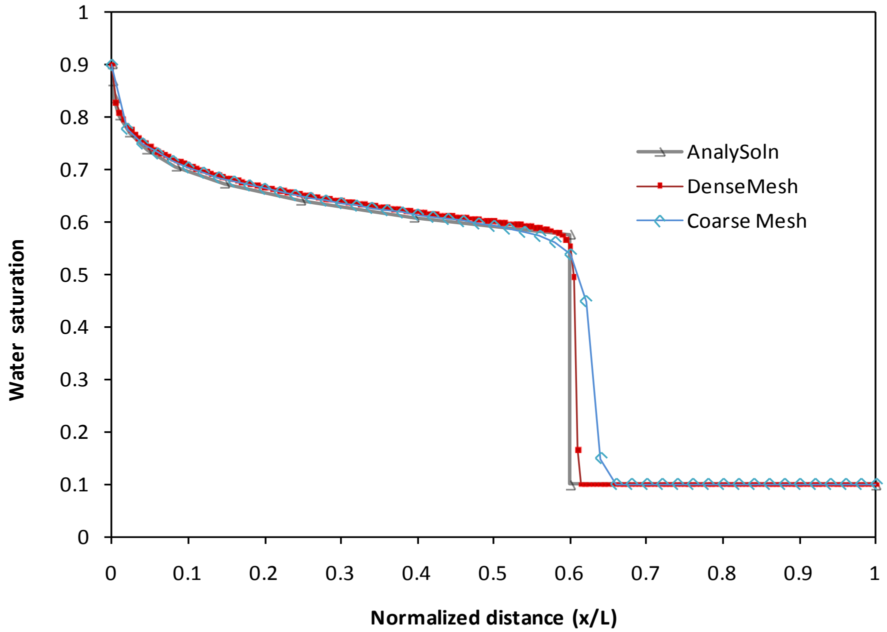
Buckley-Leverett Problem (contd.)

- **Parameters**

Properties	Values	Comment
Soil		
Intrinsic permeability **Porosity**	10^{-11} m^2 0.3	
Pore size distribution index	2.0	**Brook-Corey law**
Water residual saturation **NAPL residual saturation**	$s_{wr} = 0.1$ $s_{nr} = 0.1$	
Fluid		
Water density **NAPL (oil) density** **Water viscosity** **NAPL(oil) viscosity**	$\rho_w = 1000$ kg/m^3 $\rho_n = 900$ kg/m^3 $\mu_w = 0.001$ Pa s^{-1} (kg/ms) $\mu_n = 0.005$ Pa s^{-1} (kg/ms)	

Buckley-Leverett Problem (Results)

- **Comparison of water saturation profiles**
  - Semi-analytical solution vs. TechFlowMP results
  - Coarse and dense meshes



Location of the water front

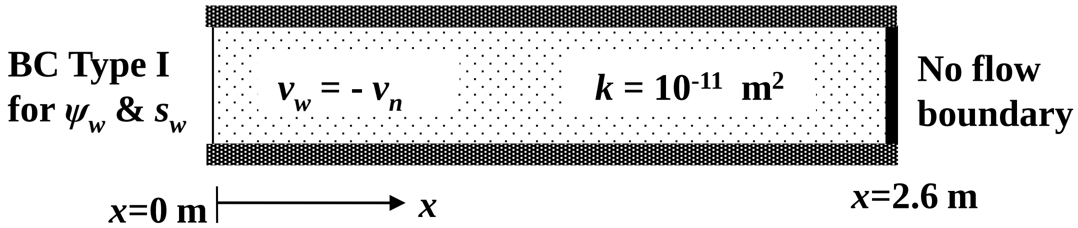
$$x_f = \frac{Q_w t}{A\phi}\left(\frac{df_w}{ds_w}\right)$$

$$f_w = \frac{1}{1 + \frac{k_{rn}}{k_{rw}}\frac{\mu_w}{\mu_n}}$$

Domain size, Length	L = 5 m	
Space step size, SD-A	Δx = 0.1 m	Coarse grid
Space step size, SD-B	Δx = 0.025 m	Dense grid

McWhorter-Sunada Problem

- **The flows of water and NAPL are initiated by the capillary pressure between two phases in a domain.**



