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# A Lagrangian, stochastic modeling framework for multi-phase flow in porous media

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**Abstract**

Many of the complex physical processes relevant for compositional multi-phase flow in porous media are well understood at the pore-scale level. In order to study $CO_2$ storage in sub-surface formations, however, it is not feasible to perform simulations at these small scales directly and effective models for multi-phase flow description at Darcy scale are needed. Unfortunately, in many cases it is not clear how the micro-scale knowledge can rigorously be translated into consistent macroscopic equations. Here, we present a new methodology, which provides a link between Lagrangian statistics of phase particle evolution and Darcy scale dynamics. Unlike in finite-volume methods, the evolution of Lagrangian particles representing small fluid phase volumes is modeled. Each particle has a state vector consisting of its position, velocity, fluid phase information and possibly other properties like phase composition. While the particles are transported through the computational domain according to their individual velocities, the properties are modeled via stochastic processes honoring specified Lagrangian statistics. Note that the conditional expectations of the particle velocities are different for different fluid phases. The goal of this paper is to present the general framework for this alternative modeling approach. Various one and two-dimensional numerical experiments demonstrate that with appropriate stochastic rules the particle solutions are consistent with a standard two-phase Darcy flow formulation. In the end, we demonstrate how to model non-equilibrium phenomena within the stochastic particle framework, which will be the main focus of the future work.


*Keywords:* Stochastic particle method; Lagrangian approach; Porous media; Multi-phase flow; PDF method

## 1. Introduction

Flow and transport processes in natural porous media are usually described using differential equations defined on the macroscopic (Darcy) scale. For slow single-phase flow in a homogeneous porous medium, Darcy's law is an expression of momentum conservation at the macroscopic scale. When multiple immiscible

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fluid phases are present (e.g., oil, super-critical $CO_2$ and water), the permeability in Darcy's original equation is replaced by an effective value to accommodate the presence of other phases in the porous medium [1]. This effective parameter is expressed as a function of phase saturation and is called relative permeability. Macroscopic capillary effects are introduced by considering different pressures in the different fluid phases. The capillary pressure relations are also usually expressed as functions of saturation.

In addition to saturation, the relative permeability and capillary pressure relations depend on the pore-scale geometry, network topology, wettability characteristics, viscosity ratio of the fluids, and saturation history. The physical interactions that take place in the rock-fluids system at the pore (microscopic) scale dictate the behavior observed at the macroscopic scale. The complexity of the small-scale dynamics has precluded the development of a general approach that links the pore-scale physics and the representation at the Darcy scale [2]. Thus, in practice the relative permeability and capillary relations, which are assumed to be appropriate macroscopic-scale descriptions, are obtained by performing laboratory flow experiments using specimens (cores) of the porous medium of interest.

This simple Darcy scale representation of the relative permeability and capillary relations is thought to be applicable for two-phase flow under strongly wetting conditions when the viscosity ratio is close to unity, and the macroscopic flow is within a relatively small range of capillary numbers [3]. In other cases of practical interest, such as EOR (enhanced oil recovery) gas injection processes and the injection and post injection periods associated with $CO_2$ sequestration in aquifers and reservoirs, the application of this simple model is questionable.

The mean flow velocity of reservoir displacement processes is quite small (a few centimeters per day) and the characteristic pore size of the medium is also very small. So the Reynolds number is much less than unity, and the flow at the pore scale is expected to usually be in the Stokes regime, in which the inertial effects are negligible and the pressure drop takes place entirely due to viscous and capillary forces. In these cases, the problem at the pore level is well defined and can be solved, if the pore scale geometry is known. However, even a small sample of a real porous medium contains millions of pores and in most cases it is very difficult to obtain the complete description of the pore scale geometry [4].

While the small scale flow dynamics are interesting, the objective is to construct a model based on relations that represent the macroscopic (Darcy scale and larger) behaviors accurately. The model must account for the dynamic effects of the pore scale physics on the large-scale flow. In the standard approach, the assumption is that the pore scale physics is accounted for in the relative permeability and capillary relations, which are obtained from experiments. However, this standard treatment is not well suited, if the flow involves complex processes such as non-equilibrium phenomena and residual trapping. In such flows, a statistical approach is more appropriate, since a small elemental volume of the porous media contains a large number of pores. Here we develop a statistical method for multi-phase transport in porous media using stochastic particles.

Particle tracking methods have been employed successfully in subsurface flow simulations. From the pioneering works of [5,6], fully Lagrangian schemes based on random walk approach have been widely employed for tracer (i.e. unit-viscosity, miscible, single-phase) transport. Extension of the particle-tracking approach to more complex geometry [7] and reactive flows in highly heterogeneous formations [8] appeared later. A hybrid Eulerian–Lagrangian method, where particle tracking is employed to represent the transport, was developed and used to model unstable first-contact miscible (two-component, single-phase flow) displacements in the presence of density and viscosity differences [9]. In these particle tracking methods, each particle represents a physical mass. The concentration of the tracked species (e.g. tracer) is obtained by averaging over the control volume. Relatively large particle numbers and fine grids are necessary to obtain reasonably accurate concentration distributions in the domain.

Several Eulerian–Lagrangian schemes have been introduced for linear tracer transport (see, e.g. [10–14]) and extended to nonlinear problems such as solving the saturation equation for two-phase immiscible flow (see, e.g., [15–17]). Fully Lagrangian methods have also been applied to reactive-tracer transport with nonlinear accumulation term (see, e.g., [18,19]; or [20] for a comprehensive review), which requires the calculation of concentration at the node of a superimposed grid [21]. Unlike particle tracking schemes, here concentrations are propagated along path lines. Streamline-based methods, which belong to this family, have been developed for modeling multi-component multi-phase displacement processes in heterogeneous domains [22]. Character-