Comparing different numerical methods for 2D-coupled water and solute transport in porous media

Presented by
Shirishkumar Baviskar* and Timo Heimovaara

Department of Geoscience and Engineering,
CiTG, Delft, Netherlands.

*Email: s.m.baviskar@tudelft.nl

International Conference on Numerical and Mathematical Modeling of Flow and Transport in Porous Media
29 September -3 October 2014, Dubrovnik, Croatia.

Context of research

- Comparison of three 2D coupled models for water and solute transport in porous media (1) COMSOL (2) FAESOR and (3) FDM-MIC model.

- Description of 2D FEM for coupled water and solute transport in porous media using FAESOR (Krysl, 2000).

- Description of 2D FDM for water flow coupled with Marker in Cell (MIC) by Gerya (2010), for solute transport in porous media.

- Model verification problems and a application problem → Comparison based on global mass balances, iteration methods, time stepping methods.

Equations Involved - Water Transport

- **Richard's Equation**

$$\frac{C_m(\Psi^{(a+1,b)})+S_w S_s}{\Delta t}\delta^{b+1}+\nabla\cdot\boldsymbol{q}=0 \ldots\ldots Eq(1.a)\ldots Head\ Based\ldots COMSOL$$

$$\frac{\theta^{a+1}-\theta^{a}}{\Delta t}+\frac{C_m(\Psi^{(a+1,b)})+S_w S_s}{\Delta t}\delta^{b+1}+\nabla\cdot\boldsymbol{q}=0 \ldots\ldots Eq(1.b).\ Mixed\ Based\ .\ FAESOR/FDM$$

$$\delta^{b+1}=(\Psi^{a+1,b+1}-\Psi^{a+1,b})\ldots\ldots Eq(2)$$

$$\boldsymbol{q}=-\boldsymbol{K}(\Psi)\nabla(\Psi+z)\ldots\ldots Eq(3)$$

- van Genuchten functions

$$\boldsymbol{K}(\Psi)=k_r\boldsymbol{K}_{\boldsymbol{sat}}\ldots\ldots Eq(4)$$

$$S_{eff}=[1+\alpha|\Psi|^n]^{-m}\ldots\ldots Eq(5)$$

$$\theta(\Psi)=\theta_r+S_{eff}(\theta_s-\theta_r)\ldots\ldots Eq(6)$$

$$k_r=S_{eff}^{1/2}[1-(1-S_{eff}^{1/m})^m]^2\ldots\ldots Eq(7)$$

$$S_w=S_{eff}+\frac{\theta_r}{\theta_s}\ldots\ldots Eq(8)$$

$$C_m=\frac{\alpha m}{1-m}(\theta_s-\theta_r)S_{eff}^{1/m}(1-S_{eff}^{(1/m)})^m\ldots\ldots Eq(9)$$

Equations Involved - Solute Transport

- **Advection Dispersion Equation**

$$\frac{\partial \theta c}{\partial t} + \nabla \cdot \boldsymbol{u} = 0 \ldots\ldots Eq(10)$$

$$\boldsymbol{u} = -\boldsymbol{D} \nabla c + \boldsymbol{q} c \ldots\ldots Eq(11)$$

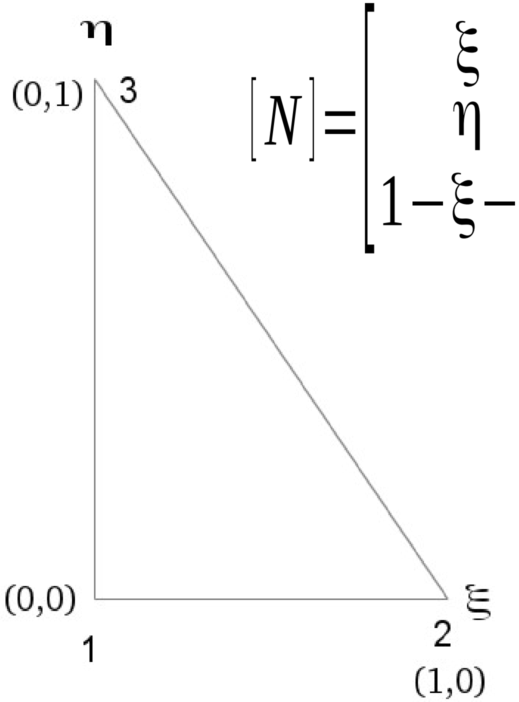
$$D_{\alpha\beta} = \alpha_T |v| \delta_{\alpha\beta} + (\alpha_L - \alpha_T) \frac{v_\alpha v_\beta}{|v|} + D_m \delta_{\alpha\beta} \ldots\ldots Eq(12)$$

$$v = \frac{\boldsymbol{q}}{\theta} \ldots\ldots Eq(13)$$

Initial and Boundary Conditions

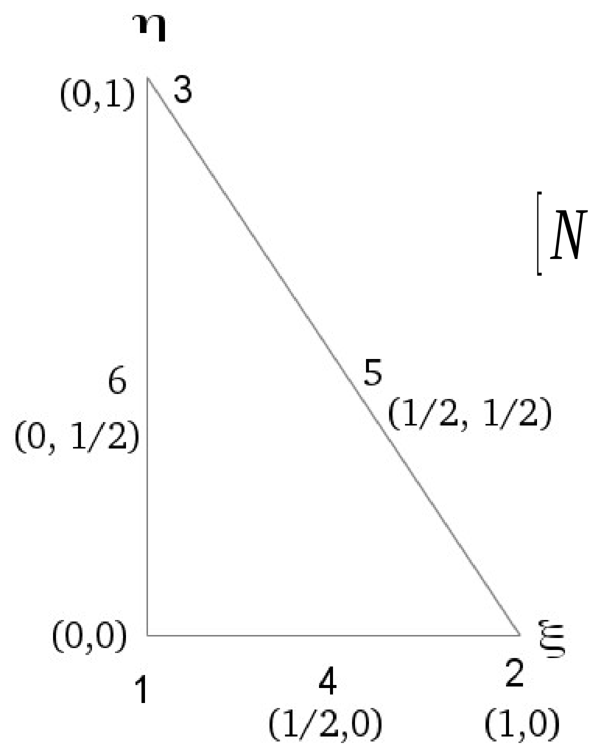
Water and Solute Transport Model	Initial Condition	Boundary Conditions	
		top horizontal edge	bottom horizontal edge
Richards Equation	$\Psi(x,z,0)=z-z_{ref}$	Neumann $\boldsymbol{q}(x,0,t)=q_{top}$	Robbins $\boldsymbol{q}(x,-1,t)=-K_{surf}(\Psi_{amb}-\Psi)$
Advection Dispersion Equation	$c(x,z,0)=c_{ini}$	Dirichlet $c(x,0,t)=c_{top}$	Robbins $c(x,-1,t)=\boldsymbol{q}\,c$

FEM - COMSOL and FAESOR



$$[N]=\begin{bmatrix} \xi \\ \eta \\ 1-\xi-\eta \end{bmatrix}$$

COMSOL



$$[N]=\begin{bmatrix} (\eta+\xi-1)(2\eta+2\xi-1) \\ \xi(2\xi-1) \\ \eta(2\eta-1) \\ -4\xi(\eta+\xi-1) \\ 4\eta\xi \\ -4\eta(\eta+\xi-1) \end{bmatrix}$$

