MNMs - Micro- and Nanoparticles transport, filtration and clogging Model - Suite

A comprehensive tool for design and interpretation of colloidal particle transport in 1D Cartesian and 1D radial systems

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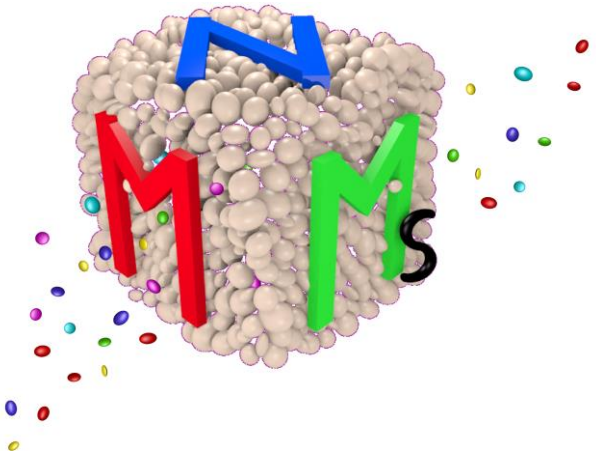
TUTORIAL



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1 Purpose of the tutorial

The purpose of this tutorial is to introduce new users of the software package MNMs 2018 to its functionalities. Several examples are given to familiarize with the major sections and modules of MNMs, and with the main concepts and procedures of pre-processing and post-processing (e.g., domain design, finite differences discretization, specification of initial and boundary conditions, data-fitting procedures, and graphical visualization of the results). In the following, after a brief presentation about the colloidal transport and the code structure, guided exercises are proposed for:

- Calculation of DLVO and extended DLVO interaction profiles
- Solute transport in 1D
- Particle transport in 1D
- Radial injection of colloidal shear thinning suspensions

2 Introduction to MNMs

MNMs (*Micro- and Nanoparticles transport, filtration and clogging Model - Suite*) is a numerical tool, developed in a Matlab environment, for the analysis of laboratory column transport tests, in saturated conditions, for colloidal particles and solutes. It represents the evolution of MNM1D (https://areeweb.polito.it/ricerca/groundwater/software/mnm1d/) and E-MNM1D (https://areeweb.polito.it/ricerca/groundwater/emnm1d/), whose features are here merged into one software.

The major tools available in **MNMs 2018** include:

- **Calculation of particle-particle and particle-collector interaction energy profiles using the DLVO (Derjaguin and Landau, Verwey and Overbeek) and extended DLVO theory.** This tool can be used to foresee the micro- and nanoparticles behavior in terms of aggregation and expected mobility.
- **Calculation of single-collector efficiency** using several correlations reported in the literature, accounting for concomitant transport mechanisms (i.e. advection, gravity and Brownian motion) and for finite size of the particles (steric effect).
- **Simulation of the transport in 1D saturated porous media of conservative solutes** (i.e. subject to advection and dispersion phenomena) **and reactive solutes** (advection, dispersion, equilibrium adsorption, first order degradation). Numerical and analytical solutions are available.
- **Simulation of the transport of colloidal particles in 1D saturated porous media**. Two concurrent interaction sites are available to simulate reversible and irreversible particle deposition following linear, blocking, ripening or straining kinetics. Particle transport simulation can be performed accounting for transients in ionic strength, and porous medium clogging, when the modification of the column porosity and permeability due to deposition of colloidal particles strongly influences the flow field. In this case, MNMs takes into account the variation of pressure drop along the column due to the medium clogging and solves the differential system coupling flow and transport equations.
- **Simulation of the transport of concentrated particle suspensions in radial coordinates.** Transport and flow equations are solved in radial geometry accounting for attachment and detachment dependency on pore fluid velocity and viscosity. The model equations can account also for the non-Newtonian (shear thinning) rheological properties of the dispersant fluid and the porous medium

clogging associated with filtration and sedimentation in the porous medium of both particles and polymeric residual undissolved particles.

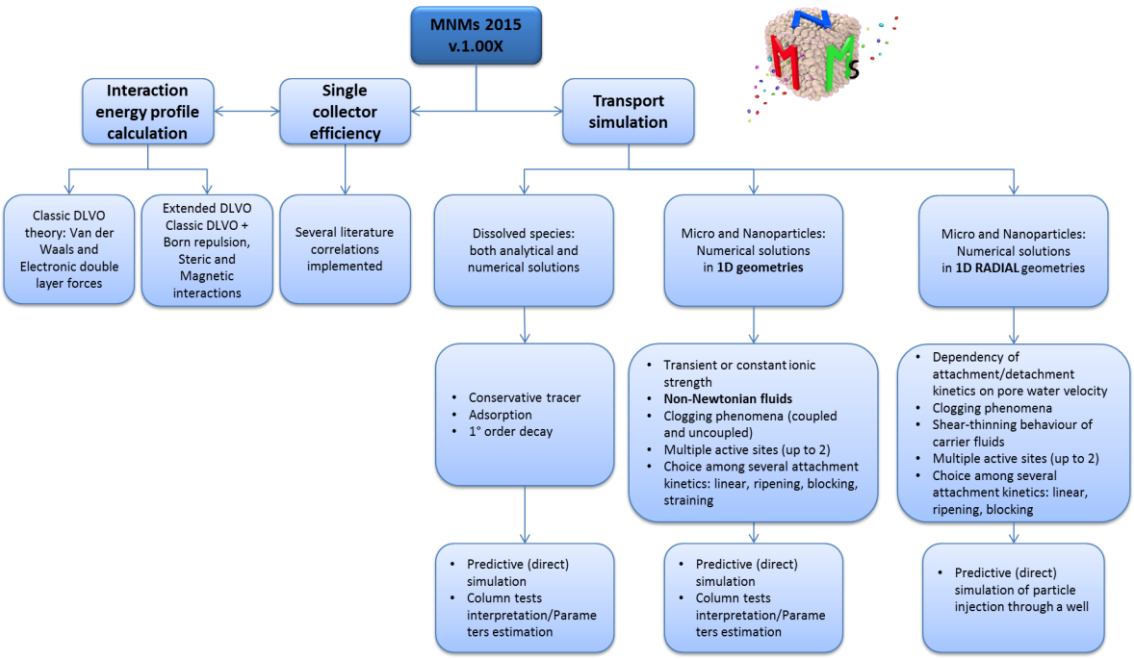

Figure 2-1: Tools included in MNMs 2018

2.1 Particle transport equations in 1D

The transport of particles is governed by advection-dispersion phenomena and by particle-particle and particle-soil physicochemical interactions. Mathematically, colloidal particles transport in saturated porous systems is usually modeled using a modified advection-dispersion equation, which accounts for non-equilibrium interactions between particles in the liquid (water) and solid (grains)phase [Tosco, Tiraferri et al., 2009]:

$$\begin{cases} \varepsilon \dfrac{\partial c}{\partial t} + \rho_b \dfrac{\partial s}{\partial t} + q_i \dfrac{\partial c}{\partial x_i} - \varepsilon D_{ij} \dfrac{\partial^2 c}{\partial x_i^2} = 0 \\ \rho_b \dfrac{\partial s}{\partial t} = f(c, s) \end{cases} \quad \textbf{(2.1)}$$

where:

ε = The porosity of the medium [-]

q_i = The Darcy's velocity [L T^{-1}]

c =The particle concentration in the mobile phase [M L^{-3}]

s = The particle concentration in the solid phase [-]

Dij =The dispersion coefficient [L^2 T^{-1}]

ρ_b = The bulk density of the solid matrix [M L^{-3}]

The first equation represents the mass balance for the particles suspended in the liquid phase. The second equation represents the mass balance for the particles attached on the solid phase, here expressed as a generic non-equilibrium exchange term that can designed in several forms, according to the mechanisms to be modelled (i.e. clean bed, blocking, ripening, etc.). Particle deposition onto the grain surface is generally

referred to as attachment, particle release as detachment. If the solid matrix is supposed to be heterogeneous regarding the affinity to colloidal particles, or different interaction mechanisms (e.g. chemical interaction and physical filtration) are considered, the function can be seen as the sum of two or more terms, one for each interaction sites that has to be modelled [Tosco and Sethi, 2009]:

$$f(c,s) = \rho \frac{\partial s_1}{\partial t} + \rho \frac{\partial s_2}{\partial t} + \ldots \qquad \textbf{(2.2)}$$

2.2 The interface

At the first run, MNMs 2018 shows an empty window with MNMs' logo. The first interaction of the user with the interface is carried out by means of the *File* menu where the user can choose the type of simulation to run: DLVO calculation, single-collector efficiency, or transport simulation (solute or particles). Once the user has selected the type of simulation, the window will be divided into two parts: the right side of the MNMs' interface is always left for output results visualization, whereas all the user-code interactions are carried out in the left side.

An overview of the interface for the three type of simulations is reported in Figure 2-2, Figure 2-3 and Figure 2-4.

