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

Presented by
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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 an application problem → Comparison based on global mass balances, iteration methods, time stepping methods.
Equations Involved - Water Transport

• Richard's Equation

\[ C_m(\Psi^{(a+1,b)}) + S_w S_s \delta^{b+1} + \nabla \cdot q = 0 \quad \text{... Eq (1. a)} \quad \text{Head Based...COMSOL} \]

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

\[ \delta^{b+1} = (\Psi^{a+1,b+1} - \Psi^{a+1,b}) \quad \text{... Eq (2)} \]

\[ q = -K(\Psi) \nabla (\Psi + z) \quad \text{... Eq (3)} \]

• van Genuchten functions

\[ K(\Psi) = k_r K_{sat} \quad \text{... Eq (4)} \]

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

\[ \theta(\Psi) = \theta_r + S_{eff}(\theta_s - \theta_r) \quad \text{... Eq (6)} \]

\[ k_r = S_{eff}^{1/2} [1 - (1 - S_{eff}^{1/m})^m]^2 \quad \text{... Eq (7)} \]

\[ S_w = S_{eff} + \frac{\theta_r}{\theta_s} \quad \text{... Eq (8)} \]

\[ C_m = \frac{\alpha m}{1-m} (\theta_s - \theta_r) S_{eff}^{1/m} (1 - S_{eff}^{(1/m)})^m \quad \text{... Eq (9)} \]
Equations Involved - Solute Transport

• Advection Dispersion Equation

\[
\frac{\partial \theta c}{\partial t} + \nabla \cdot u = 0 \quad \ldots \quad Eq(10)
\]

\[
u = -D \nabla c + qc \quad \ldots \quad Eq(11)
\]

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

\[
v = \frac{q}{\theta} \quad \ldots \quad Eq(13)
\]
## Initial and Boundary Conditions

<table>
<thead>
<tr>
<th>Water and Solute Transport Model</th>
<th>Initial Condition</th>
<th>Boundary Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Richards Equation</td>
<td>( \Psi(x, z, 0) = z - z_{\text{ref}} )</td>
<td>Neumann</td>
</tr>
<tr>
<td></td>
<td>( q(x, 0, t) = q_{\text{top}} )</td>
<td>Robbins</td>
</tr>
<tr>
<td>Advection Dispersion Equation</td>
<td>( c(x, z, 0) = c_{\text{ini}} )</td>
<td>Dirichlet</td>
</tr>
<tr>
<td></td>
<td>( c(x, 0, t) = c_{\text{top}} )</td>
<td>Robbins</td>
</tr>
<tr>
<td></td>
<td>( c(x, -1, t) = q c )</td>
<td>Robbins</td>
</tr>
</tbody>
</table>

Initial Condition:
- \( \Psi(x, z, 0) = z - z_{\text{ref}} \)
- \( c(x, z, 0) = c_{\text{ini}} \)

Boundary Conditions:
- **top horizontal edge**
  - Neumann:
    - \( q(x, 0, t) = q_{\text{top}} \)
  - Robbins:
    - \( q(x, -1, t) = -K_{\text{surf}}(\Psi_{\text{amb}} - \Psi) \)

- **bottom horizontal edge**
  - Dirichlet:
    - \( c(x, 0, t) = c_{\text{top}} \)
  - Robbins:
    - \( c(x, -1, t) = q c \)
FEM - COMSOL and FAESOR

\[
\begin{bmatrix}
\eta \\
(0,1)
\end{bmatrix}
\begin{bmatrix}
\xi \\
\eta \\
1-\xi-\eta
\end{bmatrix}
\]

\[
\begin{bmatrix}
\eta \\
(0,1)
\end{bmatrix}
\begin{bmatrix}
\xi \\
\eta \\
(2\eta+2\xi-1) \\
\xi(2\xi-1) \\
\eta(2\eta-1) \\
-4\xi(\eta+\xi-1) \\
4\eta\xi \\
-4\eta(\eta+\xi-1)
\end{bmatrix}
\]