FAESOR

FAESOR - Richards Equation

- Head based form of RE $$C\frac{\partial\psi}{\partial t}-\nabla\cdot\boldsymbol{K}[\nabla(\psi+z)]=0$$
- Applying weighted residual, Green theorem, boundary conditions

$$\int_v \eta C\frac{\partial\psi}{\partial t}dV+\int_v(\nabla\eta)\cdot\boldsymbol{K}[\nabla(\psi+z)]dV+\int_{S_2}\eta\bar{q}_n dS+\int_{S_3}\eta K_{surf}(\psi-\psi_{amb})dS=0$$

- Solution technique for RE with Picards iteration's scheme (Celia et al, 1990)

$$\boldsymbol{T}_v^b+\boldsymbol{C}_m\frac{\delta_v^{b+1}}{\Delta t}+(\boldsymbol{K}_m+\boldsymbol{H}_m)\boldsymbol{\Psi}_v-\boldsymbol{L}\boldsymbol{w}_v=0$$

- $$\boldsymbol{\Psi}_v^{a+1,b+1}=\boldsymbol{\delta}_v^{b+1}+\boldsymbol{\Psi}_v^{a+1,b}$$

FAESOR - Richards Equation

- Temporal discretization $dt = min(\Delta titer \| \Delta t_{max})$

- For convergence $$\boldsymbol{\Psi}_{v_{prime}}^{a+1,b+1} = \frac{\boldsymbol{\Psi}_{v}^{a+1,b+1} - \boldsymbol{\Psi}_{v}^{a+1,b}}{dt}$$

- Truncation error $$truncerr = \frac{\left(\boldsymbol{\Psi}_{v_{prime}}^{a+1,b+1} - \boldsymbol{\Psi}_{v_{prime}}^{a+1,b}\right) dt}{2}$$

- We have considered $\delta_r = 1 \times 10^{-3}$ and $\delta_a = 1 \times 10^{-3}$

  for $convcrit = \delta_r |\boldsymbol{\Psi}_{v}^{a+1,b+1}| + \delta_a$ and $testval = |\boldsymbol{\delta}_{v}^{b+1}| - convcrit$

- Loop for convergence with iterations and automatic time stepping

$$if\ niter \geqslant maxiter(i.e.25), \rightarrow \Delta t_{iter} = \Delta t \cdot \mu_1 (i.e\ 0.25) \rightarrow not\ converged \rightarrow niter = niter + 1$$

$$if\ niter \leq miniter(i.e.15), \rightarrow \Delta t_{iter} = \Delta t \cdot mu_2 (i.e.1.1)$$

$$max(testval) < 0, \rightarrow t = t + \Delta t \rightarrow converged$$

FAESOR - Advection Dispersion Equation

- Head based form of ADE $\theta \frac{\partial c}{\partial t} - \nabla \cdot \boldsymbol{D}[\nabla(c) - \boldsymbol{q}\, c] = 0$
- Applying weighted residual, Green theorem, boundary conditions.

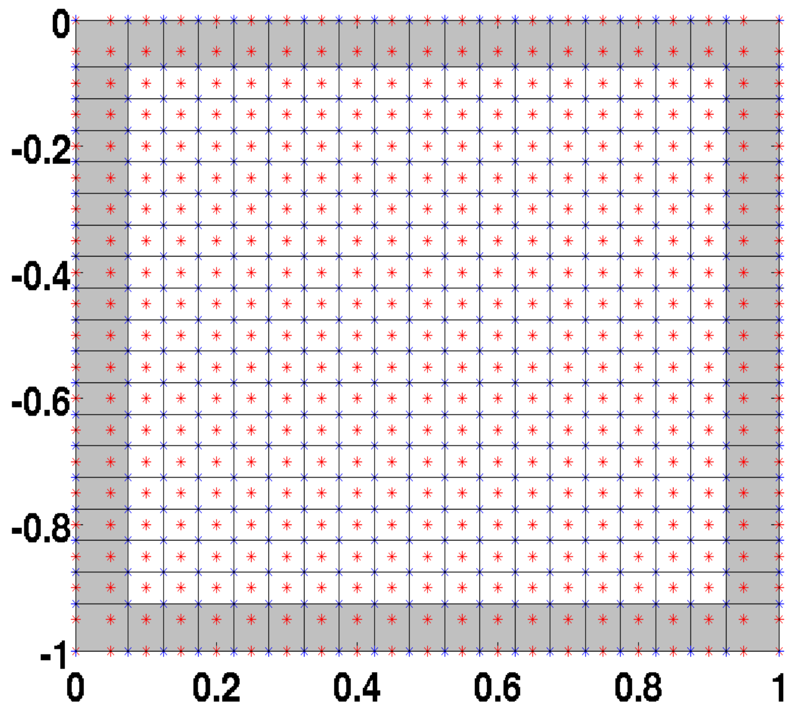
$$\int_v \eta \theta \frac{\partial c}{\partial t} dV + \int_v (\nabla \eta) \cdot \boldsymbol{D}[\nabla(c) - \boldsymbol{q}\, c] dV + \int_{S_3} \eta n \boldsymbol{q}\, c\, dS = 0$$

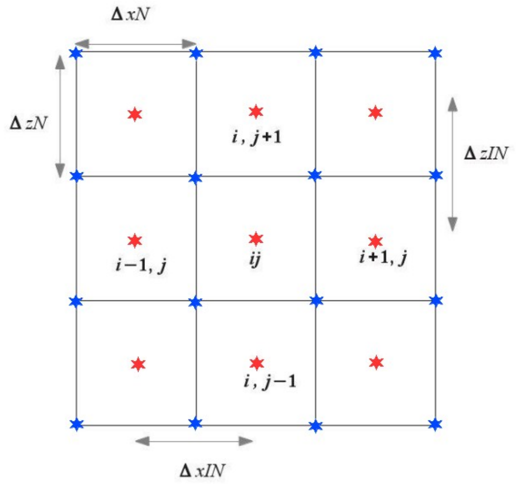
- Solution technique for ADE with Euler backward (Implicit) method.

$$\left[\frac{1}{\Delta t}\boldsymbol{T}_v + \boldsymbol{DA}_m\right]\boldsymbol{Con}_{v_{a+1}} = \left[\frac{1}{\Delta t}\boldsymbol{T}_v\right]\boldsymbol{Con}_{m_a} + \boldsymbol{Ls}_{v_{a+1}} = 0$$

