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SIMULATION OF TRANSPORT COLUMN EXPERIMENTS – TRACING TESTS*

Vratislav Žabka, Jan Šembera

Abstract

This paper presents the modelling of tracing tests in column experiments. Program Transport was used for the simulation. Its main function is not to predict results of experiments but to compare influence of individual physical and chemical processes to the experiment results. The one-dimensional advection-diffusion model is based on Finite Volume Method; it includes the triple porosity concept, sorption, retardation, and chemical reactions simulated using connected program React from The Geochemist's Workbench package or PhreeqC.

The program Transport simulates not only the processes inside the column but also preparation of entering solutions and measurement methods of outgoing solution parameters.

Features of the program Transport allow a more precise simulation of the ongoing action and study the interaction of tested solutions and rocks. In the last chapter we introduce a simple example of using the program Transport to study a physical phenomenon inside column. It is sorption of sodium ions on colloidal particles of the quartz sand.

Keywords: column experiment; tracing test; groundwater modelling; sorption

1 Introduction

Importance of modelling is rising due to frequent contamination of the groundwater. In the last twenty years, the coupling of hydrologic transport and reactive chemistry has been fast developed. The observed influence of chemical and biochemical reaction to transport is the reason for the effort to coupling of hydrologic transport and reactive chemistry.

Column experiments are important for correct set up of 3D model parameters. With column experiment we evaluate properties of the tested rock (like sorption capacity, pore volume etc.). Good understanding of processes in the column is required for correct differentiation of individual processes. Thus, the most comprehensive model of the column is needed for accurate estimation of parameters.

The Transport program includes some innovations comparing to conventional models. These innovations can be divided in three groups: 1) more precise geometrical and physical model of the column experiment; 2) major attention to the reactive

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component of the process; and 3) communication between transport and reactive component of the process.

In paragraph three we are engaged in streamlining communication between programs. The Transport program, which is being developed by authors of this paper, first computes the transport processes. Then it sends the request to one of the geochemical software PhreeqC or The Geochemist's Workbench. Geochemical program calculates chemical equilibrium and sends data back to the Transport program. Both geochemical programs are commercial and we do not intervene in their code. Thermodynamic equilibrium is calculated by finding a minimum of Gibbs function.

Every group is important for the simulation but for the purposes of this work we describe especially geometrical and physical model innovations.

2 Geometrical and physical model innovation

The simplest model of column experiment is a cylinder consisting of porous medium (Figure 1). In our case, we have used one-dimensional model based on the Finite Volume Method. The inlet is modelled by boundary condition defining species concentrations as piecewise constant functions in time. The result of the simulation is the chemical composition of the solute outgoing from the column.

The real column experiment looks slightly different and some simplifications affect computed parameters. In this chapter we briefly describe correction of two simplifications that are most relevant: 1) input and output chamber of the column and 2) output flask.

By the terms input and output chamber of the column we mean the volumes ahead of the porous medium cylinder and behind this cylinder. Those parts of the

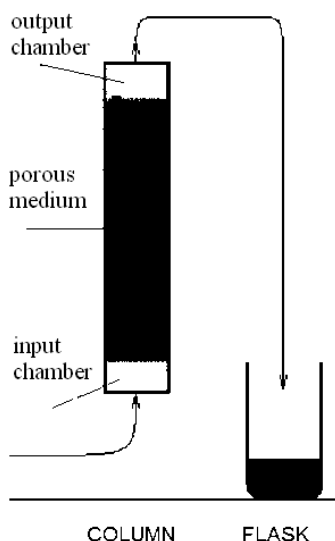


Fig. 1: *Scheme of laboratory column experiment.*

column are formed due to technology of column creation and they have various effects in various column experiments. Both chambers frequently contain another material than the column cylinder. When we do not include chambers into the model of column experiment, the parameters can be calibrated incorrectly. For better understanding we present the equation (3) for computation of concentration of one species in the input chamber. All these equations (2), (3), (4) are based on the principle of mass conservation and on the relation (1).

$$Q = \frac{C \cdot V}{t} \quad (1)$$

$$C_0(t + \Delta t) = C_0(t) + (C_{vst}(t) - C_0(t)) \frac{\Delta t \cdot Q(t)}{V_0} \quad (2)$$

where C_0 [$\text{mg}\cdot\text{l}^{-1}$] is concentration of one species in the input chamber, t [s] is the actual time, V_0 [l] is volume of the input chamber, C_{vst} [$\text{mg}\cdot\text{l}^{-1}$] is the concentration of the input solution and Q [$\text{l}\cdot\text{s}^{-1}$] is the flow rate. Another type of the simplest model extension is the model of the output flask. The solute concentrations and properties in the real column experiment are measured in the output flask. The solution outflows from the output chamber into the output flask. At a certain time the flask is replaced and analyzed. Composition of the solution in the output flask is different than composition of the solute outflowing from the column computed by the simplest model. This is the reason why we include the computation of the output flask into the model. It is described by equations (3) and (4):

$$V_{N+2}(t + \Delta t) = V_{N+2}(t) + \Delta t \cdot Q(t) \quad (3)$$

$$C_{N+2}(t + \Delta t) = \frac{C_{N+2}(t) \cdot V_{N+2}(t) + \Delta t \cdot Q(t) \cdot C_{N+1}(t)}{V_{N+2}(t + \Delta t)} \quad (4)$$

where the index $N + 1$ refers to the output chamber, and the index $N + 2$ refers to the output flask.