Properties	Values
Boundary condition	
Water pressure (x=0 m,t) Water pressure(x=5 m,t) NAPL saturation (x=0 m,t) (Water saturation (x=0 m,t)) NAPL saturation (x=5 m,t)	ψ_w = 19.885 m H_2O, BC Type I No flux/flow boundary **s_n = 0., BC Type I** **(s_w = 1., BC Type I)** No flow boundary
Initial condition	
Water saturation (x, t=0) NAPL saturation (x, t=0) Water pressure (x, t)	s_w = 0.01 **s_n = 0.99** ψ_w = 19.885 m H_2O (P_w =195000 Pa)

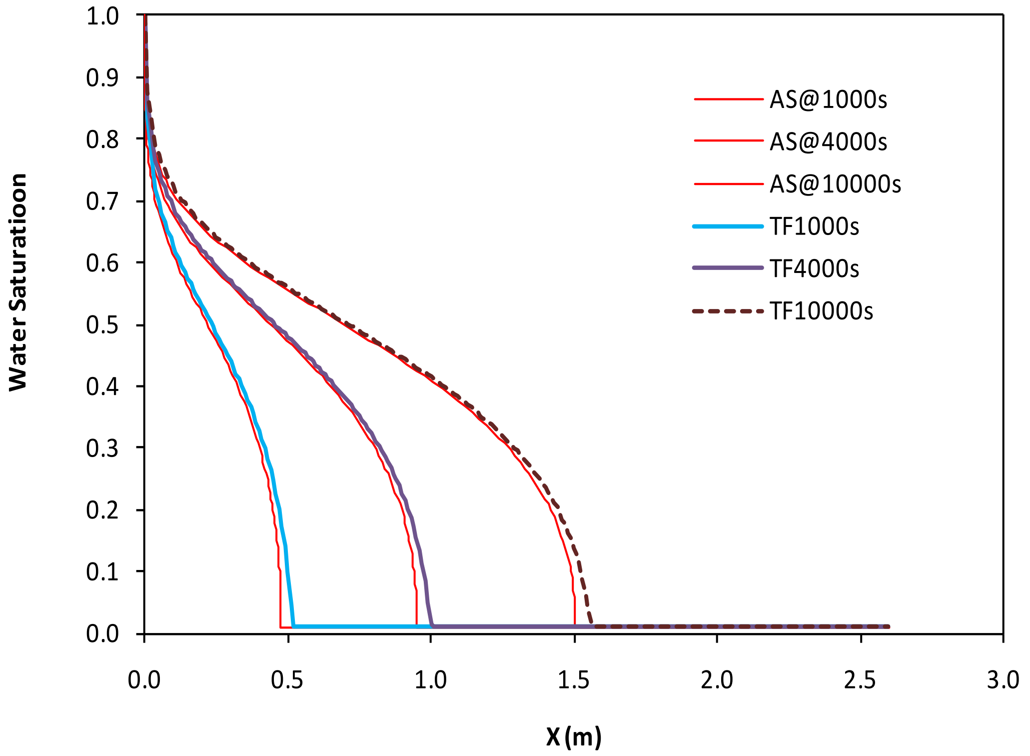
McWhorter-Sunada Problem (contd.)

Properties	Values	Remark
Soil		
Soil intrinsic permeability Porosity	10^{-11} m^2 0.3	
Pore size distribution index Entry pressure, P_d	2 5000 Pa (ψ_w=0.5099 mH_2O)*	Brook-Corey law 1 mH_2O=9806.65Pa
Water residual saturation NAPL residual saturation	s_{wr} = 0. s_{nr} = 0.	
Fluid		
Water density NAPL (oil) density Water viscosity NAPL(oil) viscosity	ρ_w = 1000 kg/m^3 ρ_n = 1000 kg/m^3 0.001 Pa s^{-1} (= kg/m s) 0.001 Pa s^{-1} (= kg/m s)	

Domain and space discretization		
Domain size, Length Space step size	L = 2.6 m Δx = 0.01 m	260 elements
Water viscosity NAPL(oil) viscosity	0.001 Pa s^{-1} (= kg/m s) 0.001 Pa s^{-1} (= kg/m s)	
Time discretization		
Simulation time Time step size	T = 10,000 s Δt = 1 – 100 s (Max. 15 iterations)	