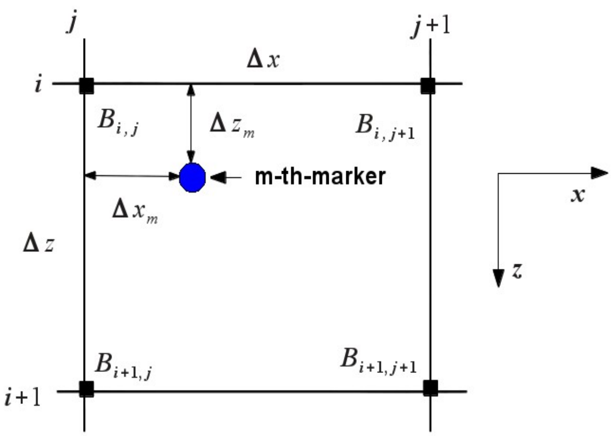
FDM - Richards Equation

$$\frac{\theta_{ij}^{a+1}-\theta_{ij}^{a}}{\Delta t}+\frac{C_m\left(\Psi_{ij}^{(a+1,b)}\right)+S_w S_s}{\Delta t}\delta_{ij}^{b+1}=-\frac{qz_{i+1/2,j}-qz_{i-1/2,j}}{\Delta z_{i-1/2,j}}-\frac{qx_{i,j+1/2}-qx_{i,j-1/2}}{\Delta x_{i,j-1/2}}$$





Marker-in-Cell



- Eulerian and Lagrangian time derivative of concentration related together by advection term

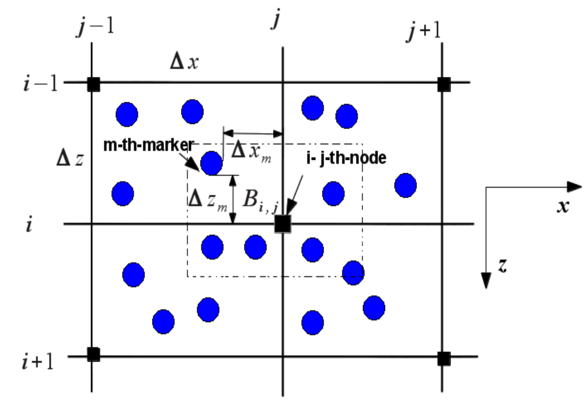
$$\frac{Dc}{Dt} = \frac{\partial c}{\partial t} + \boldsymbol{q} \cdot \nabla c$$

- Lagrangian term solved on Euler nodes

$$\frac{Dc}{Dt} = -\nabla \cdot \boldsymbol{D} \nabla c$$

- Advection term solved on Lagrangian markers

$$x_{mrk}^{tx_{mrk} + \Delta tx_{mrk}} = x_{mrk}^{tx_{mrk}} + vx_{mrk} \Delta tx_{mrk}$$
$$z_{mrk}^{tz_{mrk} + \Delta tz_{mrk}} = z_{mrk}^{tx_{mrk}} + zx_{mrk} \Delta tz_{mrk}$$



Marker-in-Cell

$$\nabla\cdot\boldsymbol{D}\nabla c=\frac{-\left(-Dz_{i+1/2,j}\dfrac{c_{i+1,j}-c_{i,j}}{\Delta z_{i,j}}\right)-\left(-Dz_{i-1/2,j}\dfrac{c_{i,j}-c_{i-1,j}}{\Delta z_{i-1,j}}\right)}{\Delta z_{i-i/2,j}}+\frac{-\left(-Dx_{i,j+1/2}\dfrac{c_{i,j+1}-c_{i,j}}{\Delta x_{i,j}}\right)-\left(-Dx_{i,j-1/2}\dfrac{c_{i,j}-c_{i,j-1}}{\Delta x_{i,j-1}}\right)}{\Delta x_{i,j-i/2}}$$

- Dispersion term on Euler Nodes
- Changes in effective concentration field on Euler nodes $\Delta c_{i,j}=c_{i,j}^{t+\Delta t}-c_{i,j}^{t}$
- New marker concentration $c_m^{t+\Delta t}=c_m^t+\Delta c_m$
- Incremental update creates small scale variation on sub-grid, $\Delta c_{i,j}=\Delta c_{i,j}^{subgrid}+\Delta c_{i,j}^{remaining}$ which can be damped by sub-grid diffusion operation
- Subgrid diffusion applied on markers over characteristic local concentration diffusion time scale

$$\Delta c_m^{subgrid}=c_{m(nodes)}^t-c_m^t\left[1-\exp\left(-d\frac{\Delta t}{\Delta t_{diff}}\right)\right]$$

$$where\ \Delta t_{diff}=\frac{1}{2D_{mx}/\Delta x^2+2D_{mz}/\Delta z^2}$$

- $\Delta c_{i,j}^{remaining}=\Delta c_{i,j}-\Delta c_{i,j}^{subgrid}$
- $c_{m(corrected)}^{t+\Delta t}=c_m^t+\Delta c_m^{subgrid}+\Delta c_m^{remaining}$

Mass Balance Check

- **Water transport** $MB(t) = Total\ additional\ mass\ inside\ domain - Total\ net\ flow\ out\ of\ domain$

  FEM - COMSOL and FAESOR

  $$MB_w(t) = \sum (\theta - \theta_0)\, dv - \left[\sum (-qx_{in}\, dz_{¿} - qx_{out}\, dz_{out}) + \sum (-qz_{in}\, dx_{in} - qz_{out}\, dx_{out}) \right] dt$$

  - FDM

  $$MB_w(t) = \sum (\theta - \theta_0)\, dv - \left[\sum (-qx_{in}\, \Delta zIN - qx_{out}\, \Delta zIN) + \sum (-qz_{in}\, \Delta xIN - qz_{out}\, \Delta xIN) \right] dt$$

- **Solute transport** $MB(t) = Total\ additional\ concentration\ mass\ inside\ domain - Total\ net\ flux\ out\ of\ domain$
  - FEM - COMSOL and FAESOR

  $$MB_s(t) = \sum (\theta c - \theta_0 c)\, dv - \left[\sum (-ux_{in}\, dz_{in} - ux_{out}\, dz_{out}) + \sum (-uz_{in}\, dx_{in} - uz_{out}\, dx_{out}) \right] dt$$

  - MIC
    - Dispersion

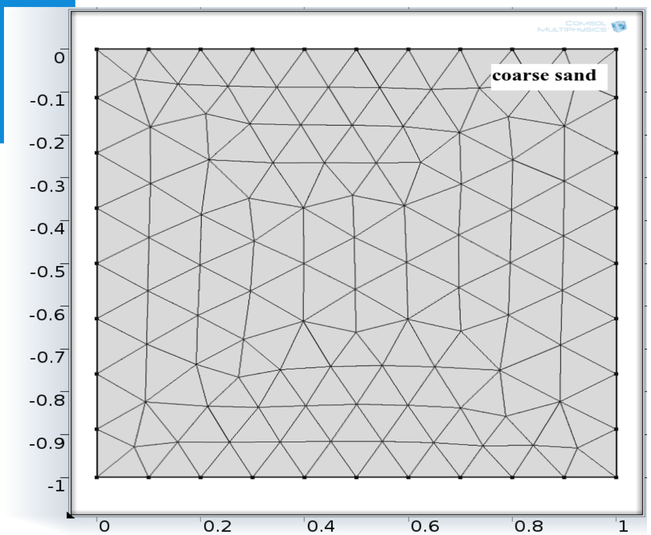
    $$MB_{sD}(t) = \sum (\theta c - \theta_0 c)\, dv - \left[\sum (-uDx_{in}\, \Delta zIN - uDx_{out}\, \Delta zIN) + \sum (-uDz_{in}\, \Delta xIN - uDz_{out}\, \Delta xIN) \right] dt$$