COMSOL

FAESOR
FAESOR - Richards Equation

- Head based form of RE
  \[ C \frac{\partial \psi}{\partial t} - \nabla \cdot K [\nabla (\psi + z)] = 0 \]

- Applying weighted residual, Green theorem, boundary conditions
  \[
  \int_v \eta C \frac{\partial \psi}{\partial t} dV + \int_v (\nabla \eta) \cdot K [\nabla (\psi + z)] dV + \int_{S_1} \eta \bar{q}_n dS + \int_{S_2} \eta K_{surf} (\psi - \psi_{amb}) dS = 0
  \]

- Solution technique for RE with Picards iteration's scheme (Celia et al, 1990)
  \[
  T^b_v + C_m \frac{\delta^{b+1}_v}{\Delta t} + (K_m + H_m) \Psi_v - Lw_v = 0
  \]

- \[
  \Psi_v^{a+1,b+1} = \delta^{b+1}_v + \Psi_v^{a+1,b}
  \]
FAESOR - Richards Equation

- Temporal discretization \[ dt = \min \left| \Delta t_{\text{iter}} \right| \Delta t_{\text{max}} \]

- For convergence

\[
\Psi_{v_{\text{prime}}}^{a+1,b+1} = \frac{\Psi_{v}^{a+1,b+1} - \Psi_{v}^{a+1,b}}{dt}
\]

- Truncation error

\[
\text{truncerr} = \frac{ \left( \Psi_{v_{\text{prime}}}^{a+1,b+1} - \Psi_{v_{\text{prime}}}^{a+1,b} \right) dt }{2}
\]

- We have considered \( \delta_r = 1 \times 10^{-3} \) and \( \delta_a = 1 \times 10^{-3} \) for \( \text{convcrit} = \delta_r |\Psi_{v}^{a+1,b+1}| + \delta_a \) and \( \text{testval} = |\delta_{v}^{b+1}| - \text{convcrit} \)

- Loop for convergence with iterations and automatic time stepping

\[
\text{if } niter \geq \text{maxiter (i.e. 25)}, \text{ } \Delta t_{\text{iter}} = \Delta t \cdot u_1 (i.e, 0.25) \text{ } \rightarrow \text{not converged } \rightarrow niter = niter + 1
\]

\[
\text{if } niter \leq \text{miniter (i.e. 15)}, \text{ } \Delta t_{\text{iter}} = \Delta t \cdot u_2 (i.e, 1.1)
\]

\[
\max (\text{testval}) < 0 \rightarrow t = t + \Delta t \rightarrow \text{converged}
\]
FAESOR - Advection Dispersion Equation

• Head based form of ADE
  \[ \theta \frac{\partial c}{\partial t} - \nabla \cdot D \nabla (c - q c) = 0 \]

• Applying weighted residual, Green theorem, boundary conditions.
  \[ \int_v \eta \theta \frac{\partial c}{\partial t} dV + \int_v (\nabla \eta) \cdot D \nabla (c - q c) dV + \int_s \eta n q c dS = 0 \]

• Solution technique for ADE with Euler backward (Implicit) method.
  \[ \left[ \frac{1}{\Delta t} T_v + DA_m \right] Con_{v+1} = \left[ \frac{1}{\Delta t} T_v \right] Con_{m+1} + Ls_{v+1} = 0 \]
FDM - Richards Equation

\[
\frac{\theta_{ij}^{a+1} - \theta_{ij}^a}{\Delta t} + \frac{C_m (\Psi_{ij}^{(a+1,b)}) + S_w S_s}{\Delta t} \delta_{ij}^{b+1} = -\frac{q z_{i+1/2,j} - q z_{i-1/2,j}}{\Delta z_{i-1/2,j}} - \frac{q x_{i+1/2,j} - q x_{i-1/2,j}}{\Delta x_{i,j-1/2}}
\]
Marker-in-Cell

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

\[
\frac{Dc}{Dt} = \frac{\partial c}{\partial t} + q \cdot \nabla c
\]

- Lagrangian term solved on Euler nodes

\[
\frac{Dc}{Dt} = - \nabla \cdot D \nabla c
\]

