Particle tracking approach to model chemical reaction transport in 3D discrete fracture networks

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Recharge area:
- Porous aquifer
- Surface water

Direction and rate of contaminant migration

Water stored underground in cracks and pores

Fractured aquifer

http://rdnwaterbudget.ca/water-101/aquifers-groundwater/
Chemical reaction: A → B → C

Source Zone

groundwater zone

Parker et al., 2010
How fast do plumes travel in fractured rock aquifers?

Direct Migration Pathway from Sewers to Well

Bedrock
Chemical reaction combine with particle tracking.
Chemical reaction: Tetrachloroethylene (PCE) degradation

http://web.utk.edu/~microlab/LoefflerLab/Chlorinated_ethenes.html

PCE: PERC, Perchloroethylene

“A volatile organic compound (VOC)”

In 1965, worldwide production was about 1 million metric tons (Fossburg 2006)

Widely used for dry cleaning and as a metal degreaser, in typewriter correction fluid, and shoe polish.

Small amounts are also retained by recently dry cleaned clothing

Bemis et al., 2014

A contaminant Cont is assumed to be subject to first-order degradation:

\[ R = \mu_w C \]  

where \( R \) is the decay rate [M L^{-3} T^{-1}] and \( \mu_w \) is the first-order rate constant for solutes in the liquid phase [T^{-1}].

Schaerlaekens et al., 1999
Work flow

Input data

Fracture data analysis

Generation of DFN

Flow simulation

Particle tracking

PCE degradation (Chemical reaction) & solute transport
2 cases simulation

- Flow simulation
- Particle tracking
- PCE degradation (Chemical reaction) & solute transport

Development
Testing
Explaining
Validation

Implement
Simple case

- Transmissivity: $1 \times 10^{-4} \text{ m}^2/\text{s}$
- Aperture: $1 \times 10^{-4} \text{ m}$
- Steady-state flow
- Boundaries condition:
  + High constant head: left side 199m
  + Low constant head: right side 198.5m
  + No flow for others faces ($Q_{\text{in}} = Q_{\text{out}}$)
- Particle releasing: 50
Particles Tracking

- Particle number: 50

Location \((x, y, z)\)

Chemical reaction

PHREEQC

10/24/2018
PCE degradation (Chemical reaction) & solute transport

<table>
<thead>
<tr>
<th>Contaminant</th>
<th>Maximum contaminant level (MCL) (EPA)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PCE</td>
<td>0.005 mg/L</td>
</tr>
<tr>
<td>TCE</td>
<td>0.005 mg/L</td>
</tr>
<tr>
<td>CisDCE</td>
<td>0.005 mg/L</td>
</tr>
<tr>
<td>VC</td>
<td>0.002 mg/L</td>
</tr>
</tbody>
</table>

Continuous injection 0.1 mg/L Pce only

PCE & TCE concentration in different time for one pathway
PCE & TCE results in different time after releasing PCE
Fracture data analysis -> Generation of DFN

**Set Properties:** $T/P/k/P_{32,rel}$
- Set S1: 198°/18°/18/26%
- Set S2: 155°/4°/15/24%
- Set S3: 264°/23°/16/18%
- Set S4: 98°/81°/11/32%

Fracture poles in K-area and delineated Univariate Fisher properties of the four fracture sets identified: $T =$ mean pole trend, $P =$ mean pole plunge, $k =$ concentration, $P_{32,rel} =$ relative fracture intensity
Selroos, 2016

- Domain size: 100 x 100 x 100 m
- Transmissivity: 1e-5 m²/s
- Aperture: 1e-4 m

<table>
<thead>
<tr>
<th>Set</th>
<th>$r_o$</th>
<th>R</th>
<th>No. fracture</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>20</td>
<td>100</td>
<td>200</td>
</tr>
<tr>
<td>2</td>
<td>20</td>
<td>100</td>
<td>193</td>
</tr>
<tr>
<td>3</td>
<td>20</td>
<td>100</td>
<td>125</td>
</tr>
<tr>
<td>4</td>
<td>20</td>
<td>100</td>
<td>261</td>
</tr>
</tbody>
</table>
- Domain size: 100 x 100 x 100m
- Boundaries condition:
  - High constant head: 99 m
  - Low constant head: 98.8 m
  - No flow for others faces ($Q_{in} = Q_{out}$)
- Transmissivity: $10^{-5}$ m$^2$/s
- Aperture: $10^{-4}$ m
- Particle releasing: 100
### Velocity and travel time of particles inside DFN