    $$uDx = D_{xx} \frac{dc}{dx} \qquad uDz = D_{zz} \frac{dc}{dz}$$

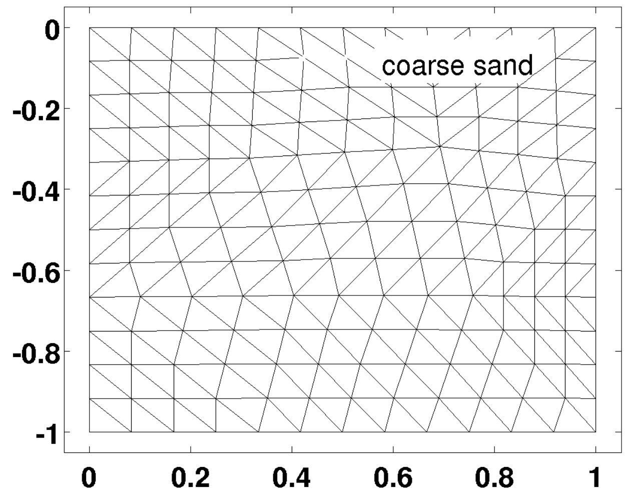
    - Advection

    $m_{outA} = \sum m_c - m_{recycled}$ (Sun, 1999)

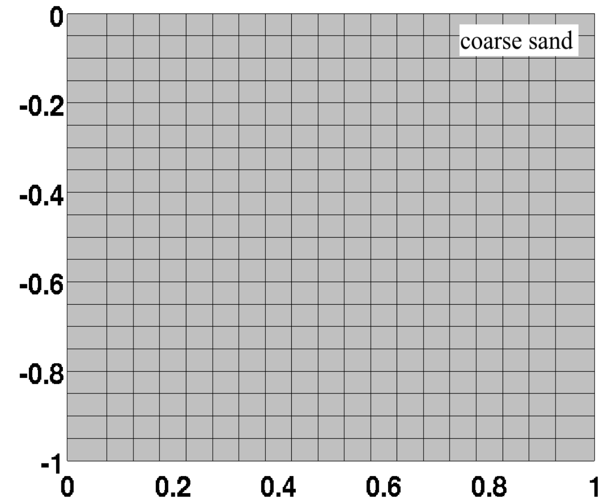
Spatial Scenarios: Model Verification



COMSOL



FAESOR
(Mesh by NETGEN (Schöberl, 2003))



FDM-MIC

Hydraulic parameters	α [1/m]	n	Θ_s [m^3/m^3]	Θ_r [m^3/m^3]	K_{sat} [m/s]
coarse sand	2.00	1.50	0.40	0.04	5.00×10^{-2}

Material Properties : Model Verification

Parameters	Problem 1	Problem 2	Problem 3
z_{ref} [m]	0.00	-1.00	-2.00
c_{ini} [kg/m^3]	1.00	1.00	1.00
q_{top} [m/s]	0	0	0
K_{surf} [1/s]	5.0 x 10^{-2}	5.0 x 10^{-2}	5.0 x 10^{-2}
Ψ_{amb} [m]	-1.00	-1.00	-1.00
c_{top} [kg/m^3]	0.00	0.00	0.00
S_s [kg/m^{2}s^2]	4.00 x 10^{-6}	4.00 x 10^{-6}	4.00 x 10^{-6}
D_m [m^2/s]	1.00 x 10^{-10}	1.00 x 10^{-10}	1.00 x 10^{-10}
α_L [m]	0.10	0.10	0.10
α_T [m]	1.0 x 10^{-2}	1.0 x 10^{-2}	1.0 x 10^{-2}

Results : Model Verification

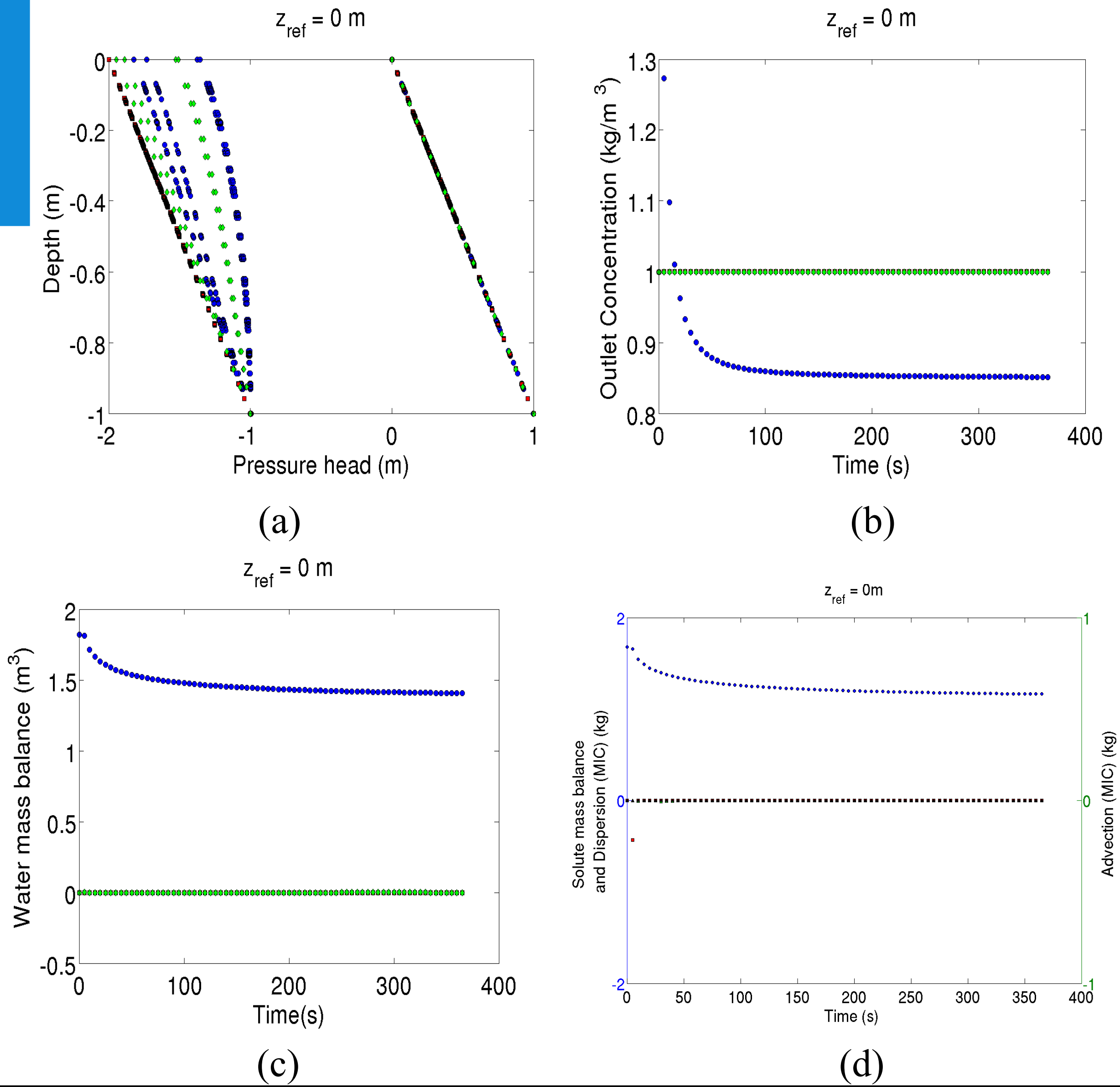
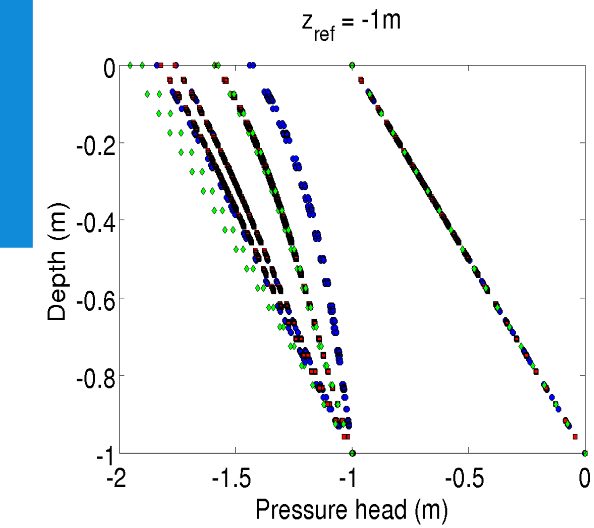
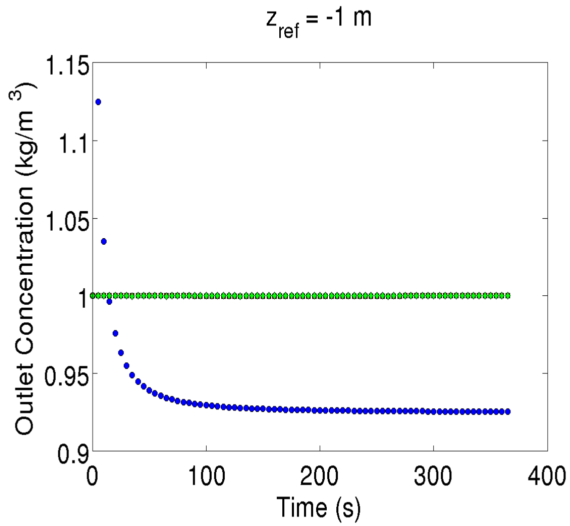