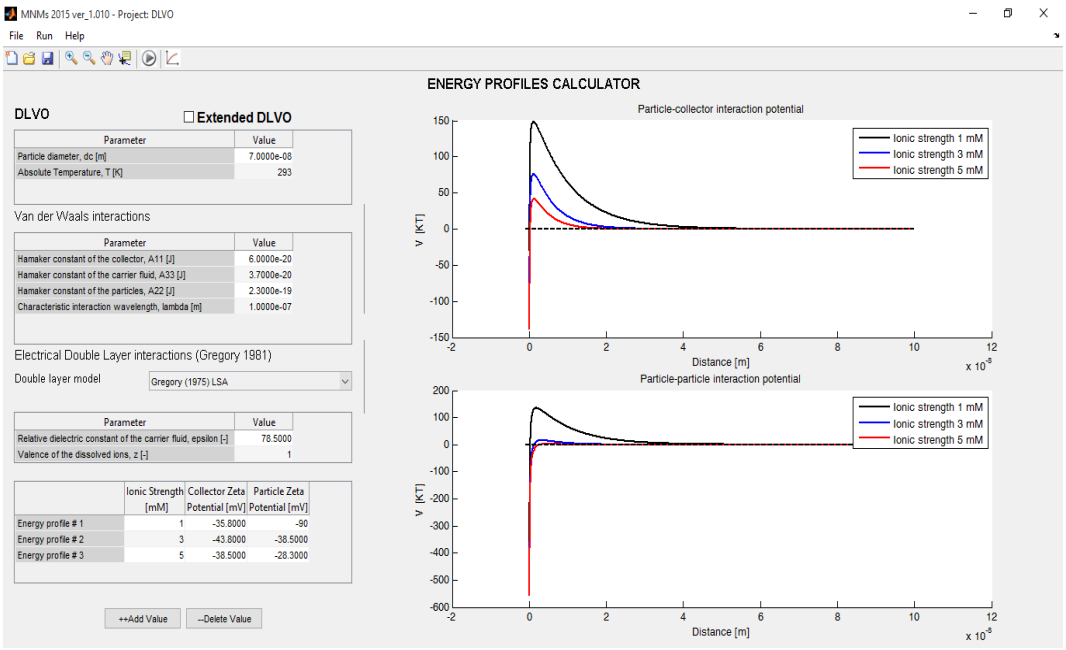

Figure 2-2: Screenshot of the DLVO calculation tool in MNMs.

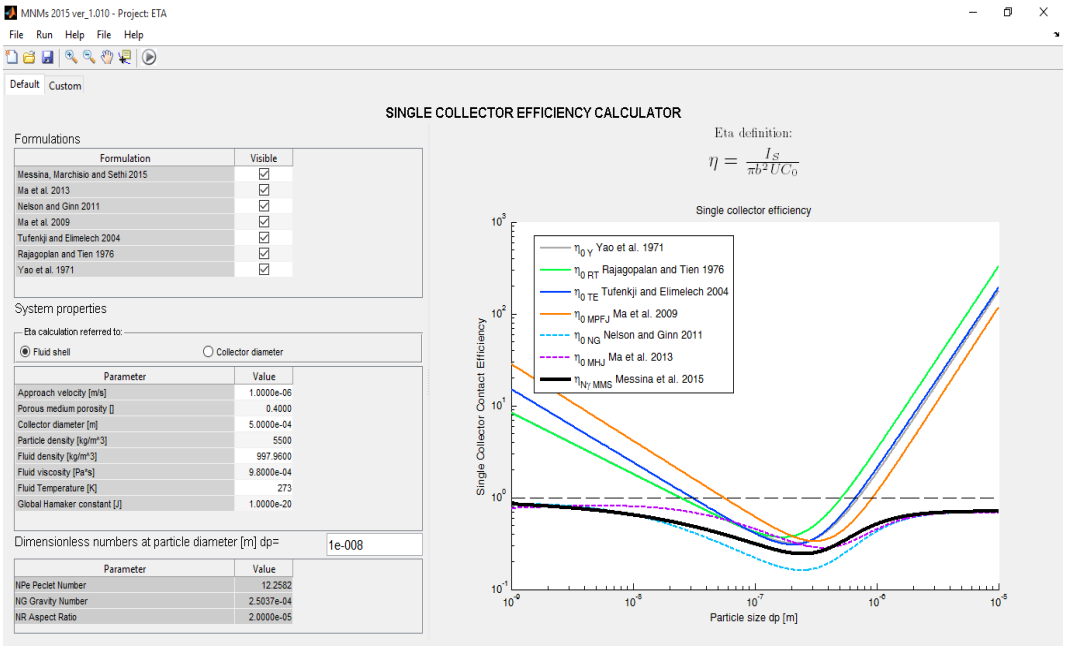

Figure 2-3: Screenshot of the single collector efficiency tool in MNMs.

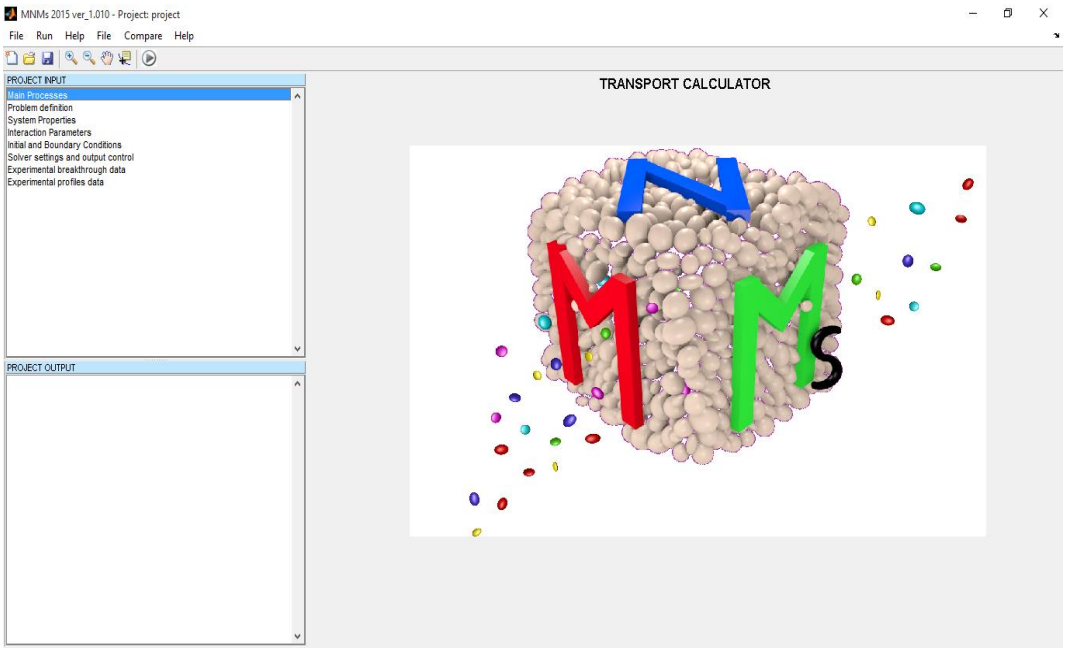

Figure 2-4: Screenshot of the main window of a transport simulation in MNMs.

3 DLVO and extended DLVO

This example refers to carboxylate-modified latex beads (60 nm) dispersed in water at three values of NaCl concentration (0.1, 10 and 100 mM). The porous medium is Quarts sand.
The zeta potential (Zetasizer Nano ZSP, Malvern) of the Quartz sand, measured at 22°C, at NaCl 0.1, 10 and 100 mM is equal to -35.8 mV, -25.2 mV, -22.2 mV, respectively.
The zeta potential (Zetasizer Nano ZSP, Malvern) of latex particles measured at 22°C, at NaCl 0.1, 10 and 100 mM is equal to -60.0 mV, -58.3 mV, -42.2 mV, respectively.
The following values for the Hamaker constant of the three materials (sand, water and latex particle) have been obtained from the literature:

- Sand $6.0 \cdot 10^{-20}$ J
- Water $3.7 \cdot 10^{-20}$ J
- Latex $4.2 \cdot 10^{-19}$ J

The default value of the characteristic interaction wavelength is provided equal to $1 \cdot 10^{-7}$ m (literature).

3.1 DLVO

- Open MNMs.
- The standard MNMs main window will be opened.
- Begin a new project clicking on the new project icon  in the toolbar. You are asked to choose which kind of project he wants to start. Click on *DLVO project*. Alternatively, go in the ***File*** menu and choose ***New…→DLVO project***.
- A standard dialog box for retrieving files will be opened. Choose the destination folder and the name of the project (e.g. DLVO in this case), then click ***Save***.
- The DLVO window will appear with a standard set of parameters and DLVO energy profiles.

Now you can calculate the DLVO interaction profiles for latex beads dispersed in water:

- Insert the data reported above.
- Press the "play" button in the toolbar or press “F5” on your keyboard to run the simulation. You will get the result reported in Figure 3-1. You can click on the figures to adjust the axes limits.

✓ **N.B.:** Do not forget to save your project!

3.2 Extended DLVO

By selecting the "**Extended DLVO**" option, Born repulsion, steric interaction and magnetic interaction are added to the classical DLVO interactions.

- Assume that our particles are now covered by a shell of a biopolymer (molecular weight 65000 g/mol, density 1.04 g/cm^3, thickness of the brush layer 150 nm). Keep default value for the other parameters.
- Run again the simulation (play button or F5 key), you will get the result reported in Figure 3-2.

Run again the calculation for iron particles with the following properties:

- Diameter 70 nm
- Hamaker constant $2.3 \cdot 10^{-19}$ J
- Zeta potential at 22°C, -38.2 mV, -35.5 mV, -28.0 mV at NaCl 0.1, 10 and 100 mM.

- Saturation magnetization 564.7 kA/m

- Calculate the extended DLVO with magnetic interaction, without (bare particles) and with (sterically stabilized particles) polymer adsorbed on the particles.