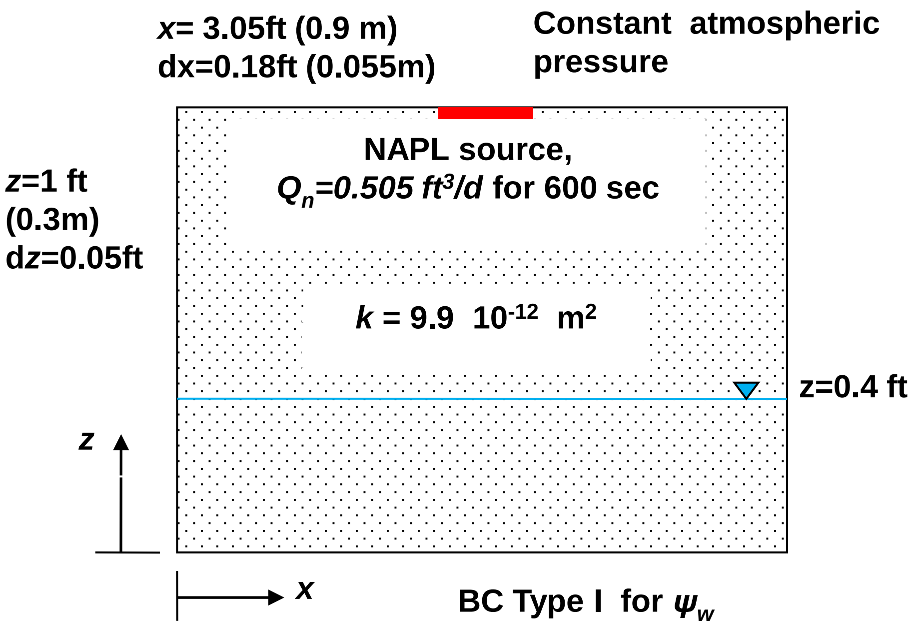
McWhorter-Sunada Problem (contd.)

- **The change in water saturation over time**
  - Semi-analytical solutions vs. TechFlowMP results
    - The global implicit scheme, upwind scheme, and Pardiso solver are implemented.



NAPL Release at the Ground Surface

- **NAPL's release into the variably saturated zone.**
  - Three phases: water, gas, and NAPL.
  - A NAPL is released for 600 sec.



Initial condition

- Water: Variable s_w
- NAPL: s_n = 0 at t=0 sec
- Water head: ψ_w = 0.4 ft H_2O

Domain and space discretization

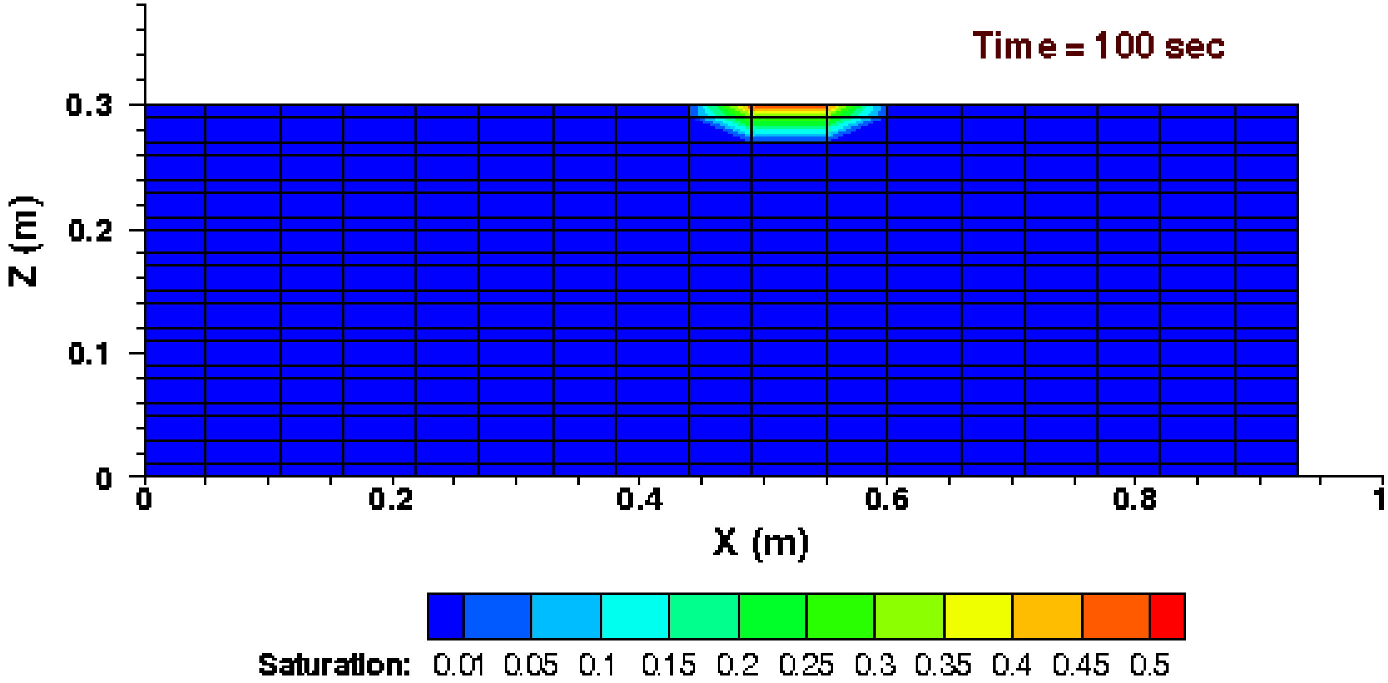
- X = 93 cm: Δx = 0.18 ft (5.47 cm)
- Z = 30.48 cm: Δz = 0.05 ft (1.524 cm)

