Use of Sγ momentums for the modeling of multiphase tracer transport in homogeneous porous media

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Keywords: Multiphase transport, Sγ momentum, break-up, coalescence, porous media.

Abstract. Droplets transport in homogeneous porous media has been found to be an attractive problem applicable in a lot of industrial and scientific sectors such as enhanced oil recovery, food production, plastics etc. As applications become wider, a predictive method for the process is warranted. To this end, it has been widely accepted that the collection of γ-order moments, Sγ, can describe the time evolution of any spatially averaged quantity like the mean diameter of spherical droplets, while it has been also found that Sγ satisfies the transport equations [1]. Here, the so-called "Sγ concept" is applied in a CFD module for the modelling of the transport processes occurred in a mixture of a continuous aqueous phase which includes a discontinuous one in the form of droplets. This mixture flows within a homogeneous porous medium under creeping or laminar flow conditions. The moments of the particle size distribution are evaluated using the local flow conditions as obtained from CFD simulations for the processes considered. To solve the transport equations, the microstructure droplets formation/destruction has been also taken into account by using already known analytical expressions for the source terms representing the break up and coalescence of the droplets [2-4]. The proposed constitutive model adequately simulates the effect of porous geometry on the droplets size distribution and could be helpful in understanding the phenomena that take place in microscopic scale.

Introduction

Given the difficulty in the description of a transient (dynamic) structure of spherical bubbles due to its high geometrical complexity, it is hard to define a globally valid model for the prediction of the time evolution for almost any process occurring in such a configuration. In the present study, the approach we take is the so-called 'moments of distribution', Sγ, where an arbitrary number of moments is used to describe the drop size distribution. The essence of the method is that the evolution of the moments of a distribution can be analyzed using a transport equation consisting of a convective term, which can be coupled to the local flow characteristics in a device. The source terms in the transport equation describe the local phenomena (break-up and coalescence) that affect on the particle size distribution. The main advantage of this approach is that analytical expressions (including probabilistic parameters) for the characteristic magnitudes could be derived, leading in successful simulations through common and rather simple CFD techniques.

The Moments of Distribution (Sγ) concept

The domain (particle) size distribution can be described by a collection of moments of the distribution as:

$$S_\gamma = n\int_0^\infty d^\gamma P(d)\mathrm{d}d \tag{1}$$

where n is the total number density and $P(d)$ is the distribution of the droplets. It is easy to show that for two different γ values, the S_γ functions can produce a useful characteristic diameter $d_{\gamma_1\gamma_2}$ according to the relation:

$$d_{\gamma_1\gamma_2} = \left(\frac{\int_0^\infty d^{\gamma_1} P(d)\mathrm{d}d}{\int_0^\infty d^{\gamma_2} P(d)\mathrm{d}d}\right)^{\frac{1}{\gamma_1-\gamma_2}} = \left(\frac{S_{\gamma_1}}{S_{\gamma_2}}\right)^{\frac{1}{\gamma_1-\gamma_2}} \text{ for } \gamma_1 \neq \gamma_2 \tag{2}$$

The main advantage of the Sγ function is that it satisfies a transport equation [1], i.e.

$$\frac{\partial S_\gamma}{\partial t} + \underline{u}\cdot\nabla S_\gamma = h_i^\gamma \tag{3}$$

where it has been assumed that the drops have the same velocity, $\underline{u}$, as the continuous bulk phase. Note that $\underline{u}$ can be obtained from the CFD flow calculations. The relevant source terms will be discussed separately below.

The source terms

To model the source terms in eq. (3), we assume an analytical expression for the particle size distribution, i.e. a log-normal distribution. Since the governing phenomena are the droplet break up, coalescence and growth, the source terms can be expressed as:

$$h_i^\gamma = h_{br}^\gamma + h_{cl}^\gamma \tag{4}$$

where h_{br}^γ and h_{cl}^γ are the respective source terms that can be modeled explicitly.