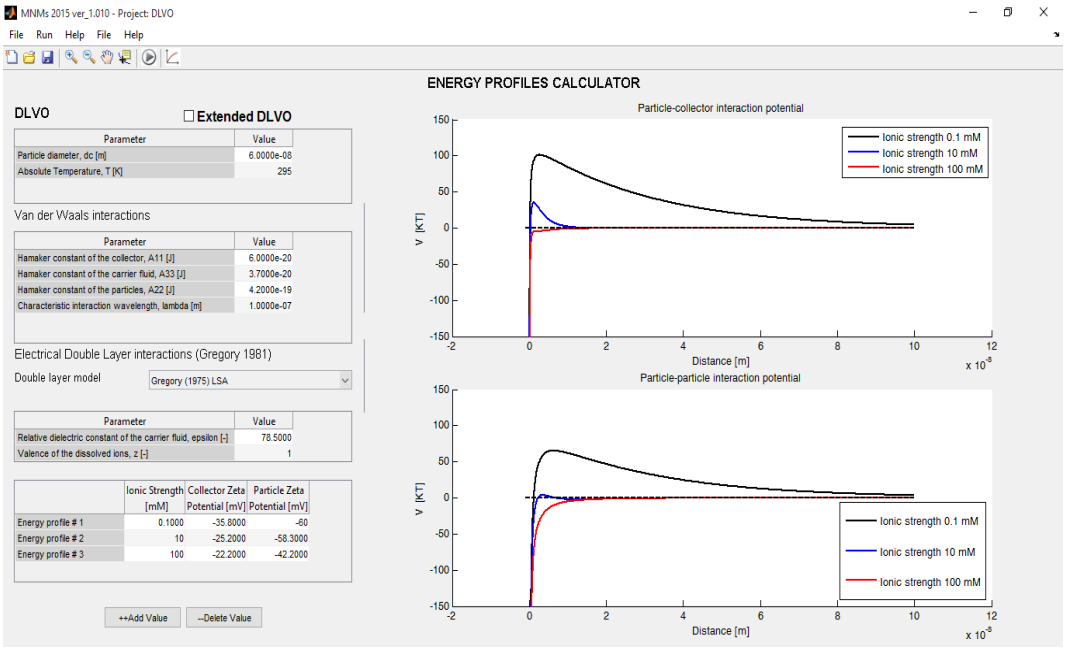

Figure 3-1: DLVO calculation for latex beads.

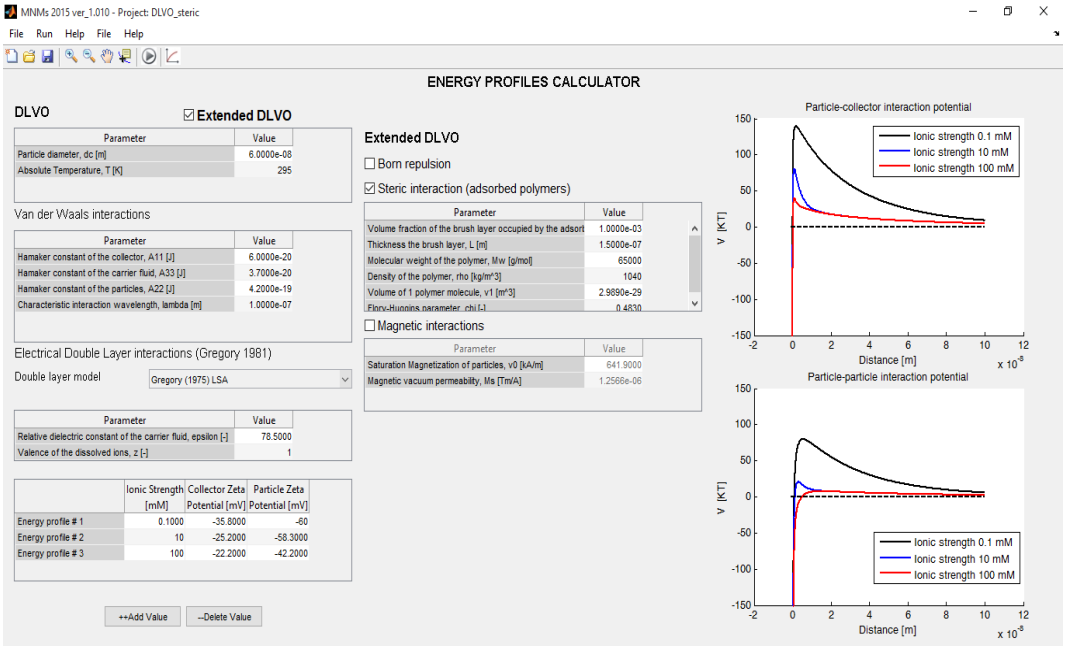

Figure 3-2: extended DLVO calculation for latex beads (steric repulsion).

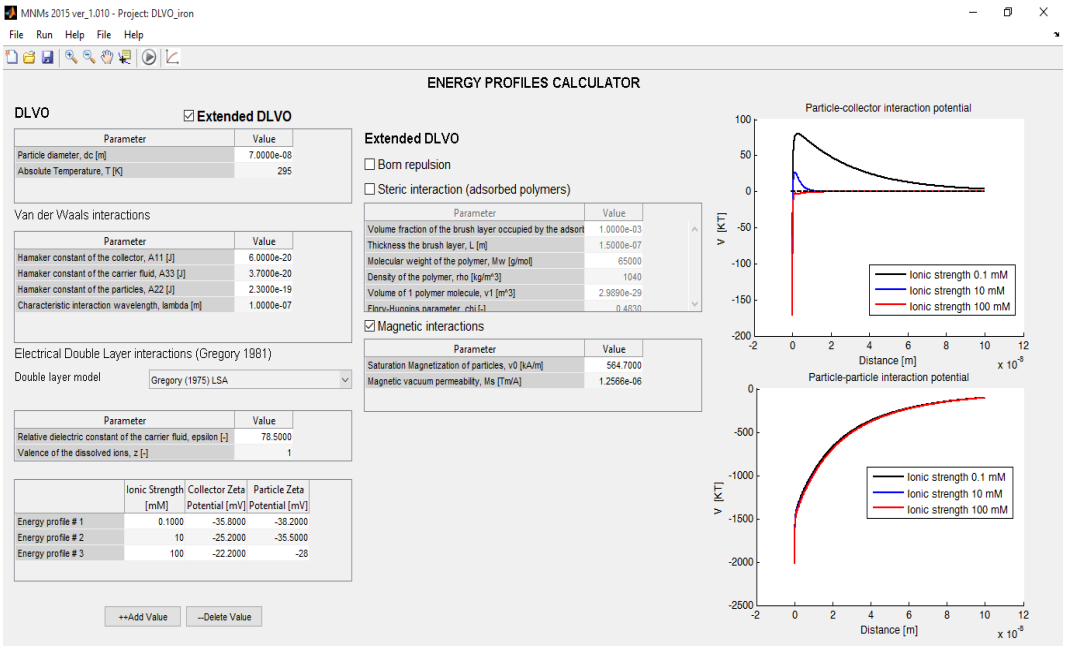

Figure 3-3: extended DLVO calculation for iron nanoparticles without steric stabilization.

4 Solute transport test

4.1 Direct (predictive) simulation of a tracer test

This example presents the direct problem (predictive simulation) of tracer transport into a 50 cm long sand column having a radius of 1 cm, filled with quartz sand with density of the bulk of 2650 kg/m^3. The injection discharge is constant during the whole simulation and is equal to $1 \cdot 10^{-7}$ m^3/s. The sand bed has an effective porosity of 0.25 and a dispersivity equal to 0.002 m.

The injection protocol involves two stress periods. The first one is free of salt and is 1000 s long and represents the column pre-conditioning, the second one is the injection of salt (C_0 = 1e-3 kg/m^3) and is 1500 s long.

4.1.1 Building the model

- Open MNMs.
- Begin a new project clicking on the new project icon  in the toolbar. Click on ***Transport simulation***. Alternatively, go in the *File* menu and choose ***New…→Transport* simulation**.
- A standard dialog box for retrieving files is opened. Choose the destination folder and the name of the project (e.g. tracer_direct in this case), then click ***Save***.
- The transport simulation window is opened. In the left side of the window two list-boxes contain all the input options (upper box) and the list of simulation output (lower box) if already available. The latter is always empty in case of new project.
- Into the ***PROJECT* INPUT** box, double click on the ***Main Processes*** line to open the first window for model input data.

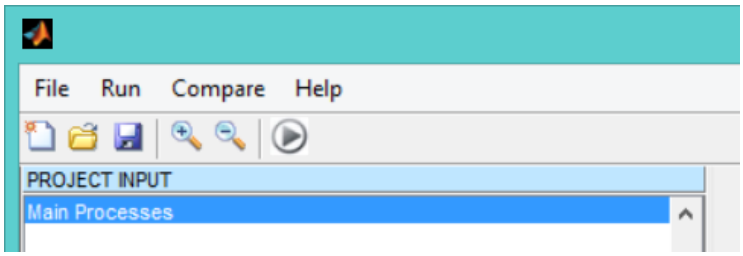

Figure 4-1: PROJECT INPUT list-box. Double click on the Main Processes item.

- The ***Main Processes*** (Figure 4-2) selection window will show. Choose **Solute transport-Analytical solution** from the radio button and click *Next*.

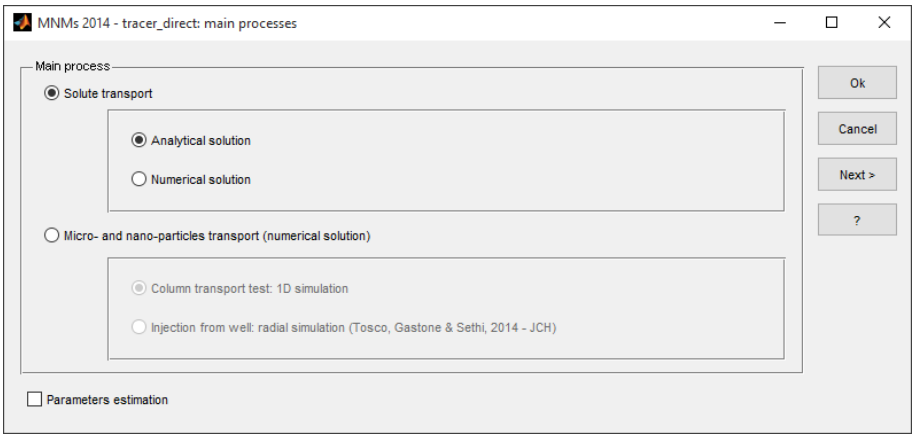

Figure 4-2: Main Processes selection window.