3 Geochemical reaction modeling

Following [1], while the coupling of hydrologic transport and chemical reaction models is an active area of research, the development of chemical reaction batch models has received much less attention. Whereas reactive parameters setting is more difficult than setting of transport parameters. Reactive transport program cannot only compute with species concentrations. Information about other solute properties is important to include. Those properties are changing along the column experiment depending on current reactions and ambient conditions.

For example, setting of the solute and external atmosphere equilibrium is important for solute properties and inside chemical reactions. Otherwise setting of precipitation processes have an effect to solute composition and sometimes also transport properties. E.g. when column experiment takes only few days, it is not possible for

hematite to precipitate; the mineral hematite is the final product of precipitation for solution including oxygen and iron but its precipitation needs at least hundreds of years and column experiments do not last as long, so we have to suppress this mineral in the thermodynamic equilibrium computations.

In the case of tracing tests, reactive component plays not such a significant role. Into the column filled with rocks whose pores are saturated with water, NaCl solution is injected. There are no chemical reactions which could significantly affect properties of the solution. But there are other physical phenomena that can influence solution properties. One of them is sorption.

4 Example of using the model – simulation of sorption

Our column experiments use quartz sand, which contain colloidal particles. According to [3], in natural waters with pH of 6–8 clay minerals are cationic. These minerals may exchange the crystal lattice ions for cations in solution because minerals surface charge is mostly negative (electrostatic sorption). Quartz clay may exchange calcite ions for sodium ions.

The effect of solute concentration on the adsorption is described by adsorption isotherms. In the simple case of equilibrium sorption, Langmuir isotherm corresponds with electrostatic adsorption the best way. To compute the concentration of adsorbate, analytical solution of equation system is used in the program Transport. Except of Langmuir isotherm equation (5) system contains also the mass conservation equation (6).

$$C_s = C_{max} \frac{C_r K_L}{1 + C_r K_L} \quad (5)$$

$$C_{s0} + C_{r0} = M = C_s + C_r \quad (6)$$

where C_s [$\text{mg}\cdot\text{l}^{-1}$] is concentration of adsorbate adsorbed of the adsorbent, C_{max} [$\text{mg}\cdot\text{l}^{-1}$] is the maximal concentration of adsorbate adsorbed of the adsorbent. K_L [$\text{mg}\cdot\text{l}^{-1}$] is the adsorption constant, C_r [$\text{mg}\cdot\text{l}^{-1}$] is the concentration of adsorbate in liquid, M [$\text{mg}\cdot\text{l}^{-1}$] is total concentration of the substance.

Custom column experiment consists in injecting a certain amount of tracers (sodium chloride) in the column, a constant flow of fresh water column. At the exit from the column mainly monitors the solution conductivity and pH.

When we simulated the situation without sorption, computed pH is changing minimally (see pH-model in Figure 2). These results did not correspond to the measurement. But simulation of conductivity fit well. When sorption of Na^+ according to the Langmuir isotherm is included into calculation, the calculated conductivity does not significantly change. The calculated pH in this case approaches the measured values much better then without sorption simulation (see pH-model with sorption in Figure 2).

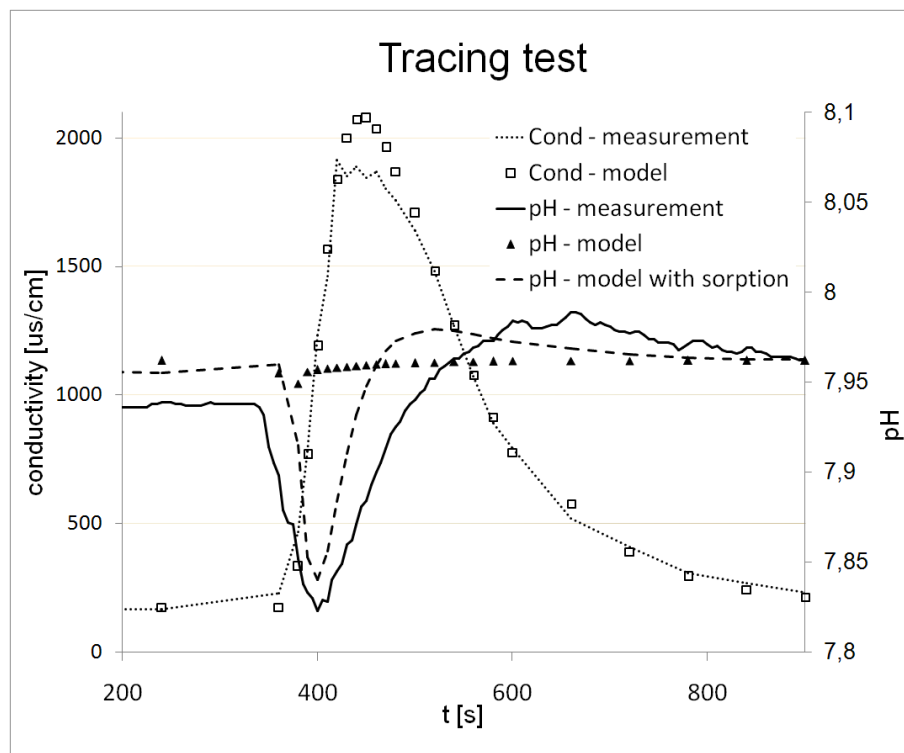


Fig. 2: Tracing test – dependence conductivity and pH on time of the experiment. It was injected 10 ml of NaCl solution ($20 \text{ g}\cdot\text{l}^{-1}$).

5 Conclusion

This paper presented changes in column experiment model that were done to improve understanding of reactive transport processes. Parameters of real column experiment can be more precisely estimated and better implemented to 3D ground-water simulation.

In the last section, possibilities of use of the program Transport for the study of physical and chemical phenomena that take place inside the column during the tracing tests were presented.

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