Break-up occurs when the droplet size is larger than a critical size d_{cr} as determined by the critical capillary number for laminar flow:

$$d_{cr} = \frac{2\sigma Ca_{cr}}{\eta_c \dot{\gamma}} \tag{5}$$

where Ca_{cr} is the critical capillary number, $\dot{\gamma}$ is the velocity gradient (shear rate for simple shear), η_c is the viscosity of the continuous phase and σ is the interfacial tension. That relationship depends on the viscosity ratio and the flow type, as has been discussed extensively [2,5]. The break-up source term, can be written as:

$$s_{br} = \int_0^\infty \left[\frac{d^\gamma}{\tau_{br}(d)}\left(N_f(d)^{\frac{3-\gamma}{3}} - 1\right)\right] n f(d)\mathrm{d}d \quad \text{for } d>d_{cr} \tag{6}$$

where $N_f(d)$ is the number of fragments formed and τ_{br} is the break-up time.

Since coalescence not only depends on the collision rate but also on the coalescence probability per collision [3], the generic form of the coalescence source term is [3,4]:

$$s_{cl} = \left(2^{\gamma/3} - 2\right)\left(\frac{6\varphi}{\pi}\right)^2 k_{coll}\, u_{rel}\left(d_{eq}\right) P_{coal}\left(d_{eq}\right) d_{eq}^{\gamma-4} \tag{7}$$

where φ is the volume fraction, d_{eq} is an equivalent (effective) diameter and $P_{coal}\left(d_{eq}\right)$ is the coalescence probability of a single collision event, calculated by using the model for partial mobile interfaces, developed by Chesters [3]. The product $k_{coll}\, u_{rel}\left(d_{eq}\right)$ represents the Smoluchowski collision rate.

Simulations

The flowchart of the simulation algorithm is shown in Figure 1. To define a realistic domain for the solution of the flow and mass transfer problem, a porous medium is constructed in the form of a spherical particle assemblage. Specifically, the representation of the biphasic domains under consideration is achieved by the random deposition of spheres of a given radius in a box of specified length. The structure is digitized and the phase function (equal to zero for solid and unity for the pore space) is determined to obtain the specified porosity (see Figure 2 for a sample medium of ε = 0.7243). The size of the digitized domains is 102×102×102 and the length of the simulation box is ten times the sphere radius.In the numerical simulations, the velocity field was computed numerically by solving the Stokes equations by taking into account the velocity vector, the pressure field and the fluid viscosity, respectively. The procedure for solving the 3D Stokes flow problem involves discretization in terms of cubic elements and was as follows [6-9]: At the pore level, a

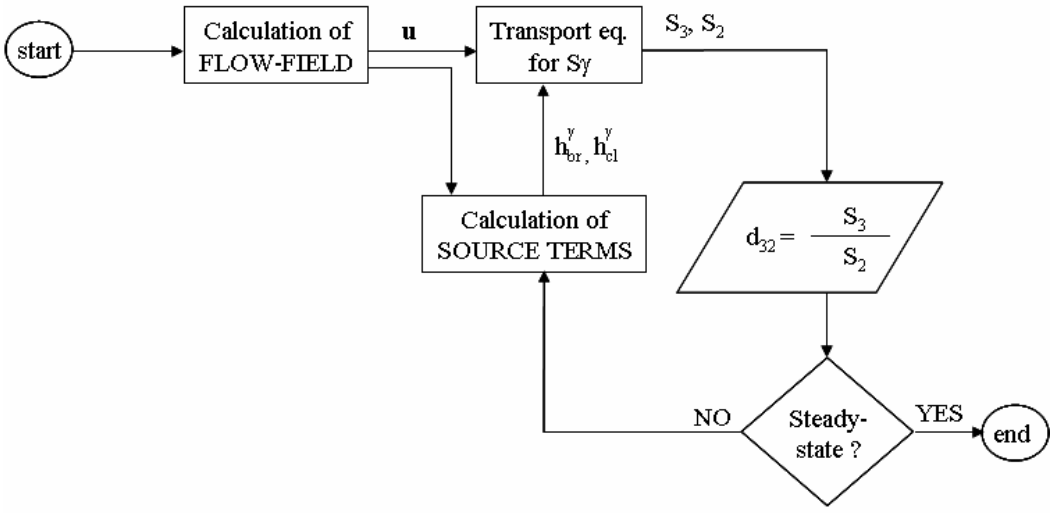

Figure 1: Flowchart of the simulation algorithm

staggered marker-and-cell (MAC) mesh is used, with the pressure defined at the center of the cell and the velocity components defined along the corresponding face boundaries. The resulting linear system of equations is solved by a successive over-relaxation (SOR) method. An initial guess for p is determined through the solution of a Laplace equation. Next, the velocity vector v is calculated from the corresponding momentum balance and the continuity equations. The pressure is corrected through an artificial compressibility equation. The above steps are repeated until convergence is reached. This numerical scheme for the determination of the velocity field has been widely validated

in terms of both the velocity field and the corresponding permeability. For the numerical solution of

