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Linking sub-pore scale heterogeneity of biological and geochemical deposits with changes in permeability

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ABSTRACT

Subsurface geochemical and biological transformations often influence fluid flow by altering the pore space morphology and related hydrologic properties such as porosity and permeability. In most coupled-processes models changes in porosity are inferred from geochemical and biological process models using mass-balance. The corresponding evolution of permeability is estimated using (semi-) empirical porosity–permeability functions such as the Kozeny–Carman equation or power-law functions. These equations typically do not account for the heterogeneous spatial distribution and morphological irregularities of the geochemical precipitates and biomass. As a result, predictions of permeability evolution are generally unsatisfactory. In this communication, we demonstrate the significance of pore-scale precipitate distribution on porosity–permeability relations using high resolution simulations of fluid flow through a single pore interspersed with crystals. Based on these simulations, we propose a modification to the Kozeny–Carman model that accounts for the shape of the deposits. Limited comparison with published experimental data suggests the plausibility of the proposed conceptual model.

1. Introduction

Subsurface biological and geochemical processes are often coupled with hydrologic processes through the accumulation (removal) of secondary materials in pore spaces and the accompanying reduction (increase) in porosity and permeability. Typical causes for mineral precipitation in porous media include production of hydrocarbons [1,2]; thermally-driven reactions near high-level waste storage sites [3] and in geothermal fields [4]; *in situ* contaminant remediation by redox reactions [5,6]; effluent disposal [7]; and carbonate mineralization during deep geological CO_2 sequestration [8]. Growth of biological material in porous media (bioclogging) is commonly observed in areas undergoing/experiencing wastewater disposal, artificial groundwater recharge, and *in situ* bioremediation [9]. Similar processes also affect granular-media filtration beds, in which filtrates are deposited within the pore space thereby reducing both porosity and permeability [10].

The morphology and growth rate of the secondary accumulations are governed by a number of factors including mineralogy of the pore walls, microbial populations, as well as chemistry, temperature and hydrodynamics of the pore fluid [11]. Conversely, the morphology and amount of secondary accumulations have significant effect on the hydrodynamics of the pore fluid. These coupled biogeochemical and hydrologic processes are commonly modeled by describing permeability evolution as a function of porosity; e.g., using the well known Kozeny–Carman relationship [12,13]

$$k = \frac{c\phi^3}{\tau^2 S^2}, \tag{1}$$

where k (m^2) is permeability, ϕ is porosity, τ is tortuosity and c is an empirical parameter that represents particle size and shape. The specific surface area per volume S ($m^2\ m^{-3}$) can be translated to the common form of surface area per unit mass (S_m ($m^2\ kg^{-1}$)) using $S = \rho_p S_m (1-\phi)$; where ρ_p is grain density. During addition of secondary materials to the pore space, all the variables of the equation can be expected to evolve. The relative evolution of permeability can be expressed as

$$k/k_0 = \frac{c/c_0}{(\tau/\tau_0)^2} \frac{(\phi/\phi_0)^3}{(S/S_0)^2}, \tag{2}$$

where the subscript 0 denotes the unaltered state.

Evolution of porosity (ϕ) can be readily infered from geochemical/biological process models using mass balance calculations [14,15]. The change in surface area (S) can be indirectly described as a function of porosity evolution if some assumptions can be made regarding the distribution of the secondary accumulations. The simplest and most commonly employed assumption is uniform distribution over the entire solid surface [14,15]. If the secondary materials do not result in complete blockage of significant proportion of the pores (e.g., early stages of precipitation in an otherwise clean sandy deposit), the change in tortuosity (τ) can be safely

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ignored. The change in the shape factor (c) is the most difficult to describe because it is inherently poorly defined and the least physical component of the model. For uniform distribution of secondary accumulations, the effect of its evolution can probably be ignored as the porosity evolution accounts for the uniform growth of the grains without substantial change in the grain shape. In summary, evolution of permeability (k) can be reasonably described as a function of porosity (ϕ) provided that the secondary materials are uniformly distributed.

From the foregoing discussions it is readily evident that description of permeability evolution in the presence of pore-scale heterogeneities of secondary deposits is particularly challenging. This challenge is compounded further by the fact that permeability evolution is described at the scale of computational grids of the flow models, which typically spans multitudes of pores. As such, the complex interplay between biologically/geochemically induced micro-heterogeneities (at pore and sub-pore scales) and macroscopic fluid flow is effectively ignored. This work was motivated to address these conceptual and scale discrepancies.

The approach taken in this paper is based on experimentally observed pore-scale features of deposits. There is ample experimental evidence clearly demonstrating the fact that secondary additions to pores are rarely uniformly distributed [16–18,9,19–21]. For example, laboratory experiments of scaling have shown that *in situ* mixing of formation water with injected seawater creates a few slender crystals that often bridge pore walls [16]. Similarly, flow visualization experiments that employed two-dimensional pore networks have shown different bacterial colony morphologies including filaments, biofilms, strands of spherical colonies (pearl necklace), and coarse aggregates [17]. Other researchers have shown bacterial biomass accumulation in granular porous media in the form of discontinuous discrete colonies within pores and pore throats [19].