- Advection term solved on Lagrangian markers

\[
\begin{align*}
x_{mrk}^{tx} + \Delta x_{mrk} &= x_{mrk}^{tx} + v_x x_{mrk} \Delta t x_{mrk} \\
z_{mrk}^{tz} + \Delta z_{mrk} &= z_{mrk}^{tx} + z x_{mrk} \Delta t z_{mrk}
\end{align*}
\]
Marker-in-Cell

• Dispersion term on Euler Nodes

\[ \nabla \cdot D \nabla c = \frac{\Delta z_{i-l/2,j}}{-Dz_{i+1/2,j} \frac{c_{i+1,j} - c_{i,j}}{\Delta z_{i,j}}} - \frac{\Delta z_{i-l/2,j}}{-Dz_{i-1/2,j} \frac{c_{i,j} - c_{i-1,j}}{\Delta z_{i-1,j}}} \]

• 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, which can be damped by sub-grid diffusion operation

\[ \Delta c_{i,j} = \Delta c_{i,j}^{\text{subgrid}} + \Delta c_{i,j}^{\text{remaining}} \]

• Subgrid diffusion applied on markers over characteristic local concentration diffusion time scale

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

\[ \text{where } \Delta t_{\text{diff}} = \frac{1}{2 \frac{D_{mx}}{\Delta x^2} + 2 \frac{D_{mz}}{\Delta z^2}} \]

• \[ \Delta c_{i,j}^{\text{remaining}} = \Delta c_{i,j} - \Delta c_{i,j}^{\text{subgrid}} \]

• \[ c_{m}^{t+\Delta t} = c_{m}^t + \Delta c_{m}^{\text{subgrid}} + \Delta c_{m}^{\text{remaining}} \]
Mass Balance Check

• **Water transport**  \( MB(t) = \text{Total additional mass inside domain} - \text{Total net flow out of domain} \)
  
  FEM - COMSOL and FAESOR
  
  \[
  MB_w(t) = \sum (\theta - \theta_0) \, dv - \left[ \sum (-qx_{in} \, dz_{in} - qx_{out} \, dz_{out}) + \sum (-qz_{in} \, dx_{in} - qz_{out} \, dx_{out}) \right] \, dt
  \]

• **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**  \( MB(t) = \text{Total additional concentration mass inside domain} - \text{Total net flux out of domain} \)
  
  • FEM - COMSOL and FAESOR
  
  \[
  MB_c(t) = \sum (\theta_c - \theta_{0c}) \, dv - \left[ \sum (-ux_{in} \, dz_{in} - ux_{out} \, dz_{out}) + \sum (-uz_{in} \, dx_{in} - uz_{out} \, dx_{out}) \right] \, dt
  \]

• **MIC**
  
  • **Dispersion**
    \[
    MB_{cD}(t) = \sum (\theta_c - \theta_{0c}) \, dv - \left[ \sum (-uDX_{in} \Delta zIN - uDX_{out} \Delta zIN) + \sum (-uDZ_{in} \Delta xIN - uDX_{out} \Delta xIN) \right] \, dt
    \]
    \[
    uDX = D_{xx} \frac{dc}{dx} \quad uDZ = D_{zz} \frac{dc}{dz}
    \]

• **Advection**
  
  \[
  m_{outA} = \sum m_c - m_{recycled} \quad (\text{Sun, 1999})
  \]
Spatial Scenarios: Model Verification

<table>
<thead>
<tr>
<th>Hydraulic parameters</th>
<th>( \alpha ) [1/m]</th>
<th>( n )</th>
<th>( \Theta_s ) [m(^3)/m(^3)]</th>
<th>( \Theta_r ) [m(^3)/m(^3)]</th>
<th>( K_{\text{sat}} ) [m/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>coarse sand</td>
<td>2.00</td>
<td>1.50</td>
<td>0.40</td>
<td>0.04</td>
<td>5.00 x 10(^{-2})</td>
</tr>
</tbody>
</table>

COMSOL
FAESOR
(Mesh by NETGEN (Schöberl, 2003))
FDM-MIC
## Material Properties: Model Verification