<table>
<thead>
<tr>
<th></th>
<th>m/d</th>
<th>TravelTime</th>
<th>d</th>
<th>Trace_Length</th>
<th>m</th>
</tr>
</thead>
<tbody>
<tr>
<td>Velocity Mean</td>
<td>15.6</td>
<td>TravelTime Mean</td>
<td>7.5</td>
<td>Trace_Length Mean</td>
<td>106.4</td>
</tr>
<tr>
<td>Velocity Std. Dev</td>
<td>10.8</td>
<td>TravelTime Std. Dev</td>
<td>2.3</td>
<td>Trace_Length Std. Dev</td>
<td>26.8</td>
</tr>
<tr>
<td>Velocity Min</td>
<td>0.6</td>
<td>TravelTime Min</td>
<td>0.06</td>
<td>Trace_Length Min</td>
<td>14.44</td>
</tr>
<tr>
<td>Velocity Max</td>
<td>387.0</td>
<td>TravelTime Max</td>
<td>12.6</td>
<td>Trace_Length Max</td>
<td>134.5</td>
</tr>
</tbody>
</table>
PCE degradation (Chemical reaction) & solute transport

Continuous injection
0.1 mg/L Pce only

PCE and TCE of one particle in difference time after releasing PCE inside DFN
PCE & TCE results in different time after releasing PCE
Conclusion

• Succeed in modeling PCE degradation and transport in 3D simple case for explaining and testing workflow
• Complex case: implement for simple case
• Estimating safety – time and distance for treatment contamination
Discussion

- Validation
- Domain size: large-domain
- Heterogeneous domain
- Point injection
Thank you
Tetrachloroethylene

- Known as PCE
- Chemical Formula C₂Cl₄
- Drying cleaning and degreasing
- Medical concerns
  - Liver failure
  - Renal Cancer
  - Lympathic and hematopoitic cancer
  - Ocular deterioration
- Drinking water
  - 3 PPB (FL)

- Dense Non-Aqueous Phase Liquid
  - DNAPL
  - Immobile
  - Concentrated
  - Spread
  - Elusive
What is the ADE?

- ADE – Advection Dispersion Equation
  - An equation used to describe solute transport through a porous media
  - Mechanisms:
    - Advection
    - Diffusion
    - Dispersion
\[
-D_L \frac{\partial C}{\partial x} \frac{\partial q}{\partial t} + \frac{\partial}{\partial t} \left( \frac{\partial C}{\partial x} + \frac{\partial^2 C}{\partial x^2} \right)
\]

Mass: \( c \delta x \delta y \)

Transport by advection:
\[
u C \delta y + \frac{\partial (uc)}{\partial x} \delta x \delta y
\]

Transport by diffusion:
\[
-D_y \frac{\partial C}{\partial y} \delta y
\]

Perea et al., 2010
Commerically Available DFN Models

- **FRAC3DVS**: A 3D finite element model for steady-state/transient, variably-saturated flow and advective-dispersive solute transport in porous or discretely-fractured porous media.

- **FRACTRAN**: A 2D finite element model for simulating steady-state groundwater flow and time-variant contaminant transport in discretely-fractured, fully-saturated porous media.

- **HydroGeoSphere**: A three-dimensional numerical model describing fully-integrated subsurface and surface flow and solute transport by T. Thomas, University of Waterloo.

- **WASY**: Advanced 3D finite element groundwater flow, heat & contaminant transport modeling by L. P. Johnson, HydroGeoSphere Inc.

**Parker, 2009**
Sources of Groundwater Contamination

- Urban runoff
- Agricultural runoff (Nitrate contamination)
- Legacy contamination (closed sites)
- Abandoned wells
- Fracking
- Leaking underground storage tanks, landfills
- Failing septic systems
- Chemical contamination (eg. PFAS & TCE)
Figure 2 Degradation pathway of PCE using first-order rate constants.