Moreover, hydrodynamics of laminar flow at pore scale dictates the effective conductance of pores to be strongly dependent on pore shape [22]. This is further corroborated by experiments that have shown that the permeability loss to be dependent not only on the quantity of secondary deposits but also on the morphology and spatial distribution of crystals [16] and microbial deposits [17,18].

The objectives of this communication are (a) to illuminate on the potential pitfalls of disregarding pore-scale heterogeneities arising from biological/geochemical processes in coupled models and (b) to introduce a simple approach for bridging the scale gaps.

2. Theoretical considerations

The underlying premise behind the approach we are introducing in this paper is that geometric description of pore evolution can be used as a modeling tool that couples the deposit forming processes (microscopic in nature) with macroscopic fluid flow. The first part of this approach involves describing the evolution of pore morphology by biological/geochemical processes. Dynamic geometric information of the pore space can be achieved using high-resolution geochemical simulation as well as time-lapse measurement of porosity and surface area and/or imaging (e.g., using X-ray computed tomography) [23–25]. The second part of the proposed approach is to devise a permeability evolution model that depends not only on the loss of total pore space, but also on the sub-pore scale heterogeneity. This paper is focused on the latter part of this modeling approach.

2.1. Flow and pore-evolution models

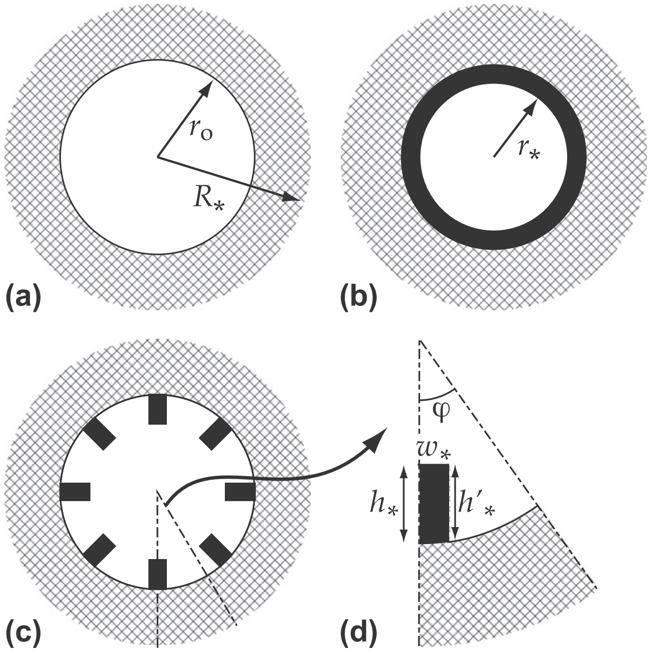

Fig. 1. Geometric model of a pore: (a) unaltered pore, (b) a pore coated with precipitate of uniform thickness, (c) a pore with eight equally spaced rectangular precipitate crystals, and (d) definitions of a unit wedge, where w_* is the half-width of the crystal, h_* is the median height of crystal, and h'_* is the height on the edge of the crystal.

Although the geometry of pores vary considerably, we can a great deal about pore-scale physical phenomena by considering simple geometrical models. In this work we focus on the cross-section of a circular pore with radius r_0 embedded inside a concentric solid matrix of radius R_* (see Fig. 1a), such that the initial porosity of the unit-cell is defined by

$$\phi_0 = \frac{r_0^2}{R_*^2}. \tag{3}$$

This cross section may be thought of as the shape of a pore-throat that controls the flow of fluid along a flow tube in a rock. We use physical rectangular Cartesian coordinates (x_*,y_*,z_*) with liquid flow along z_* direction and the cross-section situated on x_*–y_* plane. We consider two contrasting models of accumulation of secondary mineral precipitates. The simplest model entails uniform distribution of precipitates as illustrated in Fig. 1b, such that the partially plugged pore will have a radius $r_* < r_0$. In the second model, which is the main focus of this paper, we consider a pore that is interspersed with n equally spaced, rectangular crystals (see Fig. 1c). The crystals are assumed to grow perpendicular to the pore walls, consistent with reported experimental observations [16]. The smallest wedge of the pore that represents the pore geometry (containing half of a single crystal) and flow distribution has an angle of $\varphi = \pi/n$ and is illustrated in Fig. 1d. The width and median height of the half crystal are denoted by w_* and h_*, respectively.

The spatial distribution of the steady-state flow velocity (v_*) through the pore can be described by Stokes' equation

$$\nabla_*^2 v_* = \frac{1}{\mu}\frac{\mathrm{d}P}{\mathrm{d}z_*}, \tag{4}$$

where μ (Pa s) is the viscosity of the liquid and $\mathrm{d}P/\mathrm{d}z_*$ (Pa/m) is the pressure gradient that drives the liquid flow. We assume no-slip boundary condition along the pore walls, including the crystal surfaces.

The average flow velocity q (m/s) through the porous medium can also be described using the macroscopic Darcy's law as