Time discretization

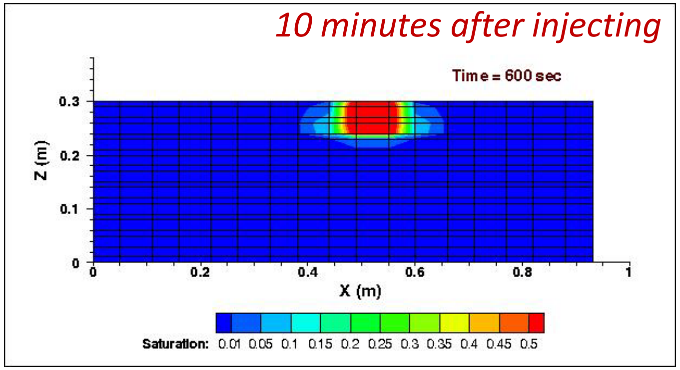
- Simulation time: T = 10 hrs (Δt = 0.01 – 8 sec)

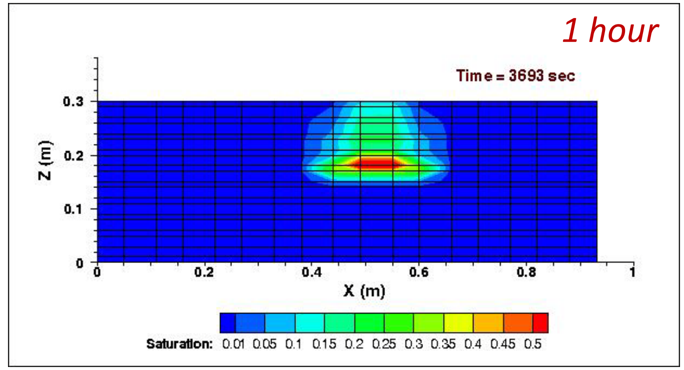
NAPL Release at the Ground Surface (contd.)

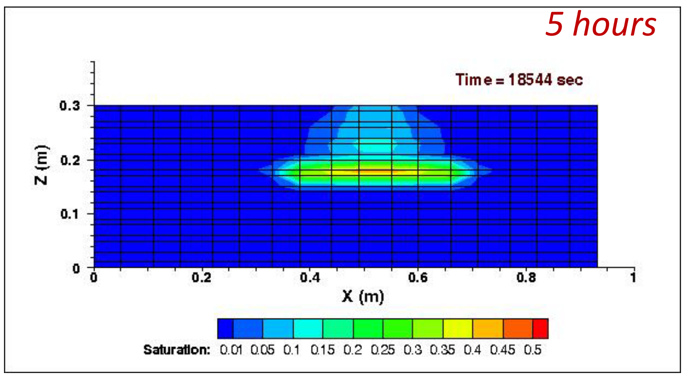
NAPL's spreading with time.

