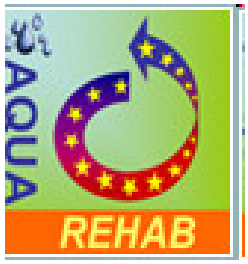

E-MNM1D
Enhanced Micro- and Nanoparticle transport Model in saturated porous media
Numerical solution of colloid trasport in 1D systems.
RELEASE: 1.0

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Reference:

Tosco T., Sethi R. (2010). *Transport of non-Newtonian suspensions of highly concentrated micro- and nanoscale iron particles in porous media: a modeling approach*. Environmental Science & Technology 44 (23), pp. 9062-9068.

E-EMNM1D (Enhanced Micro-and Nanoparticle transport Model in porous media in 1D geometry) is the evolution of MNM1D, improved and extended for the simulation of the transport of highly concentrated, non-Newtonian suspensions of colloidal particles.

The model was developed for the 1D simulation of column tests performed with iron micro and nanoparticles used in groundwater remediation, in the framework of the EU research project Aquarehab (FP7 - Grant Agreement Nr. 226565).

The model takes into accounts attachment and detachment phenomena, following one or two interaction sites (linear, blocking, ripening, straining). Moreover, the non-Newtonian nature of carrier fluids usually employed to improve stability of iron particles, as well as clogging phenomena due to particle deposition, are simulated.

The model is implemented in a Matlab environment and provided in a encrypted version (.p files), that can be run on machines that have already installed the Matlab program.The model is implemented in a Matlab environment and provided in a encrypted version (.p files), that can be run on machines that have already installed the Matlab program.

Model equations

E-MNM1D solves the coupled set of particle differential equations and constitutive relationships reported below:

1. Colloid transport equations

The transport equations for the iron particles were modelled with a physico-chemical (interactions plus straining) advection-dispersion-deposition equation:

$$\begin{cases} \dfrac{\partial}{\partial t}(\varepsilon_m c)+\dfrac{\partial(\rho_b s_1)}{\partial t}+\dfrac{\partial(\rho_b s_2)}{\partial t}=-\dfrac{\partial}{\partial x}(q_m c)+\dfrac{\partial}{\partial x}\left(\varepsilon_m D\dfrac{\partial c}{\partial x}\right) \\ \dfrac{\partial(\rho_b s_1)}{\partial t}=\varepsilon_m k_{a,1}\left(1+A_1 s^{\beta_1}\right)c-\rho_b k_{d,1}s_1 \\ \dfrac{\partial(\rho_b s_2)}{\partial t}=\varepsilon_m k_{a,2}\left(1+\dfrac{x}{d_{50}}\right)^{\beta_2}c-\rho_b k_{d,2}s_2 \end{cases}$$

where ε_m is the porosity, D is the hydrodynamic dispersion, q_m is the darcyan velocity, c is the concentration of suspended particles, s is the concentration of deposited particles (expressed as mass of deposited particles per unit mass of the porous medium), $k_{a,i}$, $k_{d,i}$, β_i (i=1,2), and A_1, are the kinetic parameters of colloid deposition and release kinetics. The first equation represents the mass balance for the liquid phase, the second and third ones the mass balance for the solid phase, following, respectively, a blocking and a straining dynamics.

The form for attachment/detachment dynamics was formulated on purpose, that can be adapted to all commonly used interaction kinetics (linear attachment, blocking, ripening dynamics).

2. Darcy's law for Newtonian and non-Newtonian fluids

The "usual" form of Darcy's law was applied also for the case of non-Newtonian fluid, provided that the true pore fluid viscosity is replaced by the apparent viscosity μ_m, that includes all non-Newtonian effects:

$$\frac{\partial p}{\partial x}=-\frac{\mu_m}{K}q_m$$

The apparent viscosity is a function of both porous medium characteristics (permeability K and porosity ε_m) and fluid properties (via a modified Cross model, see below).

3. State equations and hydrodynamic parameters

The following parameters were considered functions of the concentration of deposed or suspended particles, and/or of polymer concentration:

- Porosity available for fluid flow. The pore space available for the fluid flow ε_m can be related to the concentration of deposed particles s: increasing concentration of deposed particles, the medium porosity decreases:

$$\varepsilon_m(s) = n - \frac{\rho_b}{\rho_s} s$$

  Being n the initial porosity (i.e. before the injection of the particles), ρ_b the bulk density of the porous medium, and ρ_s the bulk density of deposited particles.

- Viscosity of the pore fluid. Dynamic viscosity of polymeric solutions is known to be a function of shear rate, polymer concentration and particles concentration. The dependence on shear rate is described by a modified Cross model:

$$\mu_m(\dot{\gamma}_m, c, c_x) = \mu_{m,\infty} + \frac{M(c)c_x}{1 + [\lambda_m(c) \cdot \dot{\gamma}_m]^{\chi_m(c)}} \quad where \quad \dot{\gamma}_m(s) = \alpha_\gamma \frac{q_m}{\sqrt{K\varepsilon_m}}$$

  where M(c) is a function that can be derived from experimental data, and depends only on the concentration of suspended particles, $\lambda_m(c)$ and $\chi_m(c)$ are two parameters of the Cross model, both functions of c, and γ_m is the shear rate of the fluid in the porous medium.

