Sensitivity Analysis of HYDRUS-1D to transient-MIM parameters: a case study related to pesticide fate in soil

B. Cheviron, Y. Coquet
UMR INRA/AgroParisTech Environnement et Grandes Cultures, Grignon, France

The Beauce groundwater, an important but contaminated ressource
- 9000 km² (6 départements)
- 20 billions of m³
- uses:
  - DWS, industries: 100-150 millions m³
  - agriculture: 300-500 millions m³

The « mobile / immobile water» model (MIM)
(Coats & Smith, 1964; van Genuchten & Wierenga, 1976, 1977)

\[
\theta_m \frac{\partial c_m}{\partial t} = \theta_m D_m \frac{\partial^2 c_m}{\partial z^2} - q_m \frac{\partial c_m}{\partial z} - \Gamma_s
\]
\[
\Gamma_s = \theta_{im} \frac{\partial c_{im}}{\partial t} = \alpha (c_m - c_{im})
\]

Steady-state water regime

Beauce soils are characterized by large immobile water contents
(at -1 cm matric potential)

(Aletto et al., 2006)
Sensitivity analysis of HYDRUS-1D to transient MIM parameters

Two possibilities for the water exchange term:

- As a function of water content:
  \[ \Gamma_w = \omega(S_m - S_{im}) \]

  At equilibrium: \( S'_m = S_{im} \), then \( \alpha_m = \alpha \) and \( n_m = n \)

  - If \( \theta_{mr} = 0 \), then \( \theta_m = \theta_{mr} \), \( n = \text{cte} \)

  \[ S_m = \frac{(\theta_m - \theta_{mr})}{(\theta_{ms} - \theta_{mr})} \]

  \[ S_{im} = \frac{(\theta_{im} - \theta_{im,r})}{(\theta_{im,s} - \theta_{im,r})} \]

- As a function of matric potential:
  \[ \Gamma_w = \omega'(h_m - h_{im}) \]

  \[ S_m = \frac{1 + (\alpha_m \eta_m)^{\alpha_m}}{1 + (\alpha_m \eta_m)_m^{\alpha_m}} \]

  \[ S_{im} = \frac{1 + (\alpha_m \eta_m)_m^{\alpha_m}}{1 + (\alpha_m \eta_m)_m^{\alpha_m}} \]

which MIM concept for transient water regime?
(Simunek et al., 2003; Köhne et al., 2004)

\[ \frac{\partial \theta_m}{\partial t} = \frac{\partial}{\partial z} \left[ K \left( \frac{\partial h}{\partial z} + 1 \right) \right] - \Gamma_w \]

\[ \Gamma_w = \frac{\partial \theta_{im}}{\partial t} \]

How to describe \( \Gamma_w \)?

Two possibilities for the water exchange term:

- As a function of water content:
  \[ \Gamma_w = \omega(S_m - S_{im}) \]

  \[ S_m = \frac{(\theta_m - \theta_{mr})}{(\theta_{ms} - \theta_{mr})} \]

  \[ S_{im} = \frac{(\theta_{im} - \theta_{im,r})}{(\theta_{im,s} - \theta_{im,r})} \]

  - If \( \theta_{mr} = 0 \), then \( \theta_m = \theta_{mr} \), \( n = \text{cte} \)

  \[ S_m = \frac{1 + (\alpha_m \eta_m)^{\alpha_m}}{1 + (\alpha_m \eta_m)_m^{\alpha_m}} \]

  \[ S_{im} = \frac{1 + (\alpha_m \eta_m)_m^{\alpha_m}}{1 + (\alpha_m \eta_m)_m^{\alpha_m}} \]

- As a function of matric potential:
  \[ \Gamma_w = \omega'(h_m - h_{im}) \]

  \[ S_m = \frac{1 + (\alpha_m \eta_m)^{\alpha_m}}{1 + (\alpha_m \eta_m)_m^{\alpha_m}} \]

  \[ S_{im} = \frac{1 + (\alpha_m \eta_m)_m^{\alpha_m}}{1 + (\alpha_m \eta_m)_m^{\alpha_m}} \]

  - If \( \theta_{mr} = 0 \), then we need \( \theta_{mr}, \eta_m \) and \( n_m \)

  \[ 3 \text{ measurements} \]

  - If \( \theta_{mr} \neq 0 \),

  \[ 4 \text{ measurements} \]
**Se-based water exchange**

\[ \theta_{m,s} = 0 \]
- 8 parameters:
  \( \theta_{m,s}, \theta_{im,s}, \theta_{i}, \omega, \alpha, n, K_s, l \)

- Hydraulic parameters \( \omega, \theta_{i}, \alpha, n, K_s, l \)
- Wind method

- Hydraulic parameters \( \theta_{m,s}, \theta_{im,s} \)
  \[ \text{One measurement } \theta_{m,s}, \theta_{im,s} \]

- Parameter \( \omega \):
  \[ \text{No direct method} \] (column exp, Köhne et al., 2004)

**Pesticide MIM transport**

\[
\begin{align*}
\frac{\partial (\theta_{m} c_m)}{\partial t} + \frac{\partial (\rho f_{im} s_m c_m)}{\partial z} &= \frac{\partial}{\partial z} \left( \theta_{m} D_{sw} \frac{\partial c_m}{\partial z} \right) - \mu_{m} c_m - \Gamma_{z} \\
\frac{\partial (\theta_{im} c_{im})}{\partial t} + \frac{\partial (\rho (1-f) s_{im})}{\partial z} &= -\mu_{im} c_{im} - \Gamma_{z} \\
\Gamma_{z} &= \omega_{i}(c_{im} - c_{im}) + \left\{ \begin{array}{ll}
\Gamma_{w} c_{im} & \text{si } \Gamma_{w} > 0 \\
\Gamma_{w} c_{im} & \text{si } \Gamma_{w} < 0
\end{array} \right.
\end{align*}
\]

- Linear adsorption \[ s = k d \cdot c \]
- Degradation rate dependent on \( \theta \)
  \[ \mu = \mu_{ref} \left( \frac{\theta}{\theta_{ref}} \right)^{\delta} \]

**Soils**

- Seed bed
- Plough layer
- BT
- Hubstone clay
- Weathered limestone

**Results**

Target output:
Concentration in soil solution at 1 m depth
Results

High sensitivity to MIM parameters

\[ \theta_{\text{MIM (ref)}} = 0.132, \quad \theta_{\text{MIM (ref)}} = 0.268, \quad \omega_{\text{MIM (ref)}} = 1.3 \text{ d}^{-1}, \quad f = 0.33 \]

Results

High sensitivity to pesticide fate parameters

\[ k_d = 0.5-0.9 \text{ L kg}^{-1}, \quad \mu = 0.0042-0.0065 \text{ d}^{-1}, \quad (\text{DT} 50 = 107-165 \text{ d}) \]

Results

[Graph showing data and equations]

\[ \text{ROV} = \frac{C - C_{\text{ref}}}{C_{\text{ref}}} / \frac{P - P_{\text{ref}}}{P_{\text{ref}}} \]

Results

[Table showing parameters and their values]
Conclusion

- HYDRUS 1D shows a high sensitivity to transient MIM parameters
- van Genuchten n parameter is also very sensitive
- Classically, concentrations are very sensitive to pesticide fate parameters (sorption coeff, degradation rate)
- Transient MIM water flow should be included in models describing pesticide fate in soils