- Set the ***System Properties*** as specified in description of the example model (Figure 4-3) and click Next.
- Keep any value in the ***Interaction parameters*** window (you are assuming a tracer species, with no interaction with the soil nor degradation) (Figure 4-4).
- In the ***Initial and boundary conditions*** menu set the initial condition equal to 0 (no tracer in the column at the beginning of the test) (Figure 4-5).
- Click the ***Add*** *stress period* button and set the duration and tracer concentration according to Table 5-1 (Figure 4-5). Click **Ok**.
- Click ***Next***. In this window you can choose between first type (Dirichlet) or third type (Robin) boundary condition and choose the time and space display settings. Choose a Dirichlet boundary condition and click ***Ok***.

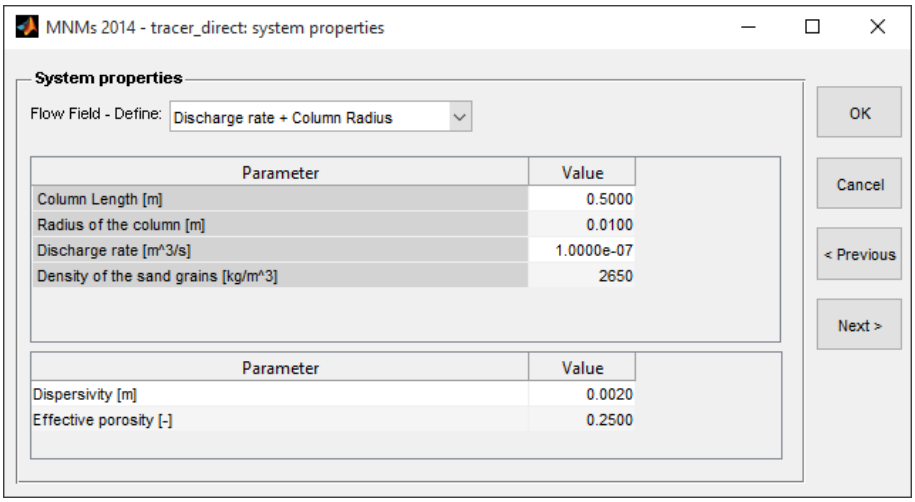

Figure 4-3: System properties menu.

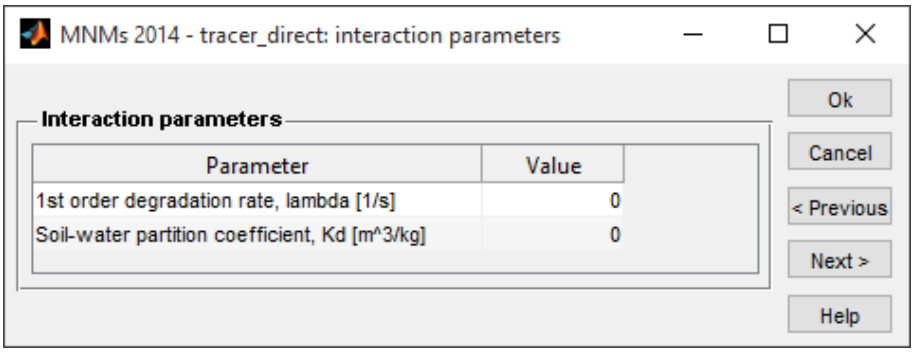

Figure 4-4: Interaction parameters menu.

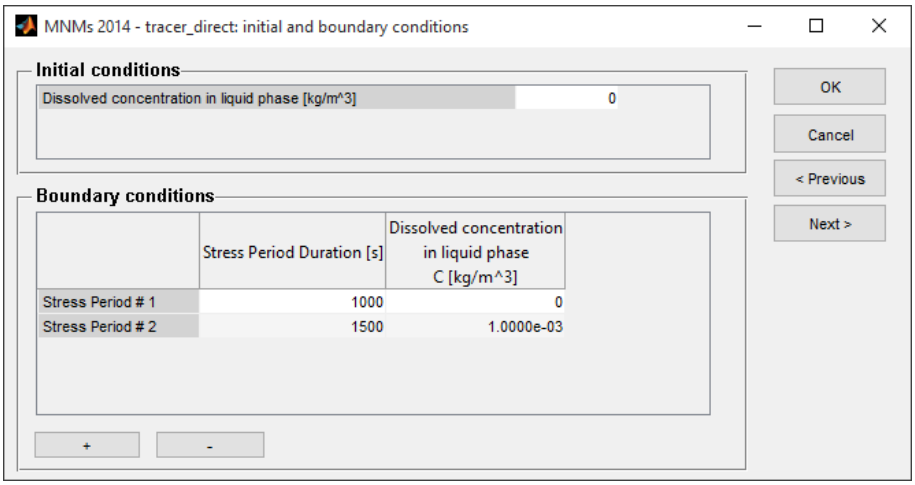

Figure 4-5: Initial and boundary conditions menu.

4.1.2 Save and run

- Save the project clicking on the save project icon in the toolbar or selecting *Save* from the ***File*** menu (only for licensed versions).
- Run the model clicking on the run project icon in the toolbar or selecting ***Run simulation*** from the ***Run*** menu or pressing "F5" on your keyboard.

✓ The model run can take few seconds up to a minute.

4.1.3 Visualize the results

The breakthrough curve of the tracer is automatically displayed in a plot in the right side of the main window (Figure 4-6). The ***PROJECT OUTPUT*** table is updated, showing the list of the available output, which are, in this case the breakthrough curve, the profile of dissolved concentration and the mass balance information.

- Save again the project to save the simulation results.
- Click on the graph to modify the axis scale, limits labels and display the grid on the graph.
- You can double click on the output items to visualize them in a separated window.

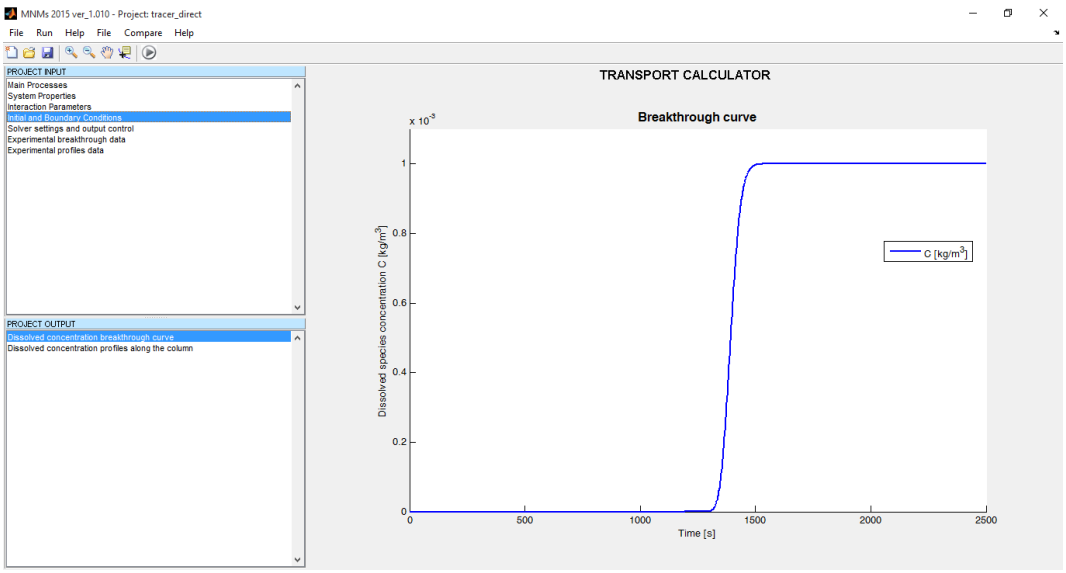

Figure 4-6: breakthrough curve.

4.2 Direct (predictive) simulation of a reactive solute transport test

- Use the same abovementioned model to run the simulation for dissolved species with a first order degradation rate of $5 \cdot 10^{-4}$ s^{-1}, run the model and save the results (in a new project file).
- Then run the same simulation for a sorbing contaminant with a soil-water partition coefficient equal to $1 \cdot 10^{-4}$ m^3/kg. Run the model and save the results (in a new project file).
- Compare the three simulations using the function "***Compare***":
    - Click on ***Compare*** → ***Breakthrough curves*** menu. The **compare simulations** window opens.
    - Click the **++ Add curve** button and select the project file of the tracer and degradation simulation.
    - All three breakthrough curves will appear on the graph for an easy comparison.

4.3 Laboratory test interpretation (inverse simulation) of a tracer test

This example presents the inverse problem (interpretation of laboratory experimental data) of a tracer transport test.

In this case we will consider an 11.5 cm long column, with inner radius 8 mm, filled with quartz sand with density of 2650 kg/m^3 and average sand grain equal to 0.4 mm. The injection discharge is $1.58 \cdot 10^{-8}$ m^3/s and is constant during the whole simulation. The clean bed porosity and the dispersivity will be determined from fitting of the experimental breakthrough curve, which is provided.