Figure: Problem 1, z_{ref} = 0m, pressure head along depth (● for COMSOL, ■ for FAESOR, ▲ for FDM) at time 0, 100, 275, 365s (a), outlet concentration along time (● for COMSOL, ■ for FAESOR, ▲ for MIC) (b), mass balance for water transport (● for COMSOL, ■ for FAESOR, ▲ for FDM) (c) and Mass balance for solute transport (● for COMSOL, ■ for FAESOR, ▲ for Dispersion term in MIC and ▲ for Advection term in MIC) (d).

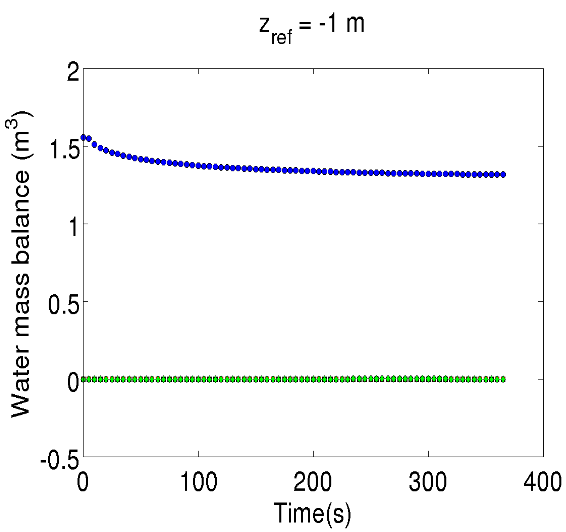
Results : Model Verification



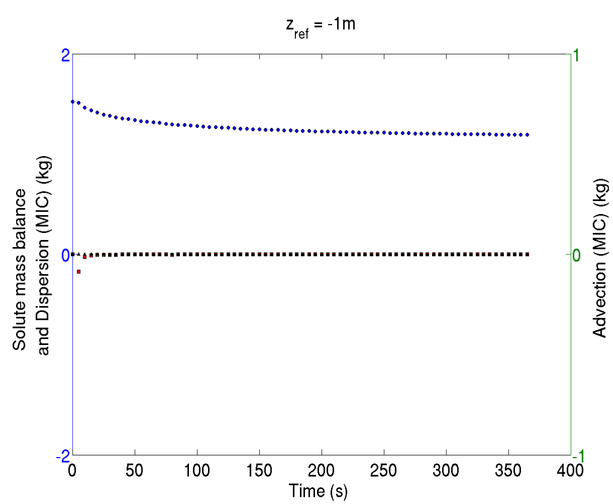
(a)



(b)



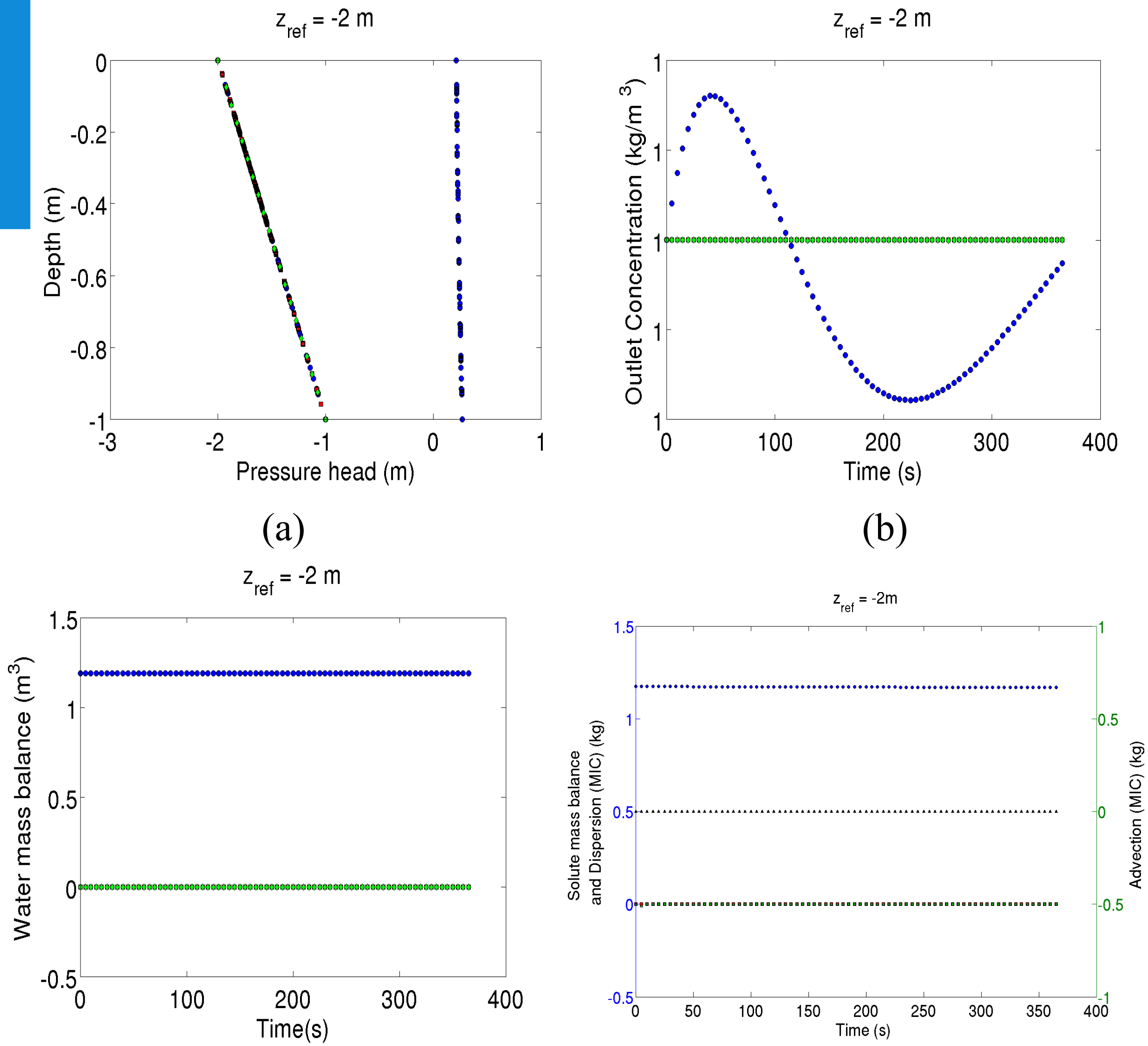
(c)



