Multiphase multi-rate mass transfer model for anomalous transport in fractured and heterogeneous media

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Anomalous transport phenomena occur in a wide range of industrial and environmental applications. For example, such phenomena are encountered in the study of heterogeneous porous media, which are of pivotal importance in modern oil & gas and aquifer remediation research. Generally, standard Fickian diffusion models fail to accurately model solute transport in complex porous media like natural soil or fracture matrices, due to the wide range of mass transfer rates between zones of mobile contaminant (advection dominated) and immobile contaminant (diffusion dominated). In fact, these transfer rates depends on the complexity and variety of the pore geometry (for example polydisperse and clustered particles or randomly shaped fractures) which is not accounted for in Fickian diffusion models.

A model that account for porous systems with multiple transfer rates between one mobile zone and a set of immobile zones is the Multi-Rate Mass Transfer (MRMT) model (Haggerty & Gorelick 1995). The MRMT is based on the multi-continuum concept, where different zones are represented as different continua communicating through first order transfer functions or linear mechanisms such as the Fick's first law (Carrera et al. 1998). In the latter case, an integral formulation of the coupling term is often employed, which takes the form of the convolution of the solute concentration with a memory function which reflects the geometry and the heterogeneity of the immobile region. While this method was initially developed for groundwater applications as a natural extension of the dual-porosity model, it has also been applied to fracture-matrix transfer (Geiger et al. 2011).

In this work, we present an implementation of the MRMT model based on the opensource finite volume library OpenFOAM that is suitable for simulating scalar transport in subsurface multiphase flows. This implementation comes as an extension of the open-source toolbox porousMultiphase-Foam (Horgue et al. 2015) that provides a series of novel features. First, we extend the Implicit Pressure Explicit Saturation (IMPES) method employed in the toolbox to non-orthogonal grids and strongly coupled systems by mean of a set of fixed point Picard iterations. Second, we implement a MRMT model for the solute concentration, which gives rise to a set of coupled equations, one for each immobile region. These equations are discretized implicitly in time, resulting in a semi-implicit method consisting in a pressure coupling loop enclosing a concentration coupling loop.

We discuss the numerical aspects of the MRMT model, comparing accuracy and performance of a monolithic solution of the MRMT equations (which are linearly coupled) against a segregated algorithm. Furthermore, results from the MRMT are compared against a range of test cases to assess its accuracy and efficiency. Our code is made available to the public through GitHub.

References:

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