

MNM1D - Micro- and Nanoparticle transport Model in saturated porous media
Numerical solution of colloid trasport in 1D systems.
RELEASE: 0.9

Tiziana Tosco and Rajandrea Sethi (2008)
DITAG, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129, Torino, Italy
tiziana.tosco[at]polito.it, rajandrea.sethi[at]polito.it

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1. Governing equations

Transport of colloids is governed by advection-dispersion phenomena, and by particle-particle and particle-soil physico-chemical interactions (Kretzschmar et al., 1999). In some cases, other important interactions can play a significant role, eg. acid-base interactions, steric repulsions (in the presence of long-chain polymers adsorbed on the particle surface), and magnetic interactions (as in the case of iron nanoparticle suspensions used for groundwater remediation) (Viota et al., 2005; Saleh et al., 2008; Tiraferri and Sethi, 2008).

Colloidal particle transport in saturated porous systems is usually modeled using a modified advection-dispersion equation. It describes the dual-phase, non-equilibrium interactions between particles in the liquid (water) and solid (grains) phase. Colloid deposition on the grain surface is generally referred to as attachment, colloid release as detachment. Classical filtration theory CFT (also called clean-bed filtration theory) considers first-order attachment kinetics, while detachment is supposed to be negligible (Logan et al., 1995). However, this theory was shown not to be appropriate in many cases: non-linear kinetic attachment behaviors, namely blocking or ripening effects, are often observed, and cannot be described using the CFT (Privman et al., 1991; Adamczyk et al., 1994; Johnson and Elimelech, 1995; Ryan and Elimelech, 1996; Ko and Elimelech, 2000; Bradford et al., 2002; Tufenkji and Elimelech, 2005). Besides, one of the most relevant factors affecting particle mobility was shown to be the solution chemistry (Mcdowellboyer, 1992; Ryan and Gschwend, 1994a, b; NocitoGobel and Tobiasson, 1996; Roy and Dzombak, 1996). In this sense, advanced theories in modeling colloid release have been proposed by Grolimund et al. (Grolimund and Borkovec, 2001, 2006).

To date, several 1D forms of the model have been proposed, taking into account the various phenomena described above. However, all these models can be described by a general form of the modified advection-dispersion equation, which includes a general exchange term for the liquid-solid phase transfer:

$$\begin{cases} n \frac{\partial c}{\partial t} + \rho_b \frac{\partial s}{\partial t} = nD \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} \\ \rho_b \frac{\partial s}{\partial t} = f(c) \end{cases} \quad (1)$$

where c is the colloid number concentration in the liquid phase [L^{-3}], s is the number colloid concentration in the solid phase [L^{-3}], ρ_b is the bulk density of the solid matrix [$M L^{-3}$], D is the

hydrodynamic dispersion coefficient [$L^2 T^{-1}$], v is the darcyan velocity [$L T^{-1}$], and n is the porosity of the packed bed [-].

The generic non-equilibrium exchange term $f(c)$ describes the mass transfer between solid and liquid phase, and can be designed in several forms, according to the mechanisms that have to be modeled. In particular, if a linear exchange term is hypothesized, $f(c)$ becomes:

$$f(c) = nk_a c - \rho_b k_d s \quad (2)$$

where k_a is the attachment coefficient [T^{-1}], and k_d is the detachment coefficient [T^{-1}]. On the other hand, when blocking phenomena occur, i.e. when the colloid concentration in the solid phase is limited to a fixed value s_{max} , $f(c)$ is expressed as

$$f(c) = nk_a \left(1 - \frac{s}{s_{max}} \right) c - \rho_b k_d s \quad (3)$$

If the collector grains, i.e. the porous matrix, is homogeneous, only one interaction site type is included in the model. On the contrary, if the solid matrix is supposed to be heterogeneous for the affinity to colloidal particles, two or more interaction site types can be modeled, leading to

$$f(c) = \frac{\partial s_1}{\partial t} + \frac{\partial s_2}{\partial t} + \dots \quad (4)$$

Finally, if the influence of hydrochemical parameters, i.e. ionic strength, is to be included into the model, the partial differential equations for colloid transport are to be coupled with the advection-dispersion equation for a conservative tracer, that allows simulating transients of salt concentration. Attachment/detachment coefficients can then be tied to the tracer concentration. Empirical functions, based on laboratory results and theoretical considerations, have been proposed by the authors of this paper in order to state a functional relationship between ionic strength and attachment, detachment and blocking coefficients (Tosco et al., 2009).

