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Influence of eddies on conservative solute transport through a 2D single self-affine fracture

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ABSTRACT

The solute transport regime is highly dependent upon the heterogeneity of the flow field. In this study, the influence of eddies on conservative solute transport through a two-dimensional (2D) single self-affine fracture was investigated by the Navier-Stokes flow and solute transport simulations. The self-affine rough fracture was generated by the successive random additions (SRA) technique. The simulations showed that eddies had significant influence on the spatial evolution of the solute plume through the fracture. Analysis of breakthrough curves (BTCs) and residence time distributions (RTDs) presented that the solute transport through the fracture was non-Fickian and the developing eddies enhanced the typical non-Fickian characteristics (i.e., "early arrival" and "heavy tail") in BTCs for a step tracer injection. Increasing the Reynolds number caused the increasing exponent of the power-law tail with the developing eddies. Fitting the non-Fickian BTCs with the classical inverse model (advection–dispersion-equation, ADE) led to a non-negligible error due to the presence of eddies. The continuous time random walk (CTRW) inverse model with truncated power law transition rate probability was alternatively employed and the fitting results showed the robust capability of CTRW in capturing the eddy-induced non-Fickian transport. It was found that the value of parameter β of CTRW decreased as the total eddy volume increased, indicating that the developing eddies might increase the magnitude of non-Fickian transport. Furthermore, the dilution index presenting the exponential of the Shannon entropy of a concentration probability distribution was used to quantify the uniformity of concentration distribution within the fracture. We could conclude that eddies provided strong resistance for solute transport and significantly delayed the mass exchange between the main flow channel and the eddy-controlled zones. Consequently, the delayed mass exchange process directly determined the magnitude of tails in BTCs. The results may enhance our understanding of the role of eddies in the solute transport through fractures.

1. Introduction

Characterizing fluid flow and solute transport through fractures is important for the understanding of conservative and reactive contaminant transport, enhanced oil recovery, remediation of non-aqueous phase liquids (NAPLs), nuclear waste disposal and carbon capture and storage [1,2]. Fractures that occur ubiquitously in geological formations is usually simplified as a pair of smooth and parallel plates. However, neglecting the roughness of fractures is still challenging for explaining and describing the behaviors of flow and solute transport, especially for the non-Fickian (anomalous) transport that is often associated with "early arrival" and "heavy tail" in breakthrough curves (BTCs). Therefore, studying conservative solute transport through rough fractures is critical for the development of solute transport theory.

Solute transport is normally assumed to follow Fickian behaviors. The corresponding governing equation for Fickian transport is the well-known advection–dispersion equation (ADE) [3], where the dispersion coefficient is assumed to be spatially and temporally constant. The Fickian ADE can accurately predict Gaussian-shaped BTCs. However, the extensive field and experiment studies [4–6] revealed that the BTCs was not always Gaussian and the Fickian transport model is inappropriate for explaining non-Gaussian-shaped BTCs. Generally, there are two typical characteristics of non-Gaussian-shaped BTCs for a pulse plume. First, the arriving time of the concentration peak in BTCs is earlier than that predicted from the Fickian transport model, which reflects that there may be a preferential path for the solute transport [7]. This is the

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so-called “early arrival” phenomenon. Second, the tail after concentration peak in BTCs lasts longer than that predicted from the Fickian transport model. This “heavy tail” could possibly be interpreted in terms of multi-rate mass exchange process between mobile and immobile domains [8,9], the absorption of fracture wall [10,11], the permeable rock matrix [12], as well as the presence of eddies inside the fracture [13–15]. Although the non-Fickian solute transport has been studied in different research areas such as heat conduction or mass transport [16], fast crystallization process [17], percolation through the porous media [5], and diffusion in solid polymers [18], in this study, we focused on the influence of eddies on solute transport through a single self-affine fracture.

Since the Fickian transport model associating with a Gaussian-shaped BTCs is derived based on the assumption that geological formations are statistically homogeneous and stationary, the heterogeneity of geological formation that occurs at all scales is considered to be primarily responsible for the ubiquitous non-Fickian transport [1]. The heterogeneous geological formation leads to heterogeneous flow field even at small scales [19]. The non-Fickian transport has been observed even in a single rough fracture. Bauget and Fourar [20] studied the solute transport in a transparent replica of a real single fracture and they found that the Fickian ADE is incapable of modeling the “heavy tail” behavior. Qian et al. [21] experimentally studied the influence of non-Darcian flow on the solute transport in a single fracture and they concluded that the “heavy tail” induced by non-Darcian flow was difficult to explain by using Fickian ADE. In order to model the non-Fickian characteristics such as “early arrival” and “heavy tail”, several appealing mathematical models were developed. This included the continuous time random walk (CTRW) [22–24]; the fractional advection-dispersion equation (FADE) [25]; the mobile-immobile method (MIM) [26]; and the boundary layer dispersion [27]. The CTRW model was proved to be capable of capturing both Fickian and non-Fickian transport. There are many successful applications of inverse CTRW model for characterizing non-Fickian BTCs. For example, the non-Fickian BTCs in the heterogeneous porous media [22,23] and single variable-aperture fracture [20,28]. However, it still needs to investigate the capability of CTRW capturing the eddy-induced non-Fickian characteristics in a single self-affine fracture.