(d)

Figure: Problem 2, z_{ref} = -1m, pressure head along depth (● for COMSOL, ■ for FAESOR, ▲ for FDM) at time 0, 100, 275, 365s (a), outlet concentration along time (● for COMSOL, ■ for FAESOR, ▲ for MIC) (b), mass balance for water transport (● for COMSOL, ■ for FAESOR, ▲ for FDM) (c) and Mass balance for solute transport (● for COMSOL, ■ for FAESOR, ▲ for Dispersion term in MIC and ▲ for Advection term in MIC) (d).

Results : Model Verification

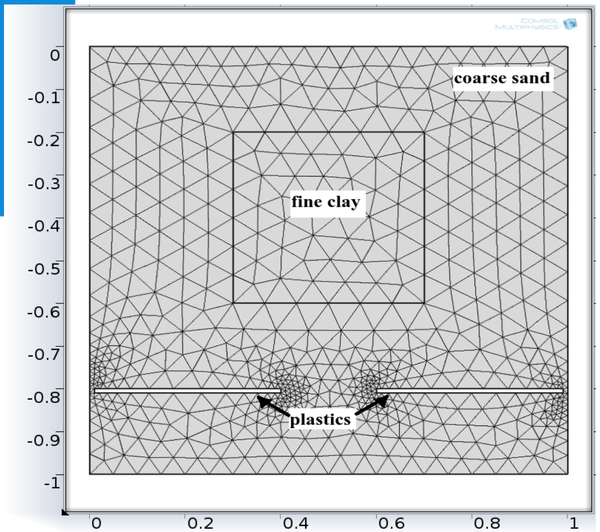


(a) (b)

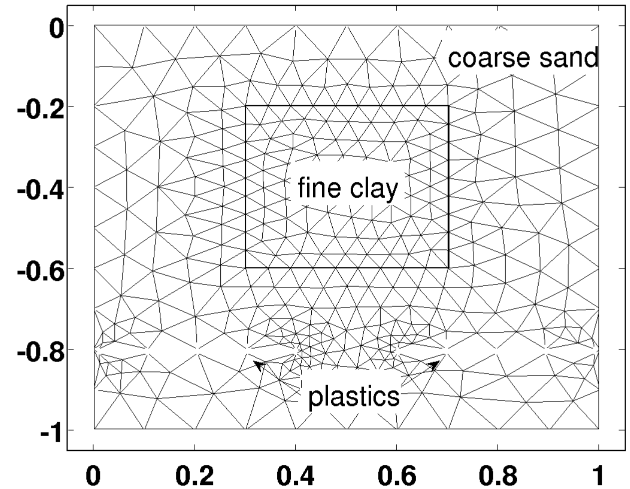
(c) (d)

Figure: Problem 3, z_{ref} = -2m, pressure head along depth (● for COMSOL, ■ for FAESOR, ▲ for FDM) at time 0, 100, 275, 365s (a), outlet concentration along time (● for COMSOL, ■ for FAESOR, ▲ for MIC) (b), mass balance for water transport (● for COMSOL, ■ for FAESOR, ▲ for FDM) (c) and Mass balance for solute transport (● for COMSOL, ■ for FAESOR, ▲ for Dispersion term in MIC and ▲ for Advection term in MIC) (d).

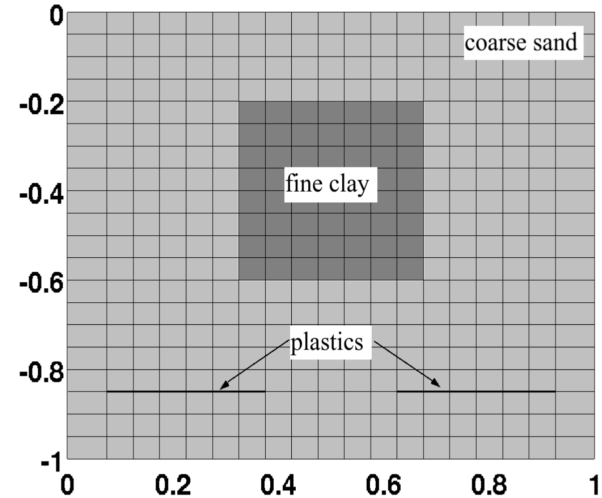
Spatial Scenarios : Application Problem



COMSOL



FAESOR



FDM-MIC

Hydraulic parameters	α [1/m]	*n*	Θ_s [m³/m³]	Θ_r [m³/m³]	K_{sat} [m/s]
coarse sand	2.00	1.50	0.40	0.04	5.00×10^{-2}
fine clay	1.00	2.50	0.45	0.08	5.00×10^{-5}

Material Properties: Application Problem

Parameters	Application Problem
z_{ref} [m]	-2.00
c_{ini} [kg/m^3]	1.00
q_{top} [m/s]	-5.0 x 10^{-3}
K_{surf} [1/s]	5.0 x 10^{-2}
Ψ_{amb} [m]	-1.00
c_{top} [kg/m^3]	0.00
S_s [kg/m^{2}s^2]	4.00 x 10^{-6}
D_m [m^2/s]	1.00 x 10^{-10}
α_L [m]	0.10
α_T [m]	1.0 x 10^{-2}