- Permeability coefficient. Following Kozeny, the permeability of a porous medium depends on the third power of porosity, and on the square of the specific surface area of the matrix, through a constant. When colloids depose on the soil grains, the pore space available for the fluid flow decreases, and the specific surface area increases, thanks to a further contribution of deposed particles. Therefore, both contributions were considered and the permeability coefficient was obtained by their combined effects:

$$K(s) = K_0 \left(\frac{\varepsilon_m}{n} \right)^3 \left(\frac{a_0}{a_0 + \vartheta a_p \frac{\rho_b}{\rho_p} s} \right)^2$$

where K_0 is the clean bed permeability (corresponding to porosity n and specific surface area a_0), ϑ is the fraction of the surface area of the deposited particles a_p that contributes to the increase of the surface area of the matrix, and ρ_p is the density of the particles.

Coupling of flow and transport was solved under the hypothesis that clogging of the porous medium is not a repent process, thus handling the problem as a quasi-stationary phenomenon. The proposed formulation relies on the hypotheses of 1D horizontal quasi-stationary flow, constant discharge, negligible compressibility of particles, porous matrix, pore fluid and particles deposits. The structure of the coupling among the model equations is summarized in Figure 1.

The set of model equations was implemented in a finite-differences code, that represents the extension of the MNM1D model. The system is solved iteratively using a Picard's iteration scheme.

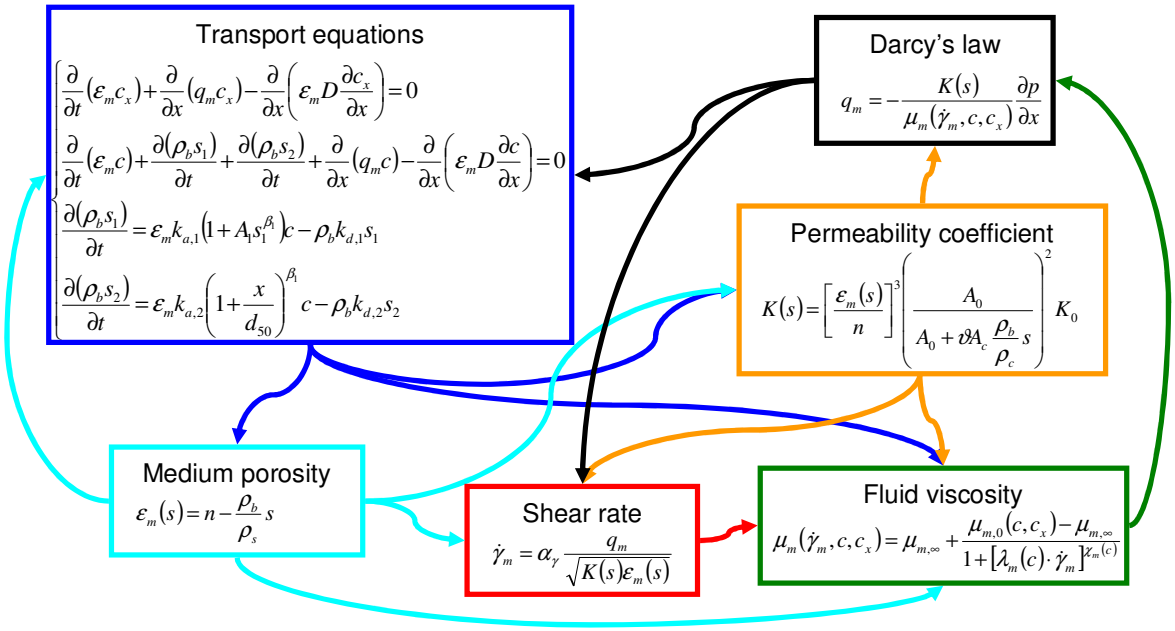

Figure 1: Scheme of the coupled model equations for micro- and nanoscale iron transport

The E-MNM1D code: running the model

The E-MNM1D code is provided as not compiled, encrypted .p Matlab files. Input and output are managed from an excel interface.

The code can be downloaded as a compressed archive. When extractive files, the .p codes have to be saved in the same folder. The excel file containing the model parameters and the results of the simulation can be renamed by the user, and can be saved in any folder.

Input/output is managed from the same Excel file (input in the first data sheet, output in the second one). All data concerning model and physical system parameters, and initial and boundary conditions are to be provided in the data sheet "Model and physical system".

The following sections are included in the Excel file:

- Basic data for the model (discretization, convergence criteria)
- Physical system (column geometry, porous medium and particles properties, flow data)
- Fluid properties (composition, density, rheological properties)
- Colloid parameters (clogging parameters, deposition and release kinetic models and parameters).
- Initial and boundary conditions for the transport problem

A short description of each required parameter and specific instructions on how to compile the data sheet are provided in the Excel file.

Output results are provided in the data sheet "output". Moreover, concentration breakthrough curves and pressure drop over time are plotted and saver in Matlab. Also the Matlab workspace is saved, named basing on the Excel file name, in the same folder.

For running a new simulation, follow these steps:

- open the excel file, insert your data, save and close the file

- open Matlab, run the main file in Matlab by typing the main file name, MAIN_FILE_EMNM1D.p

- when the simulation is finished, Matlab will re-open the excel file for you.