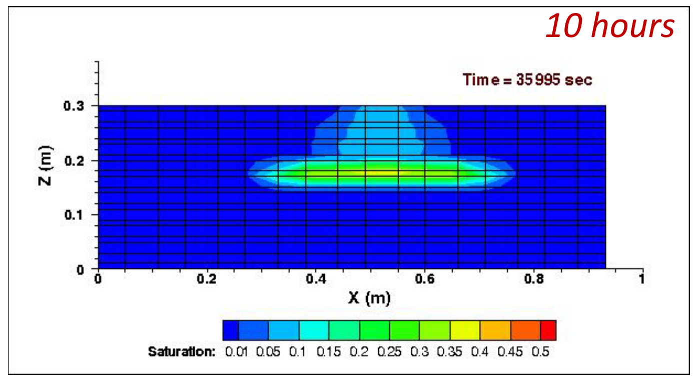


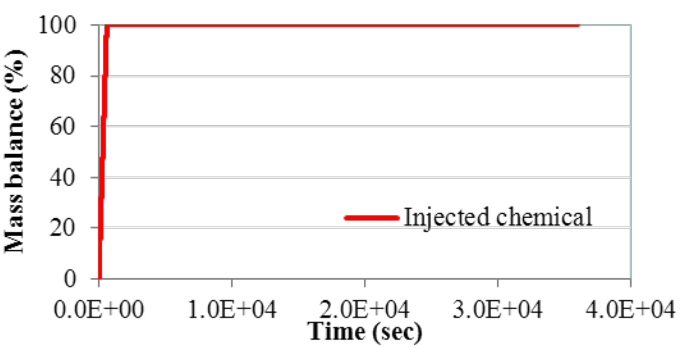
NAPL Release at the Ground Surface (contd.)









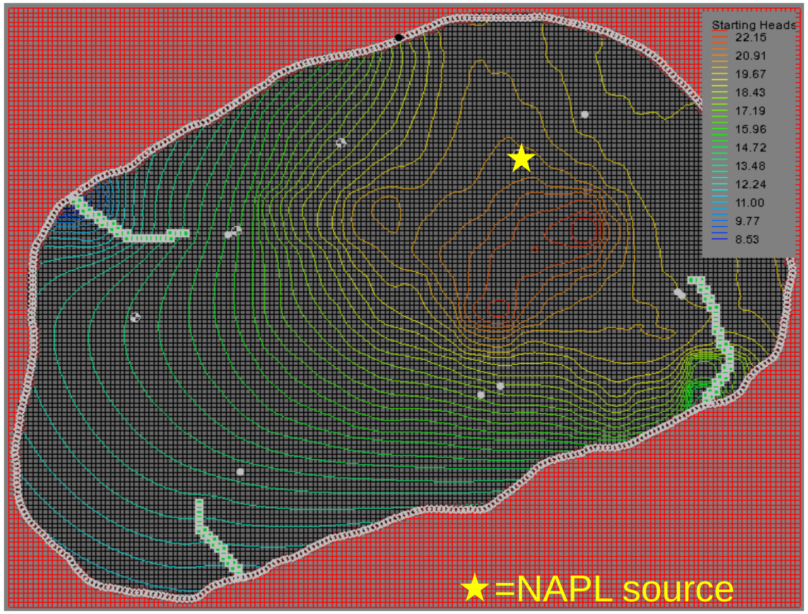


- The spreading of the released NAPL is expected to be completely within a relatively short period of time.
- The immobilized NAPL becomes a long-lasting contaminant source.

GW Pollution in the Hadnot Point Industrial Area

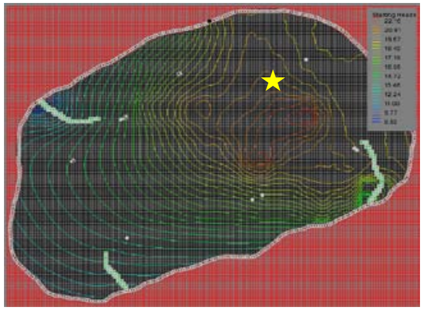
- **HPIA, Camp Lejeune, NC.**

Parameters	Description
Domain size	Length in x-axis: 8200.0 ft (**Δx=50 ft**) Length in y-axis: 6450.0 ft (**Δy=50 ft**) Depth: from 7.47161 ft to -240.744 ft Origin: (X= 2497210.0 ft, Y=335640.0, Z=0.0)
Grid	Total number of rows (Cells i): 129 Total number of columns (Cells j): 164 Total number of layers (Cells k): 7 Number of nodes: 171,600 Number of cells: 148,092 (No. active cells: 99,352; inactive cells: 48,740)
Elevation	Number of elevation data: 148,092 Minimum value: -240.744 ft Maximum value: 7.47161 Mean: -98.2263, Median: -77.2142 Reference time: 12/30/1988
Stress period	240 (from 1/1/11942 to 1/1/1962 = 7305 days)



Application to GW Pollution in HPIA (contd.)

- **NAPL at HPIA, Camp Lejeune, NC.**



  - Contaminant sources are immobilized NAPLs.
  - The dissolution of the immobile NAPL and its transport in the whole domain will be investigated.

  - The migration of the NAPL can be analyzed within a very limited region around the source area.

Thank you.

Questions?

References

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