The test protocol involves a pre-flushing (tracer concentration $C_0 = 0$) of 610 s, followed by a tracer injection of 1830 s ($C_0 = 1 \cdot 10^{-3}$ kg/m^3) and a post-flushing of 3550 s ($C_0 = 0$).

4.3.1 Building the model

- Open MNMs.
- Begin a new project clicking on the new project icon  in the toolbar. Click on *Transport simulation*. Alternatively, go in the ***File*** menu and choose ***New…*** → ***Transport* simulation**.
- A standard dialog box to retrieve files is opened. Choose the destination folder and the name of the project (e.g. *tracer_inverse* in this case), then click ***Save***.

- Into the *PROJECT* INPUT box, click on the ***Main Processes*** line to open the first window for model input data.
- The ***Main Processes*** selection window is opened. Choose **Solute transport-Analytical solution** from the radio button. Select the thick on the Parameters Estimation option and click ***Next.***

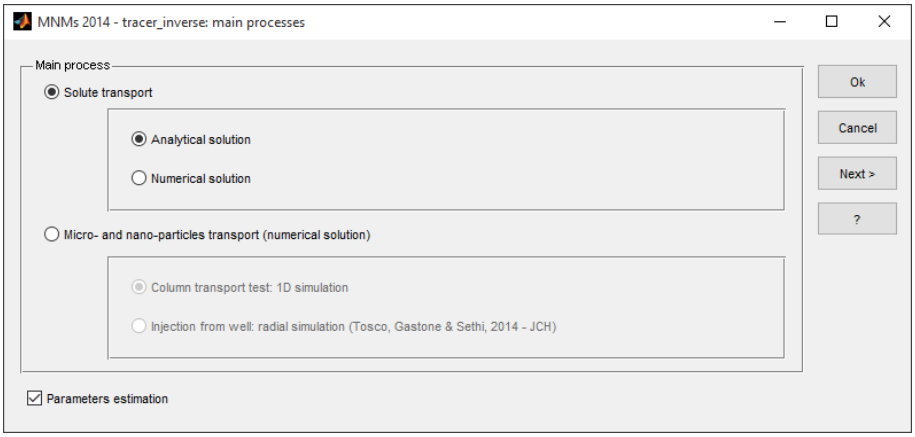

Figure 4-7: Main Processes selection window.

- Set the ***System Properties*** as specified in description of the example model (Figure 4-8) and click ***Next***. This window is similar to the one of the direct mode simulations, except for the last part, where the parameters to be fitted are reported (porosity and dispersivity). Here you can select which parameter(s) is to be fitted, which is the initial guess of the parameter and the variation range (lower and upper boundaries). All these parameters can be modified by the user. For column tests, to use the average size of sand grains (in this case, 0.4 mm) as the initial value for dispersivity.

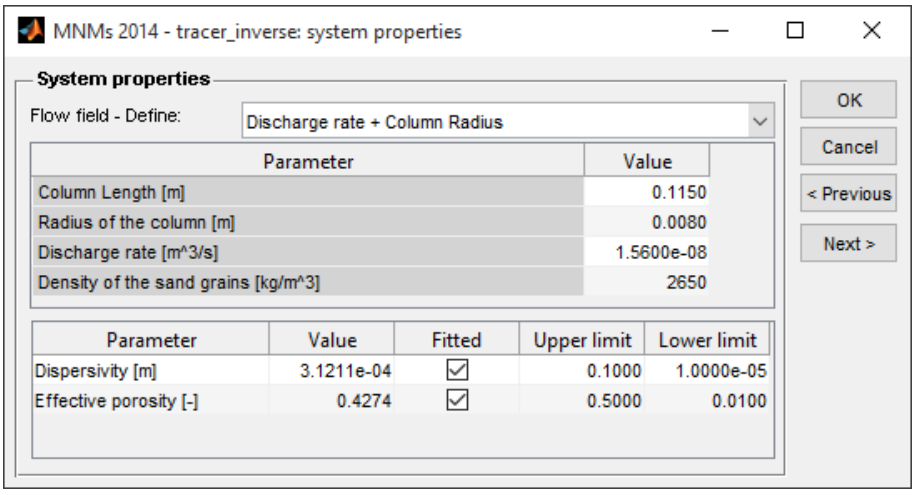

Figure 4-8: System properties menu.

- Do not enter parameters for degradation and sorption, instead click ***Next***.
- In the ***Initial and boundary conditions*** menu set the initial condition equal to 0 (no tracer in the column at the beginning of the test) (Figure 4-9).
- Click the ***Add stress period*** button and set the duration and salt concentration. Click ***Next***.

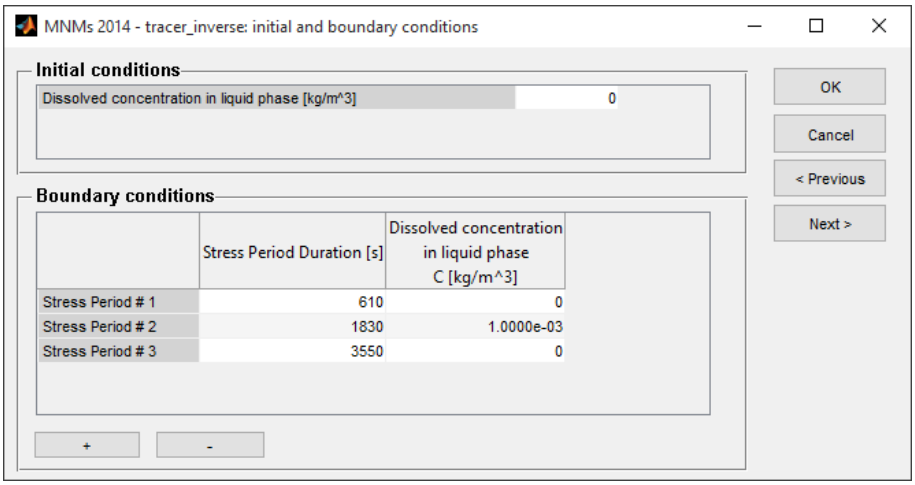

Figure 4-9: Initial and boundary conditions menu.

- In this window you can choose between first type (Dirichlet) or third type (Robin) boundary condition and choose the time and space display settings. Choose a Dirichlet boundary condition and click ***Next***.
- The window for the ***Experimental data*** will appear (Figure 4-10). Experimental data can be uploaded from an external text file (*tracer_inv_data.txt* in our test) clicking on the button ***Import Data***. Click ***Ok***.

4.3.2 Save and run

- Save your file.
- Press ***Run*** *or* F5 key on your keyboard.
- A bar will show the progress of the code. In the end, the fitted curve is displayed along with the fitted coefficients (Figure 4-11).

✓ **N.B.:** If the inversion function doesn't converge to an acceptable solution, check and adjust the initial guess values. It is suggested to carry out a ***Manual calibration*** before run the inverse simulation in order to get reliable initial guesses.

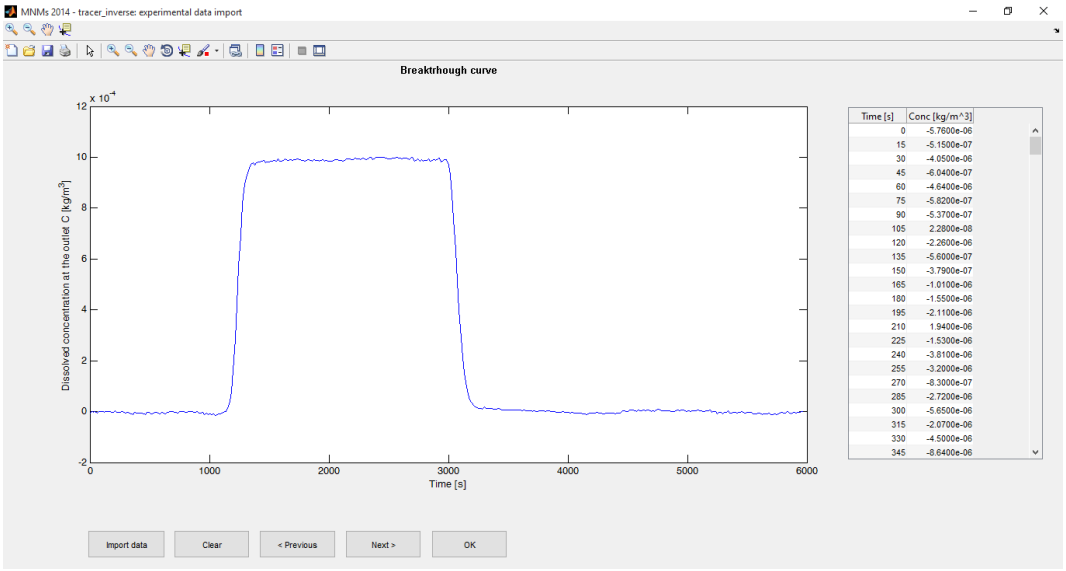

Figure 4-10: Experimental data uploading.