In addition, recently, serval authors [29–33] found that the non-Fickian transport characteristics could result from the fact that there is a fundamental difference between spreading and mixing processes of the solute. Spreading describes the spatial extent of a solute plume, which can be quantified by the apparent dispersion (i.e., the rate of increases of the second central spatial moment of the solute); Mixing is driven by diffusion and can be deemed as increases the actual volume occupied by the solute. Distinguishing spreading and mixing process is important for fundamentally understanding of the inherent relationship between the non-Fickian characteristics of BTCs and the spatial concentration distribution of the solute inside the fracture. For example, the mixing process that dilutes the solute determines the peak concentration of the plume while the spreading process controls the arriving time of the plume. Although spreading and mixing are highly coupled, various measures to quantify the mixing have been developed. This includes the dilution index [34] and scalar dissipation rate [35,36].

The main objective of this study was to investigate how developing eddies influences conservative solute transport through a 2D single self-affine fracture. A 2D single self-affine fracture was generated by the successive random additions (SRA) technique. The flow field and the spatial evolution of solute were analyzed under flow conditions with Reynolds number (Re) ranging from 30 to170. The characteristics of residence time distributions (RTDs) and BTCs were used to determine the influence of eddies on solute transport. Subsequently, two inverse models (i.e., the classical ADE and CTRW model) were tested for their capacity of characterizing the eddy-induced non-Fickian transport. Furthermore, the dilution index was used to quantify the uniformity of concentration distribution within the fracture, which highlighted the influence of eddies on the mass exchange process.

2. Modeling approach

2.1. Single self-affine fracture generation

Many studies reported that the geometry of natural fracture walls generally shows self-affine properties. Following the seminal work of Mandelbrot and Pignoni [37], the height of the self-affine rough fracture wall can be described as,

$$\lambda^H h(x) = h(\lambda x) \tag{1}$$

where λ is the arbitrary constant, called scaling factor, and the exponent H is a measure of the fracture roughness and defined as the Hurst exponent with the range from 0 to 1. To generate self-affine fractures, the specific Hurst exponent must be assumed. A large number of experimental studies reveal that the Hurst exponent of the natural rock fracture wall varies between 0.47 and 0.85. The Hurst exponent is proved to be depended on the mineral component of rocks. The characteristic Hurst exponent of the fracture wall is around $H = 0.8$ for granite and basalt, whereas $H = 0.47 \pm 0.05$ for sandstone [38]. However, our primary objective here is not to perform an exhaustive analysis for the different Hurst exponent of the fracture walls. The Hurst exponent $H = 0.8$ that suggested to be universal by the previous works [39] was assumed in the current study.

Once the Hurst exponent of the fracture wall was specific, several methods are available to generate the self-affine fracture wall (e.g., the successive random additions (SRA) and the Fourier transformation). In this study, we adopted the SRA technique [40] to generate the self-affine fracture wall. The details of the SRA technique can be also found in our previous works [39,41]. From the generated self-affine fracture wall to the single self-affine fracture, we used the shear displacement model [42] to construct the single self-affine fracture, associating with the local aperture as a function of longitudinal distance (see Fig. 1). The length of the generated fracture was $L = 160$ mm. To improve the possibility of the presence of eddies, we used a relatively large standard deviation $\sigma_b = 1.74$ mm and mean aperture $\bar{b} = 3.35$ mm , which resulted in the coefficient of variation, $\sigma_b/\bar{b}$ equal to 0.52.

2.2. Flow model

The flow field in a single self-affine fracture is solved directly by using the Navier-Stokes and continuity equations, which is assumed as the isothermal, incompressible, and homogenous single Newtonian steady flow,

$$\nabla \cdot \boldsymbol{u} = 0 \tag{2}$$

$$\rho(\boldsymbol{u} \cdot \nabla \boldsymbol{u}) - \nabla(\mu \nabla \boldsymbol{u}) = -\nabla p \tag{3}$$

where ρ is the density of fluid, $\boldsymbol{u} = [u, w]$ is the velocity vector, p is the total pressure, and μ is the dynamic viscosity of fluid. In this study, we adopted standard water properties at 20 °C, e.g., $\rho = 998.2$ kg/m^3 and $\mu = 1.002 \times 10^{-3}$ Pa·s. The single self-affine fracture walls were considered as the non-slip boundaries. The steady-state flow was induced from left to right by a given pressure drop over the entire fracture, which is a Dirichlet boundary condition. The flow model was solved based on the Finite Element Method (FEM) and was implemented in COMSOL Multiphysics package (COMSOL Inc., Burlington, MA, USA). It should be noted