The MNM1D code here described solves the colloid transport problem in transient ionic strength conditions, considering two interaction sites (site S_1 , with blocking, and site S_2 , with a linear attachment model). Consequently, equation (1) becomes

$$\left\{ \begin{array}{l} n \frac{\partial c_t}{\partial t} = nD \frac{\partial^2 c_t}{\partial x^2} - v \frac{\partial c_t}{\partial x} \\ n \frac{\partial c}{\partial t} + \rho_b \frac{\partial s_1}{\partial t} + \rho_b \frac{\partial s_2}{\partial t} = nD \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} \\ \rho_b \frac{\partial s_1}{\partial t} = n \left(1 - \frac{s_1}{s_{\max,1}(c_t)} \right) k_{a,1}(c_t) c - \rho_b k_{d,1}(c_t) s_1 \\ \rho_b \frac{\partial s_2}{\partial t} = n k_{a,2}(c_t) c - \rho_b k_{d,2}(c_t) s_2 \end{array} \right. \quad (5)$$

where c_t is the conservative salt concentration [$M L^{-3}$], s_1 is the particle concentration on solid phase [L^{-3}] for blocking sites of type 1 (reversible attachment with blocking), $s_{\max,1}(c_t)$ is the maximum particle concentration for sites 1 and depends on the salt concentration, $k_{a,1}(c_t)$ and $k_{d,1}(c_t)$ are the coefficients for sites 1, s_2 is the particle concentration on solid phase [L^{-3}] for linear sites of type 2, and $k_{a,2}(c_t)$ and $k_{d,2}(c_t)$ are the corresponding coefficients.

2. Model implementation

The model equation (5), coupled with the functional relationships reported in (Tosco et al., 2009), was implemented in a Matlab environment using a finite-differences model. The Euler implicit scheme was employed for time derivatives:

$$n \frac{\partial c}{\partial t} \cong \frac{n}{\Delta t} (c_j^{n+1} - c_j^n) \quad (6)$$

where k is the index for the time step, and j is the index for the space discretization nodes.

Both upwind and central-in-space schemes were implemented for space derivatives, giving the user the possibility of choosing the most suitable solution technique for the transport problem to be simulated:

$$\left\{ \begin{array}{l} nD \frac{\partial^2 c}{\partial x^2} \cong \frac{nD}{\Delta x^2} (c_{j+1}^{n+1} - 2c_j^{n+1} + c_{j-1}^{n+1}) \\ nv \frac{\partial c}{\partial x} \cong \frac{nv}{\Delta x} [\gamma c_{j+1}^{n+1} + (1-2\gamma)c_j^{n+1} - (1-\gamma)c_{j-1}^{n+1}] \end{array} \right. \quad (7)$$

where $\gamma = 0.5$ for the central-in-space scheme, and $\gamma = 1$ for the upwind scheme.

As the problem is non linear, due to the presence of the blocking function in the exchange term for interaction site of type 1, the model implements a Picard iterative scheme. Controls were introduced to avoid numerical oscillations.

The model can be used for direct problems. An application of the MNM1D code for the solution of the inverse problem (at the moment, not available for download) was presented by the authors (Tosco et al., 2009), where it was applied for fitting a set of laboratory tests run in transient ionic strength conditions. In that case, both interaction sites were considered to be active, but the code allows to inactivate one of them when the solid matrix can be considered homogeneous.

3. The MNM1D code: running the model

The MNM1D code is provided as a group of encrypted p-files that are to be run in Matlab. Input and output are managed from an excel interface.

The code release R0.9 is for direct simulations, and can be run on every release of Matlab. In case of very old releases, some problems could be found with functions that were not yet implemented in them.

The code can be downloaded as a compressed archive. When extracting files, the p-files are to be saved in the same direction. The excel file containing the model parameters and the results of the simulation can be renamed by the user, and can be saved anywhere desired. Code files are MAIN_FILE_R0_9.p, colloid_peaks.p, and colloid_fitting_constant_I.p.

Before running MNM1D, open the excel input/output file, insert your data in the input folder following the instructions reported in details near each parameter, and save it. It is suggested you close the excel file before running MNM1D, as otherwise you will be asked by Excel to save it a number of times at the end of the simulation (when MNM1D writes the output). Do not change the structure of the excel file.

When all parameters are defined, open Matlab, choose the directory where you saved the code files, and type MAIN_FILE_R0_9 to run the code (you will not be able to see and open the code files in Matlab, as they are saved in the p-file encrypted format). You will then be asked to chose your data xls file. At the end of the simulation, MNM1D saves the output in the second folder of your xls document.

The model run can take few seconds up to a minute, according to your CPU and complexity of the simulation.

4. Bibliography

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