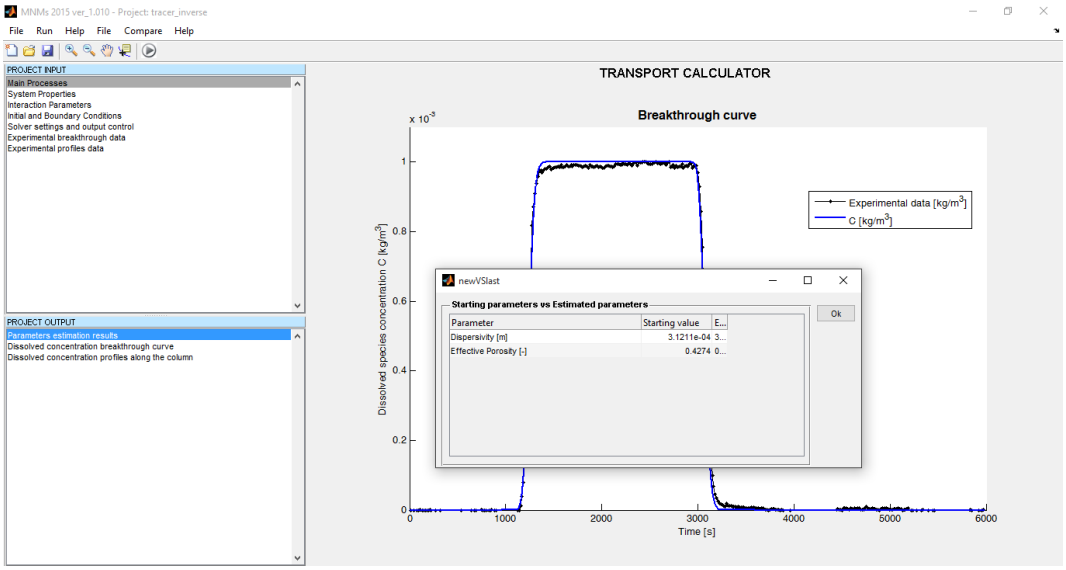

Figure 4-11: Inverse model results.

4.3.3 Visualize the results

- You can explore the functionalities of the ***PROJECT OUTPUT*** menu and of the Manual calibration tool (***Run/Manual calibration***).

5 Particle transport simulation

Simulate 1D transport of a stable dispersion of ferrihydrite (Feh) nanoparticles. At the pore scale, particle mobility is controlled by physicochemical interactions among particles and porous medium, which result in dynamic deposition and release phenomena. Column transport tests of injection of ferrihydrite nanoparticles through saturated sand-packed columns at concentrations used in field applications is simulated and interpreted in the following.

The system is composed by a 0.113 m long column having an inner diameter of 16 mm. The column is filled with quartz sand having an average effective porosity of 0.464, an average dispersivity of $2.82 \cdot 10^{-4}$ m and density of sand grains equal to 2650 kg/m^3.

During the whole simulation, a constant discharge equal to $1.56 \cdot 10^{-8}$ m^3/s is applied to the column inlet, resulting in a pore volume time of approximately 680 s.

The simulation is 7800 s long. The injection protocol involves three stress periods. The first one, almost 1 PV long, is free of Feh particles and is necessary for the column pre-conditioning. The nanoparticles are then injected for 1 h and then again the column is flushed with particles-free water. Ionic strength of water is maintained at the constant value of 1mM during the whole duration of the simulation. The injection protocol is shown in Table 5-1.

Table 5-1: Injection protocol.

	Duration	Input particle concentration	Input ionic strength
Stress period	(s)	(kg/m^3)	(mM)
1st	600	0	1
2nd	3600	$7.5 \cdot 10^{-3}$	1
3rd	3900	0	1

In a range of ionic strength values between 1 and 5 mM, Feh particles exchange between liquid and solid phase can be described with good approximation by an attachment-detachment kinetics with a Langmuirian blocking function. Therefore, in the example model only one active site will be used to simulate the ferrihydrite transport.

5.1 Direct Simulation

Working in Direct Mode, it is possible to calculate the breakthrough curves of the Feh at the column outlet and the concentration profiles of the deposited particles at the end of each stress period.

5.1.1 Building the model

- Open MNMs.
- Begin a new project clicking on the new project icon  in the toolbar. Click on ***Transport simulation***. Alternatively, go in the ***File*** menu and choose ***New…→Transport simulation***.
- A standard dialog box to retrieve files is opened. Choose the destination folder and the name of the project (e.g. Feh_direct in this case), then click ***Save***. If an existing file name is selected, the previous file will be overwritten after user's confirmation.
- Into the ***PROJECT INPUT*** box, click on the ***Main Processes*** line to open the first window for model input data.

- The ***Main Processes*** (Figure 5-1) selection window will be opened. Choose **Micro- and nano-particles transport** from the radio button and click ***Next***.

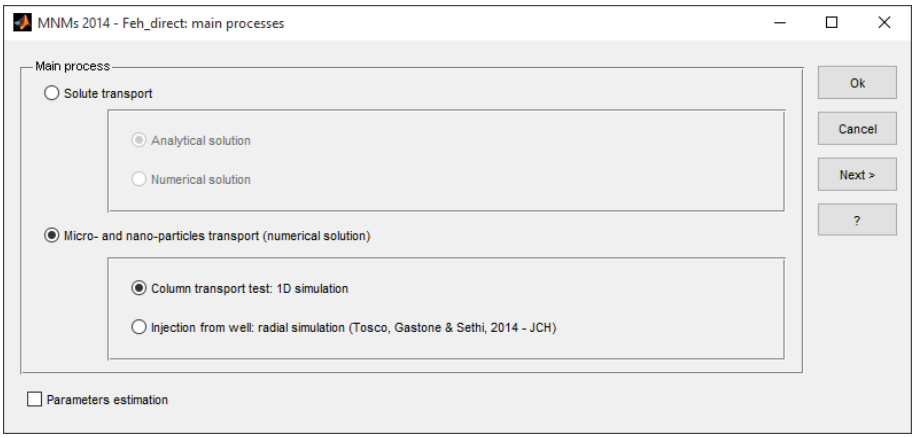

Figure 5-1: Main Processes selection window.

- The ***Problem definition*** window is opened.
- Leave all the predefined options for type of simulation, type of model and number of active sites. At the ***Type of kinetics*** entry for site 1 choose ***Blocking*** from the pop-up menu (Figure 5-2). Click ***Next***.

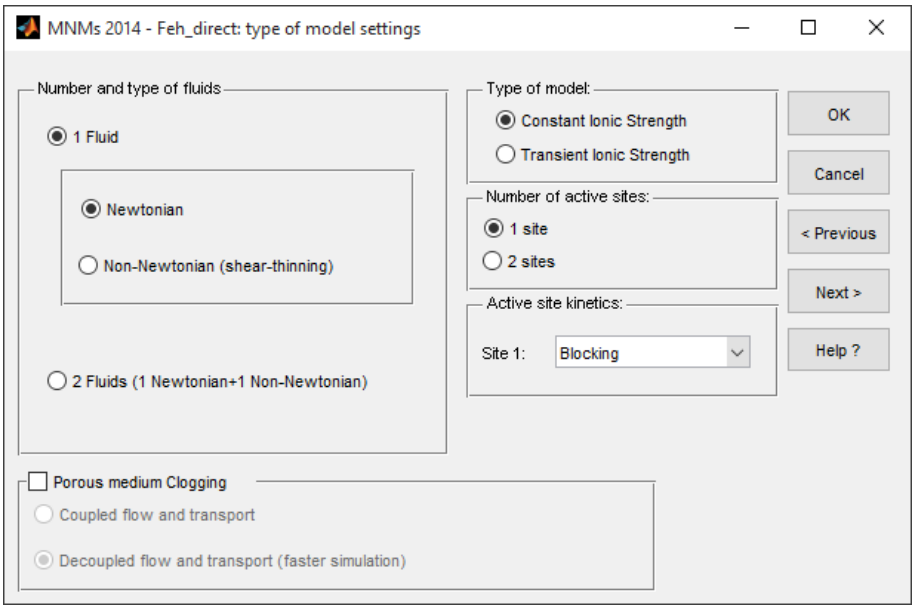

Figure 5-2: Problem definition menu.

- Set the ***System Properties*** as specified in description of the example model (Figure 5-3) and click ***Next***.

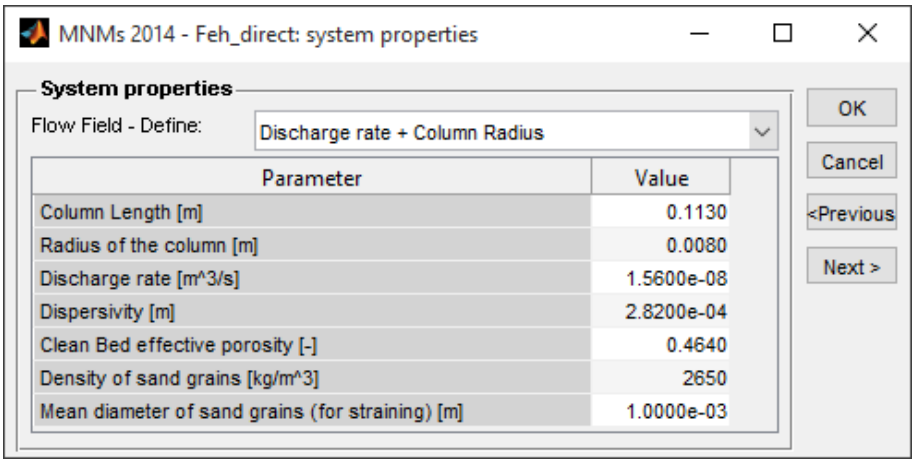

Figure 5-3: System properties menu.

- Insert the attachment and detachment coefficients and the maximum blocking concentration in the ***Kinetic coefficients*** mask as shown in Figure 5-4. Click ***Next***.