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Problem 1</th>
<th>Problem 2</th>
<th>Problem 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$z_{ref} [m]$</td>
<td>0.00</td>
<td>-1.00</td>
<td>-2.00</td>
</tr>
<tr>
<td>$c_{ini} [kg/m^3]$</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$q_{top} [m/s]$</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$K_{surf} [1/s]$</td>
<td>$5.0 \times 10^{-2}$</td>
<td>$5.0 \times 10^{-2}$</td>
<td>$5.0 \times 10^{-2}$</td>
</tr>
<tr>
<td>$\Psi_{amb} [m]$</td>
<td>-1.00</td>
<td>-1.00</td>
<td>-1.00</td>
</tr>
<tr>
<td>$c_{top} [kg/m^3]$</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>$S_s [kg/m^2s^2]$</td>
<td>$4.00 \times 10^{-6}$</td>
<td>$4.00 \times 10^{-6}$</td>
<td>$4.00 \times 10^{-6}$</td>
</tr>
<tr>
<td>$D_m [m^2/s]$</td>
<td>$1.00 \times 10^{-10}$</td>
<td>$1.00 \times 10^{-10}$</td>
<td>$1.00 \times 10^{-10}$</td>
</tr>
<tr>
<td>$\alpha_L [m]$</td>
<td>0.10</td>
<td>0.10</td>
<td>0.10</td>
</tr>
<tr>
<td>$\alpha_T [m]$</td>
<td>$1.0 \times 10^{-2}$</td>
<td>$1.0 \times 10^{-2}$</td>
<td>$1.0 \times 10^{-2}$</td>
</tr>
</tbody>
</table>
Results: Model Verification

Figure: Problem 1, \( z_{ref} = 0 \text{m} \), 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

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

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

Hydraulic parameters

<table>
<thead>
<tr>
<th>Material</th>
<th>$\alpha$ [1/m]</th>
<th>$n$</th>
<th>$\Theta_s$ [m$^3$/m$^3$]</th>
<th>$\Theta_r$ [m$^3$/m$^3$]</th>
<th>$K_{sat}$ [m/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>coarse sand</td>
<td>2.00</td>
<td>1.50</td>
<td>0.40</td>
<td>0.04</td>
<td>5.00 x 10^{-2}</td>
</tr>
<tr>
<td>fine clay</td>
<td>1.00</td>
<td>2.50</td>
<td>0.45</td>
<td>0.08</td>
<td>5.00 x 10^{-5}</td>
</tr>
</tbody>
</table>
## Material Properties: Application Problem

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Application Problem</th>
</tr>
</thead>
<tbody>
<tr>
<td>$z_{ref}$ [m]</td>
<td>-2.00</td>
</tr>
<tr>
<td>$c_{ini}$ [kg/m³]</td>
<td>1.00</td>
</tr>
<tr>
<td>$q_{top}$ [m/s]</td>
<td>$-5.0 \times 10^{-3}$</td>
</tr>
<tr>
<td>$K_{surf}$ [1/s]</td>
<td>$5.0 \times 10^{-2}$</td>
</tr>
<tr>
<td>$\Psi_{amb}$ [m]</td>
<td>-1.00</td>
</tr>
<tr>
<td>$c_{top}$ [kg/m³]</td>
<td>0.00</td>
</tr>
<tr>
<td>$S_s$ [kg/m²s²]</td>
<td>$4.00 \times 10^{-6}$</td>
</tr>
<tr>
<td>$D_m$ [m²/s]</td>
<td>$1.00 \times 10^{-10}$</td>
</tr>
<tr>
<td>$\alpha_L$ [m]</td>
<td>0.10</td>
</tr>
<tr>
<td>$\alpha_T$ [m]</td>
<td>$1.0 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

**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

Time=365  Surface: Liquid volume fraction (1)  Arrow Surface: Darcy’s velocity field

Time=365  Surface: Concentration (mol/m²)  Arrow Surface: Darcy’s velocity field

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 Picard's 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


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• 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?