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Simulation of reactive materials in column and reservoir tests. Sensitivity analysis for a linear coupled model

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Abstract

This paper presents results of simulations of reactive deformable porous material studied in configurations corresponding to the two classical methods of identification of transport parameters: column and reservoir tests. In order to quantify the relative importance of input parameters of the model which influence the material behavior in response to a chemical load, the sensitivity analysis is performed. The obtained results can be useful in selection of efficient methods of identification of chemo-mechanical parameters and in particular, finding the optimum source and time period of the tests.

Keywords: Reactive materials; Sensitivity analysis; Reservoir and column test

1. Introduction

The class of reactive (or chemically sensitive) materials includes wide range of natural media such as clays and soft tissues and many artificial materials, mostly hydro-gels and porous polymers which are developed and applied as smart or multifunctional media. The modeling of the reactive materials should include response to mechanical and chemical leads and is associated with description of deformations, flow and transport. Mechanically driven deformations of porous materials are incorporated in the theory of consolidation. The evolution of physicochemical interactions within or between elements of solid material (particles) due to change in pore fluid chemistry is the most important cause of non-mechanical deformations of the materials. The flow and advective–diffusive transport in very low permeability materials like clay and gels are limiting cases of the more coupled transport phenomena, which include osmosis and ultrafiltration. This is due to the fact that clay and some other gels act as semi-permeable membranes.

Models of consolidation coupled with transport of chemicals in reactive materials within purely macroscopic approach are based on theory of chemo-consolidation, [1,2] the theory of poroelasticity with chemical effects [3], or theory of mixtures [4–6] and are related to reversible [1,3] or irreversible [7] deformations of solids matrix. The other approaches use the averaging techniques [5,8] starting from continuum or molecular level.

A significant component of any modeling is identification of material parameters. This becomes a particularly nontrivial task for such complex behavior as exhibited by reactive materials for which there is essential lack of complete set of the parameters. The very important for indirect identification of the material parameters or functions are simulations of experimental tests. The simulations based on analytical or numerical solutions are useful in sensitivity analysis and then design of procedures that are efficient from the point of view of the actual estimation process.

The subject of this paper is the analysis of numerical models of reactive deformable porous materials studied in configurations corresponding to the two classical methods of identification of transport parameters: column and reservoir tests. The tests which are usually used to determine transport parameters of undeformable porous

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materials are considered here as potential methods which incorporate chemically induced deformations and couplings resulting from interaction of mechanical and chemical loads. First, using linear chemo-mechanical models of the tests the 1D numerical simulations are developed. The solutions are applied to perform thorough sensitivity analysis concentrated on studies of influence of material parameters present in the models on observable outputs – concentration, pressure and displacement.

2. The mathematical model

2.1. Equations of 1D linear chemo-poroelasticity

The appropriate basis of modeling the flow fluid and transport of chemicals coupled with chemically induced deformations of porous materials is the non-equilibrium thermodynamics and theory of two-phase multi-component porous materials. The model includes balance equations, and constitutive relations describing specific features of coupled reactive transport and chemo-mechanical response. The complete derivations of used here equations for model of chemically sensitivity materials and transport of single contaminant are presented in [9]. Starting from the one dimensional linearized equation of mechanical equilibrium for solid and fluid phase and adopting the assumption of constant mechanical load on the surface of sample the two equilibrium equations fall into the equation for pore pressure coupled with concentration of the substance

$$(1+a\alpha^2M)\frac{\partial p}{\partial t}-(\gamma+a\alpha dM)\frac{\partial c}{\partial t}-\frac{f_0^2M}{b}\frac{\partial^2 p}{\partial x^2}+\frac{f_0Mb_1}{b}\frac{\partial^2 c}{\partial x^2}=0, \tag{1}$$

where p determines the local value of pore pressure, c is the mass concentration of solute in pore fluid; $d=\alpha\gamma+\delta$, $1/a=2\mu+\lambda-\alpha^2M$, while the parameters μ, α, λ and M are known as Biot's parameters of poroelasticity, δ and γ represent the chemo-mechanical couplings measuring respectively change of total stress and pore pressure due to the increment of concentration; b and b_1 are coefficients of viscous and chemo osmotic drag which can be expressed by hydraulic conductivity k, osmotic permeability k_c, specific weight γ_1 and porosity f_0

$$b=\gamma_1 f_0^2 k^{-1},\ b_1=k_c b/f_0 \tag{2}$$

The linear form of transport of substance in reactive materials is

$$R\frac{\partial c}{\partial t}-K_2\frac{\partial p}{\partial t}+v_0^f\frac{\partial c}{\partial x}-D\frac{\partial^2 c}{\partial x^2}+D_1\frac{\partial^2 p}{\partial x^2}=0, \tag{3}$$

where v_0^f denotes the velocity of advective transport (in the linear model the constant value), $R=1+K_1$ is known as the retardation factor, K_1 and K_2 are parameters related to the intensity of mass exchange (between fluid and solid phase), D is coefficient of dispersive transport (representing in general both diffusion and mechanical dispersion) and D_1 denotes coefficient of ultrafiltration.

Assuming that the total stress T in material is constant in time, the deformation of skeleton due to mechanical and chemical loads can be determined from the constitutive relationship, written for the local strain, which is defined by the following expression [9]:

$$\varepsilon=a(T+\alpha p-dc), \tag{4}$$

where $T=-p$.

Then, using relationship (5), the settlement or swelling S(t) of the layer of material of thickness L can be defined as

$$S(t)=\int_0^L \varepsilon dx=\int_0^L a(T+\alpha p-dc)dx. \tag{5}$$

2.2. Boundary and initial conditions

We consider the chemo-mechanical problems related with two different tests of porous materials: A – the column test and B – the reservoir test, shown schematically in Fig. 1.

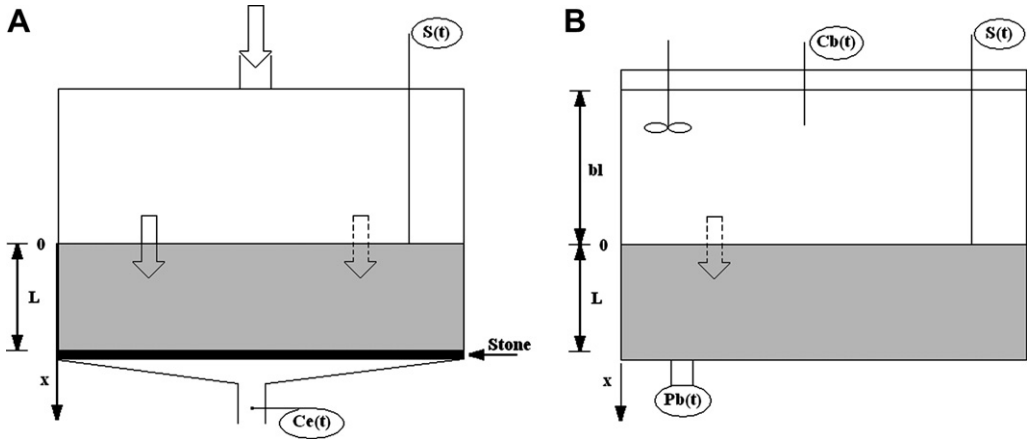

Fig. 1. The schematic view of experimental configuration of chamber with sample for column (A) and reservoir (B) test.