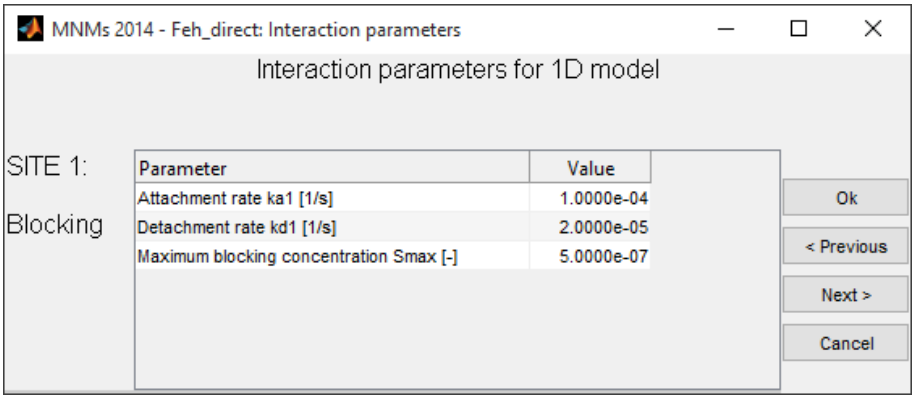

Figure 5-4: Particle Parameters menu window.

- In the ***Initial and boundary conditions*** menu set all the initial condition equal to 0 (clean column at the beginning of the test) except for the salt concentration that must be equal to 1 (background ionic strength value) (Figure 5-5).
- Click the ***Add*** *stress period* button and set the duration, particle concentration and salt concentration according to Table 5-1 (Figure 5-5). Click ***Next***.
- In the ***Solver settings and output control*** window you can set the solver settings and output control. Leave all the predefined settings. Click ***Ok*** we skip the last two windows, which can be used to import experimental data to be compared visually with your direct simulation).

5.1.2 Save and run

- Save the project clicking on the save project icon in the toolbar or selecting *Save* from the ***File*** menu (only for licensed versions).
- Run the model clicking on the save project icon in the toolbar or selecting ***Run simulation*** from the ***Run*** menu or pressing ***F5***.
  The model run can take few seconds up to a minute, according to your CPU and complexity of the simulation.

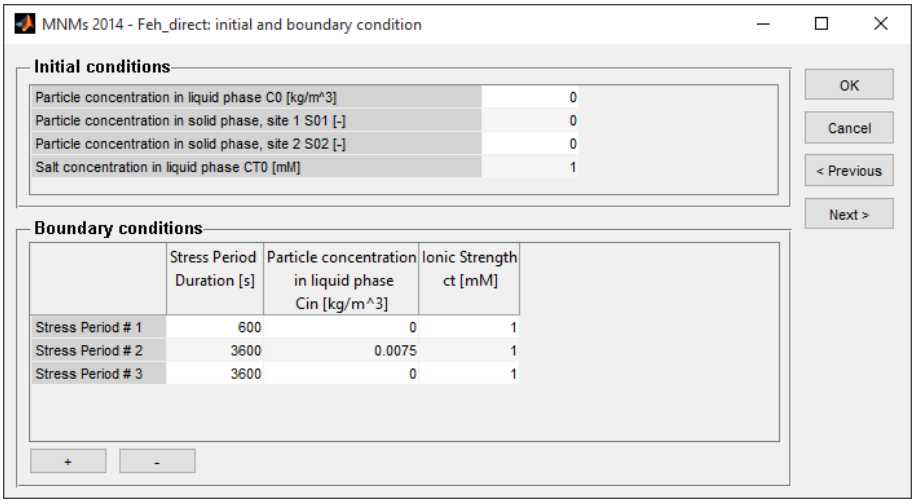

Figure 5-5: Initial and boundary conditions menu.

5.1.3 Visualize the results

The breakthrough curve of particle concentration in liquid phase and of ionic strength is automatically displayed in a plot in the right side of the main window. The ***PROJECT OUTPUT*** table is updated, showing the list of the available outputs: breakthrough curves in liquid phase and concentration profiles in liquid and solid phase.

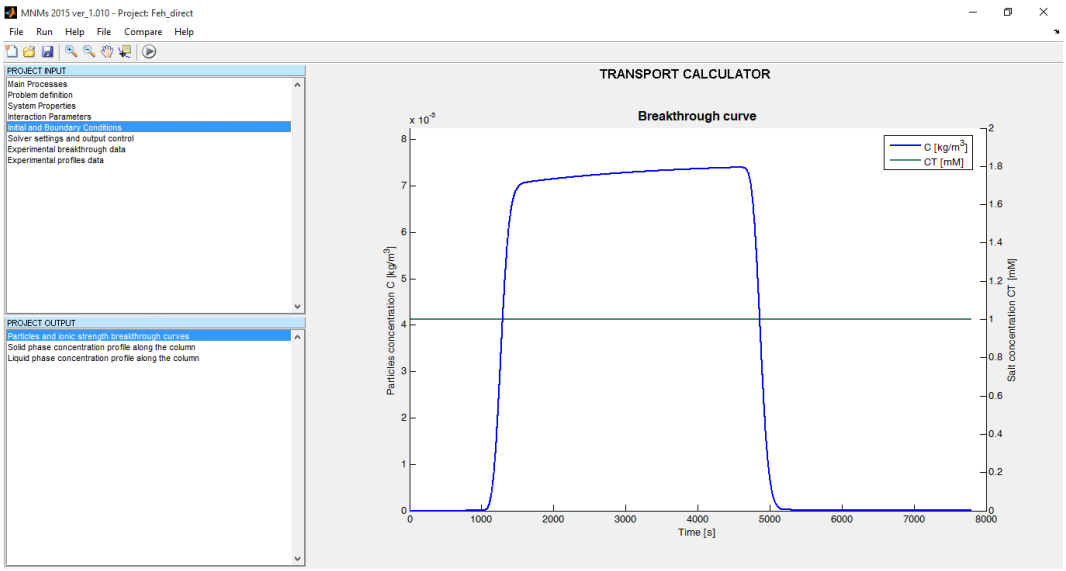

Figure 5-6: Software window after running the model

- Save again the project to save the simulation results.
- Click on the graph to modify the axis scale, limits labels and display the grid on the graph.
- Click on the ***Solid phase concentration profile along the column*** entry in the ***PROJECT OUTPUT*** table in order to open the specific result window (Figure 5-7).
- The particle transport parameters can also be tuned manually from Run/Manual calibration/Breakthrough curve (Figure 5-8).
- In the ***Manual Calibration*** window right click on a sliders to modify its maximum and minimum values. A slider can disappear if the coefficient value is outside the sliders range. In this case, please set suitable values of the sliders limits.

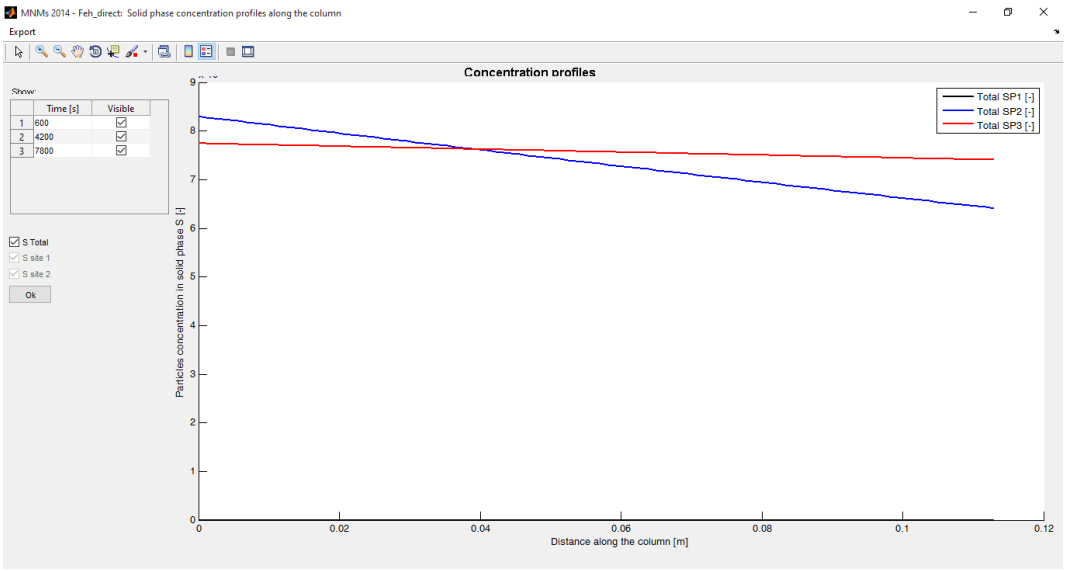

Figure 5-7: Concentration profiles along the column of the particle in solid phase. One curve for each stress period.

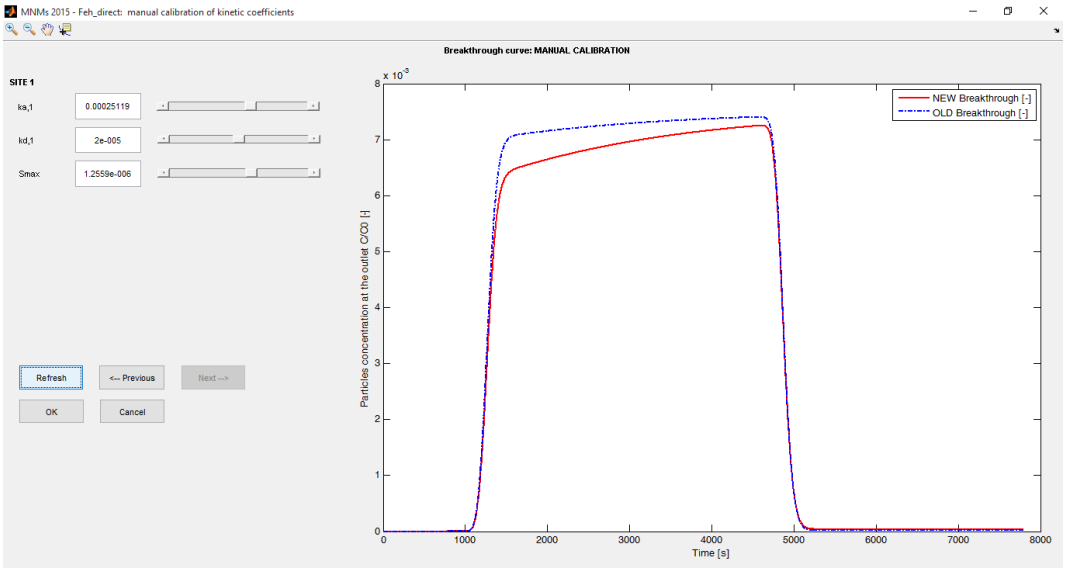

Figure 5-8: Manual calibration window.