Table 1 Definition of parameters and their values for the PCE biodegradation problem (from Case 1 and 2 in Sun et al., 2004). Rate parameters are for a reference temperature of 20°C.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Values</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Verification</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Velocity</td>
<td>$v$</td>
<td>0.4</td>
<td>m d$^{-1}$</td>
</tr>
<tr>
<td>Dispersion coefficient</td>
<td>$D$</td>
<td>0.4</td>
<td>m$^2$ d$^{-1}$</td>
</tr>
<tr>
<td>First-order degradation rate 1</td>
<td>$k_1$</td>
<td>0.075</td>
<td>d$^{-1}$</td>
</tr>
<tr>
<td>First-order degradation rate 2</td>
<td>$k_2$</td>
<td>0.070</td>
<td>d$^{-1}$</td>
</tr>
<tr>
<td>First-order degradation rate 3</td>
<td>$k_3$</td>
<td>0.020</td>
<td>d$^{-1}$</td>
</tr>
<tr>
<td>First-order degradation rate 4</td>
<td>$k_4$</td>
<td>0.035</td>
<td>d$^{-1}$</td>
</tr>
<tr>
<td>First-order degradation rate 5</td>
<td>$k_5$</td>
<td>0.055</td>
<td>d$^{-1}$</td>
</tr>
<tr>
<td>First-order degradation rate 6</td>
<td>$k_6$</td>
<td>0.030</td>
<td>d$^{-1}$</td>
</tr>
<tr>
<td>First-order degradation rate 7</td>
<td>$k_7$</td>
<td>0.000001</td>
<td>d$^{-1}$</td>
</tr>
<tr>
<td>Distribution factor, TCE to cis-DCE</td>
<td>$\alpha_1$</td>
<td>0.72</td>
<td>-</td>
</tr>
<tr>
<td>Distribution factor, TCE to trans-DCE</td>
<td>$\alpha_2$</td>
<td>0.15</td>
<td>-</td>
</tr>
<tr>
<td>Distribution factor, TCE to 1,1-DCE</td>
<td>$\alpha_3$</td>
<td>0.13</td>
<td>-</td>
</tr>
<tr>
<td>Yield coefficient, PCE to TCE</td>
<td>$y_1$</td>
<td>0.79</td>
<td>-</td>
</tr>
<tr>
<td>Yield coefficient, TCE to DCE</td>
<td>$y_2$</td>
<td>0.74</td>
<td>-</td>
</tr>
<tr>
<td>Yield coefficient, DCE to VC</td>
<td>$y_3$</td>
<td>0.64</td>
<td>-</td>
</tr>
<tr>
<td>Yield coefficient, VC to ETH</td>
<td>$y_4$</td>
<td>0.45</td>
<td>-</td>
</tr>
<tr>
<td>Fracture property</td>
<td>Upper fracture domain (&lt; 70 m)</td>
<td>Lower fracture domain (&gt; 70 m)</td>
<td></td>
</tr>
<tr>
<td>-------------------</td>
<td>--------------------------------</td>
<td>--------------------------------</td>
<td></td>
</tr>
<tr>
<td>Fracture Orientation</td>
<td><strong>Univariate Fisher</strong>&lt;br&gt;Trend/Plunge/kappa/$P_{32,\text{rel}}$&lt;br&gt;Set S1: 198°/18°/18/26%&lt;br&gt;Set S2: 155°/4°/15/24%&lt;br&gt;Set S3: 264°/23°/16/18%&lt;br&gt;Set S4: 98°/81°/11/32%</td>
<td><strong>Univariate Fisher</strong>&lt;br&gt;Trend/Plunge/kappa/$P_{32,\text{rel}}$&lt;br&gt;Set S1: 65°/17°/20/15%&lt;br&gt;Set S2: 344°/38°/18/24%&lt;br&gt;Set S3: 281°/29°/16/30%&lt;br&gt;Set S4: 174°/22°/17/10%&lt;br&gt;Set S5: 175°/75°/19/21%</td>
<td></td>
</tr>
<tr>
<td>Fracture Location</td>
<td><strong>Rectangular (Uniform)</strong></td>
<td><strong>Rectangular (Uniform)</strong></td>
<td></td>
</tr>
<tr>
<td>Fracture Intensity-Size</td>
<td><strong>Power law</strong>&lt;br&gt;$P_{32} (r &gt; r_0) \approx P_{10,\text{corr}} = 2.4 \text{ m}^{-1}$&lt;br&gt;$k_r = 2.6$, $r_0 = 0.1 \text{ m}$, $r_{\text{max}} = 564 \text{ m}$</td>
<td><strong>Power law</strong>&lt;br&gt;$P_{32} (r &gt; r_0) \approx P_{10,\text{corr}} = 0.30 \text{ m}^{-1}$&lt;br&gt;$k_r = 2.6$, $r_0 = 0.1 \text{ m}$, $r_{\text{max}} = 564 \text{ m}$</td>
<td></td>
</tr>
<tr>
<td>Fracture Transmissivity*</td>
<td><strong>Power law</strong>&lt;br&gt;$T = 10^{\log(a r^b) + \sigma_{\log(T)}} N(0,1)$&lt;br&gt;$a = 9E-9 \text{ m}^2/\text{s}$, $b = 0.7$, $\sigma = 1$</td>
<td><strong>Power law</strong>&lt;br&gt;$T = 10^{\log(a r^b) + \sigma_{\log(T)}} N(0,1)$&lt;br&gt;$a = 5.3E-11 \text{ m}^2/\text{s}$, $b = 0.5$, $\sigma = 1$</td>
<td></td>
</tr>
</tbody>
</table>