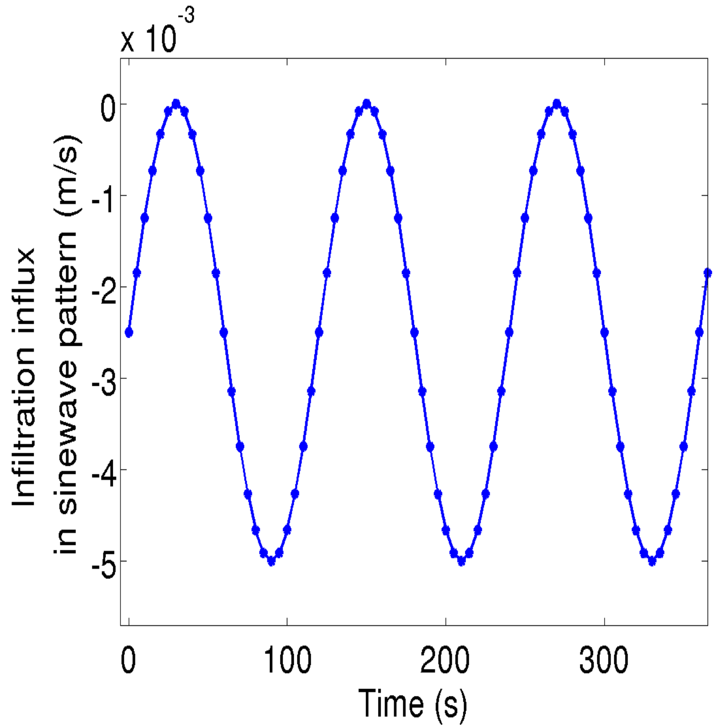


Figure: Infiltration for application problem.

Results: Application Problem

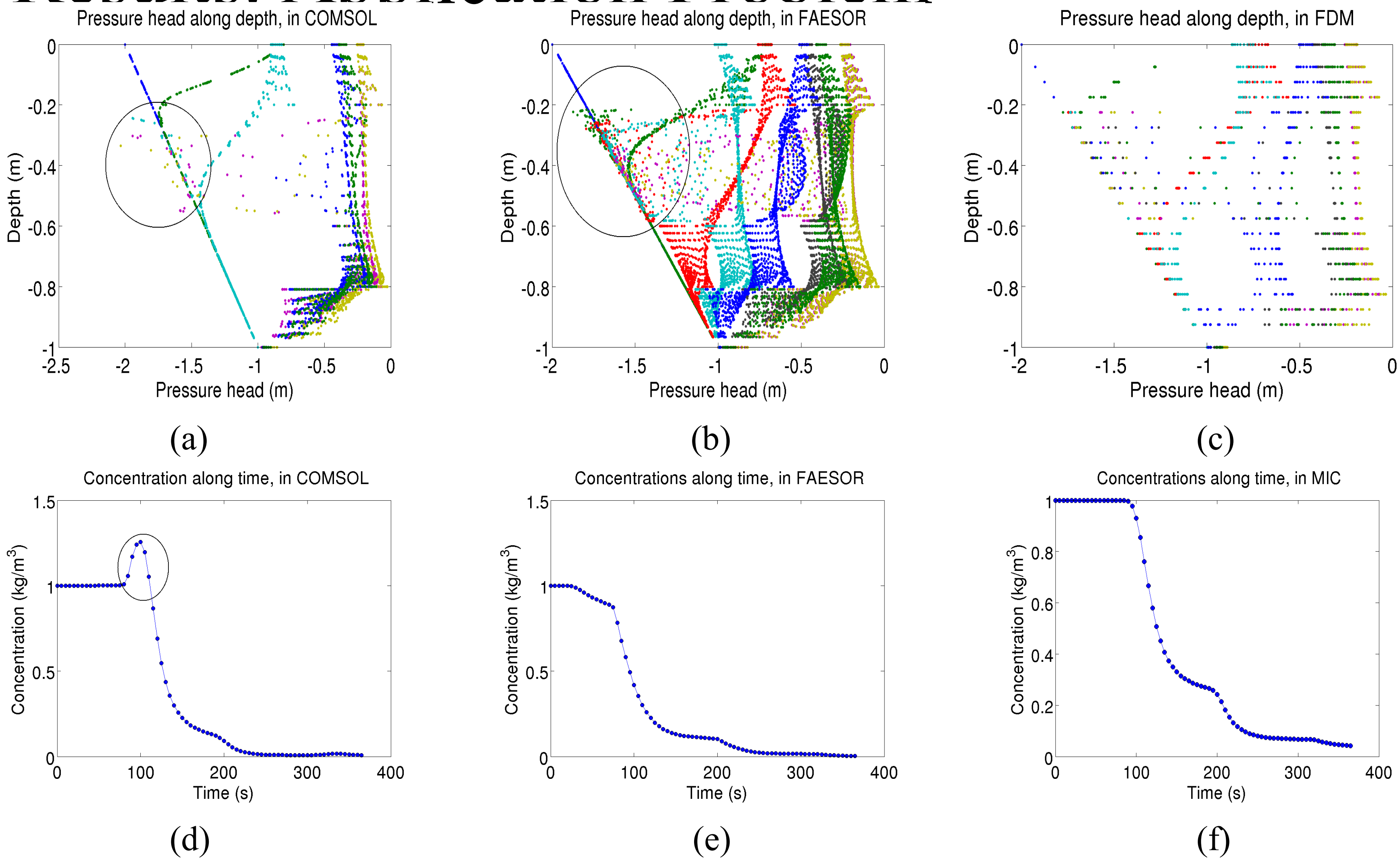


Figure: Pressure head along depth at time 0,5,25,85,100,250,365s for COMSOL (a), FAESOR (b) and FDM (c). Outlet concentration along Time for COMSOL(d), FAESOR (e), and MIC (f).