5.2 Inverse simulation

Use the same column system of the previous example. Simulate transport of ferrihydrite in a NaCl 1 mM background solution. In this case, we need new kinetic coefficients in order to be able to simulate the nanoparticle transport. Assume to have measured the concentration of the particles in the liquid phase at the column outlet during the laboratory test. You can use these test results to estimate the values of the kinetic coefficients that better approximate the real case.

- Open the previous project Fe_direct by clicking on the open project icon or by the ***File*** menu.
- Save the project changing the name into **Fe_inverse** using the *Save as…* entry in the ***File*** menu.
- Double click on ***Main processes*** in the *PROJECT INPUT* table and *change* the Type of simulation from Direct to **Inverse simulation**. Click ***Ok***.
- In the ***Interaction parameters*** window, specify **Initial value, Upper limit** and **Lower limit** for each coefficient (Figure 5-9). Select the coefficients you want to fit.
- Import the experimental data (file Feh1mM.txt) using the following window and click ***Ok***.

- Run the model to fit the data.

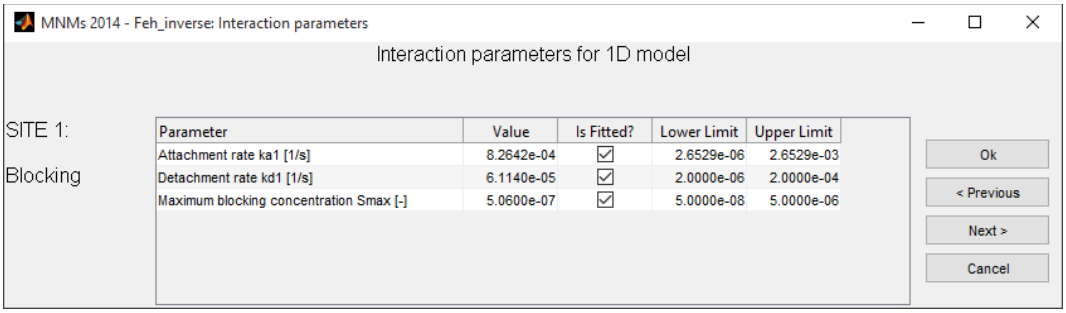

Figure 5-9: Kinetic coefficients menu for inverse simulation.

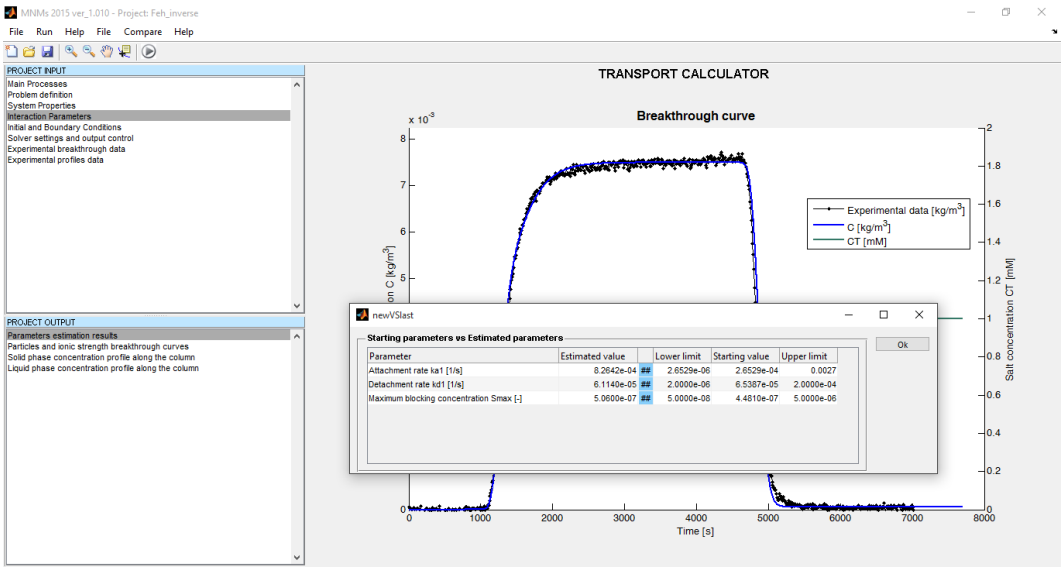

Figure 5-10: fitting results for the ferrihydrite test.

6 Particle transport simulation (2 sites)

Consider a 0.115 m long column with inner diameter of 0.8 cm, filled with quartz sand, where a tracer test and later on a particle transport tests are performed.

The tracer test was performed fist, by injecting a tracer (KCl) at an inlet concentration of 0.42 mg/l and applying a constant discharge of $1.30 \cdot 10^{-8}$ m^3/s for 1300 s. The column is initially saturated with DI water, and at time t=0 the tracer is injected. The experimental breakthrough curve of the tracer test is provided in the file *tracer_Latex.txt*.

The particle transport test was then performed injecting latex microspheres (1 micron in diameter) at an inlet concentration of 1.2 mg/l dispersed in a 30 mM KCl solution. The test protocol included a pre-flushing with particle-free solution, a particle injection, and a post flushing, following the protocol reported in Table 6-1. The experimental data are provided in the file *BTC_Latex.txt*. In this case the applied discharge rate is $1.56 \cdot 10^{-8}$ m^3/s.

Table 6-1: Injection protocol.

	Duration	Input particle concentration	Input ionic strength
Stress period	(s)	(kg/m^3)	(mM)
1st	600	0	30
2nd	3600	$1.2 \cdot 10^{-3}$	30
3rd	3900	0	30

Based on the information provided:

- Determine porosity and dispersivity from data fitting of the tracer test (if necessary refine the spatial discretization of the domain to avoid numerical artifacts).
- Try to fit the particle transport test using one interaction site (suggestion: blocking irreversible).
- Try to fit the particle transport test using two interaction sites, one linear and one with blocking.

7 Radial simulation

The exercise simulate the injection of a shear thinning suspension of microscale zerovalent iron having the following composition:

- Iron microparticles concentration 20 g/l
- Guar gum concentration 3 g/l (use rheological model from Gastone et al., 2014, with default model coefficients)
- Ionic strength 3 mM.

The suspension is injected in a sandy aquifer through a screened well with a diameter equal to 0.52 m at a discharge rate of 1 m^3/h per unit length of well screen. The injection lasts for 2 hours.

The properties of the particles are:

- Diameter 1.2 µm
- Density 7.7 g/cm^3
- Density of the layer of attached particles 3 g/cm^3
- Specific surface area $6 \cdot 10^6$ m^2/m^3

The aquifer properties are

- Dispersivity 0.3 m
- Clean bed porosity 0.26
- Clean bed permeability $1.3 \cdot 10^{-10}$ m^2
- Density of aquifer grains 2.65 g/cm^3
- Average size of sand grains 0.34 mm
- Specific surface area of the porous medium 5400 m^2/m^3
- Ionic strength 12 mM.

- As for the particle interaction parameters, use the default values (from Tosco et al., 2014). Use the single collector efficiency formulation proposed By Yao (1971).

✓ N.B. Pay attention to the multi-window structure of the ***System Properties*** window! (Figure 7-1).

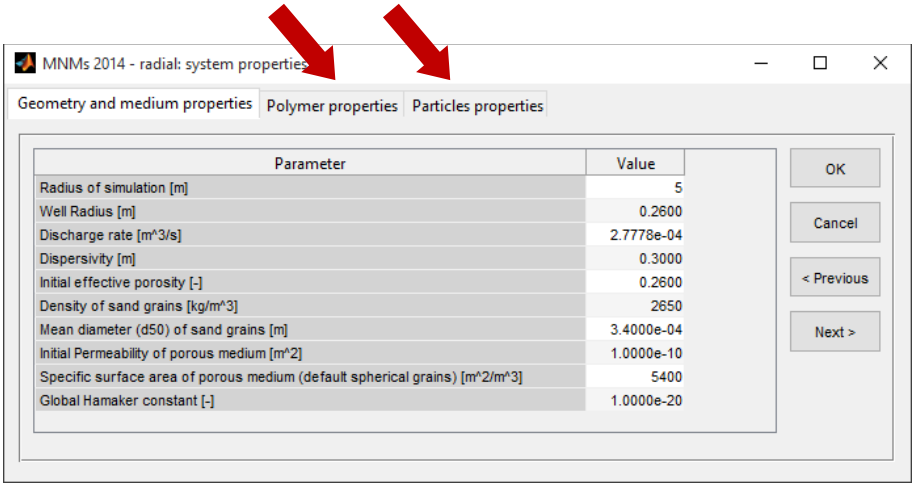

Figure 7-1: System properties window for radial simulations.

- Use a third type boundary condition.
- Run the simulation and save the results. You can then "play" with the polymer concentration and discharge rate.

8 References

- Tosco T.; Tiraferri A.; Sethi R. Ionic Strength Dependent Transport of Microparticles in Saturated Porous Media: Modeling Mobilization and Immobilization Phenomena under Transient Chemical Conditions. *Environmental Science & Technology* **2009**, *43*(12), 4425-4431.
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