Results: Application Problem

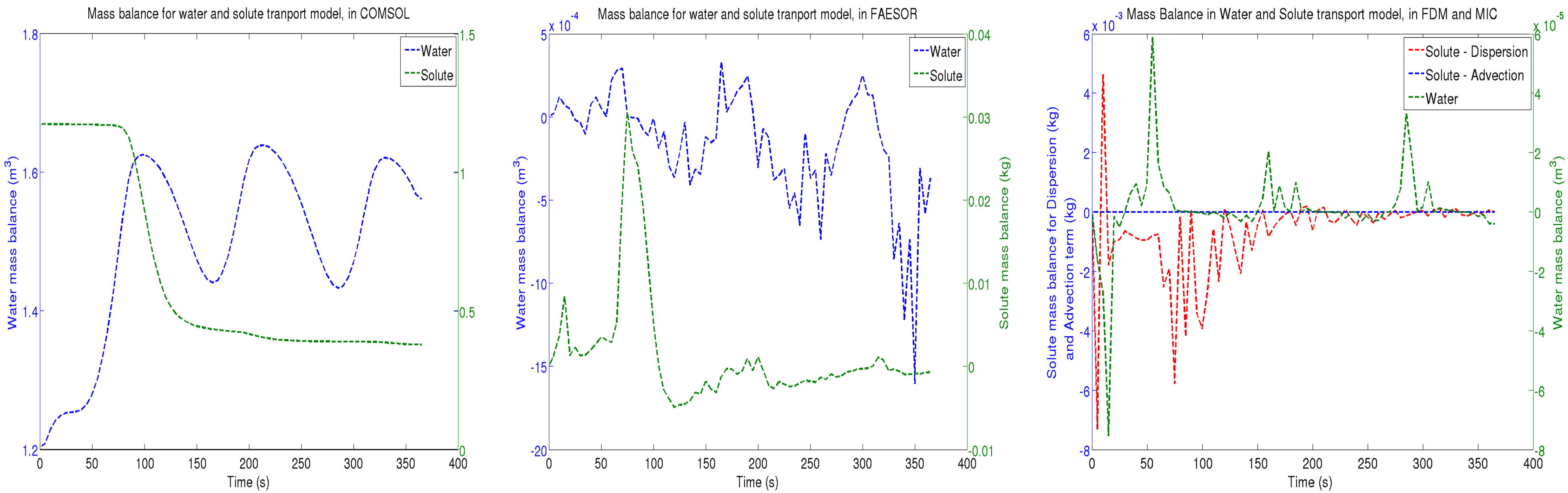
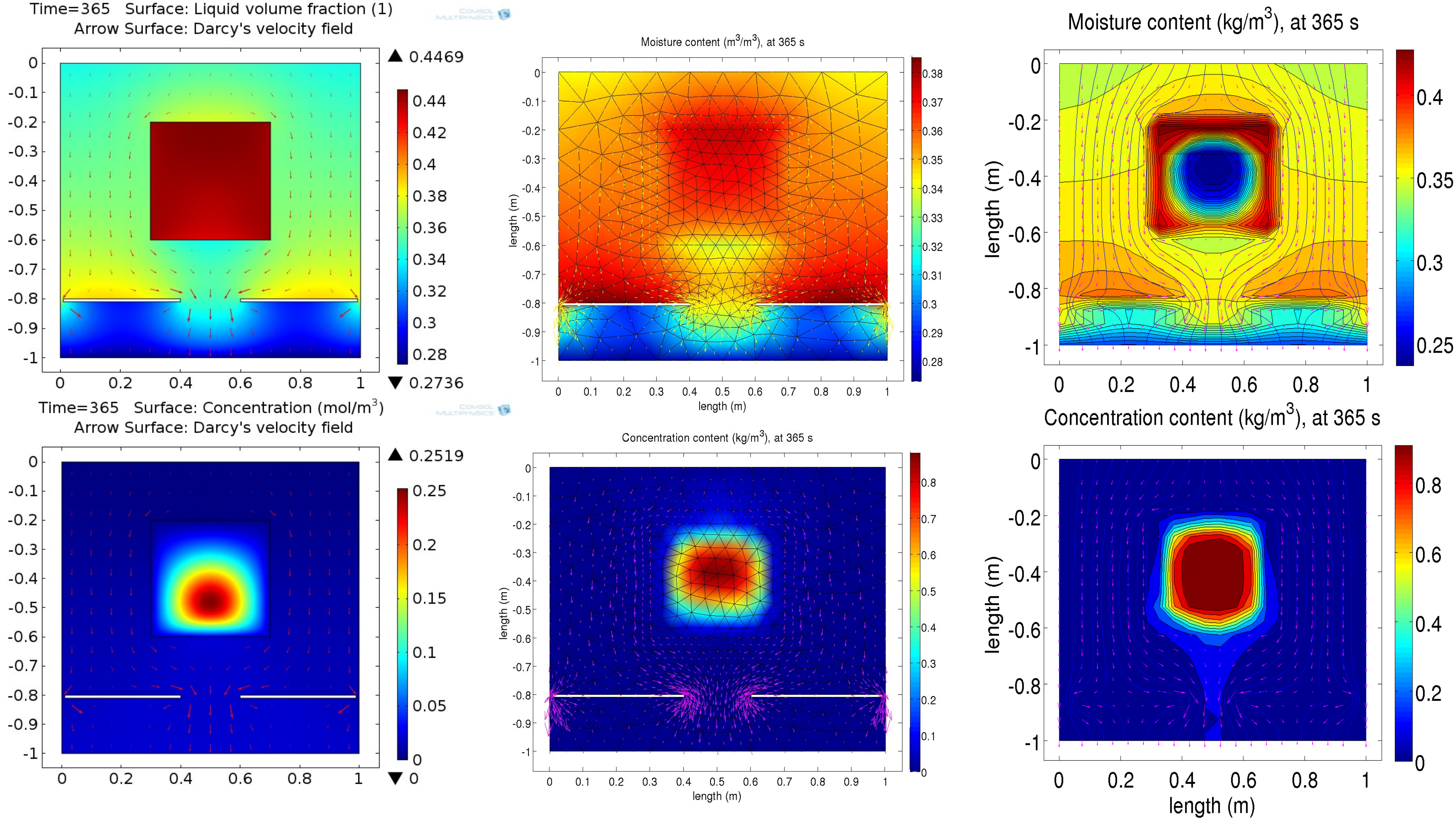


Figure: Mass balances for water and solute transport models for different numerical methods

Results: Application Problem



COMSOL FAESOR FDM-MIC

Discussions

- In FEM
  - larger amount of test functions reduces residual error thus numerical approximation becomes more accurate. FAESOR (secondary nodes) better results than COMSOL (default primary nodes).
  - COMSOL (Richards Equation is default head based) → $\frac{\theta^{(a+1)}-\theta^{(a+1)}}{\Delta t} \neq C \frac{\Psi^{a+1}-\Psi^{a}}{\Delta t}$

    in FAESOR (Richards equation is mixed based) is linearized using with Picards iteration and thus mass balance is improved.

- In FDM, placement of hydraulic conductivities and computation of darcy's velocities on internodes, gives better results.

- Automatic time stepping methods and time step dependent on iterations improves mass balance

Discussions

- During computation of advection term by conventional Euler method, the concentration front produces negative values. And produces values higher than boundary and initial conditions.

- MIC approach of calculating dispersion term on Euler nodes and advection term on Lagrangian markers reduces this error.

- MIC has better mass balance than other convention Euler based methods, described in this research (i.e. COMSOL and FAESOR).

Conclusions

- FAESOR better than COMSOL considering mass balance
- FDM method for water transport and MIC method for solute transport delivers better performance considering mass balance.
  - Could be used to validate lab and field experiments
  - Disadvantage not applicable for irregular geometry unlike FAESOR or COMSOL

References

- Celia, M., Bouloutas, E., and Zarba, R., (1990). A general mass-conservative numerical solution for unsaturated flow equation, Water Resources Research 26, 1483-1496.
- Gerya, T.V (2010). Numerical Geodynamic Modeling. Cambridge University Press.
- Krysl, P. (2000), Thermal and stress analysis with finite element method, accompanied by the MATLAB toolbox FAESOR, Pressure cooker express.
- Schöberl. J, 2003, NETGEN- 4.3, Department of Computational Mathematics and Optimization, University of Linz, Austria.
- Sun, N. (1999), A finite cell method for simulating the mass transport process in porous media, Water Resources Research 35(12), 3649-3662.

Questions ?

Thank You