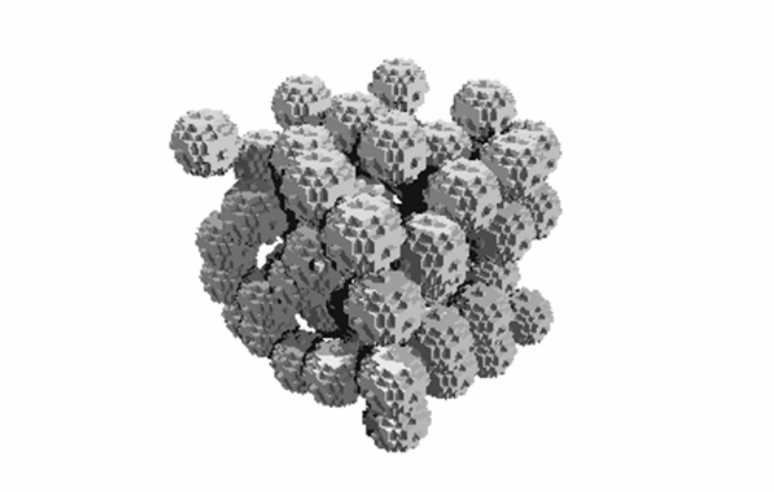

Figure 2: Stochastically constructed 3-D sphere assemblage

the transport boundary value problems, a non-uniform two-step Mac-Cormack method with upwinding [10] was used for discretization, with the resulting linear systems of equations solved using again SOR. For all the simuations, the porosity was 0.7243 and the Peclet number was set to 300 (having the spheres' radius as characteristic length), which is adequately represent the fully convective regime.

Results and Discussion

The time evolution of the droplet size is presented in Figure 3. A maximum followed by a

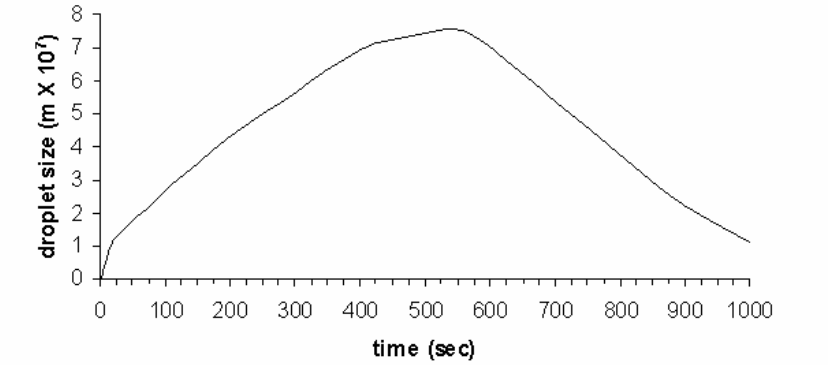

Figure 3: Droplets' size (d_{32}) distribution

minimum in size were observed due to the competition between the hydrodynamic phenomena (see discussion below). Finally, the droplet size increases monotonically for the longer time scales. This dynamic behavior of the system is clarified in Figure 4, where the relative significance of the source terms is shown. The individual source terms have been normalized on their maximum, i.e. $S_{br}=S_{br}/MAX\{S_{br}\}$, $S_{cl}=S_{cl}/MAX\{S_{cl}\}$, in order to be in the same graph. One can observe that during the first 550 seconds, coalescence dominates over the break-up as the particles are small, therefore, the droplet sizes increase. At t=550 sec the significances of break-up and coalescence are equal, thus the particle size goes through a maximum. After 550 seconds, break-up becomes more significant than coalescence, thus particle size decreases to a size, which is almost analogous to that of the initial population. It is worth noticing that the time considered for the simulation is critical for the

validity of the results since longer time periods correspond to rough iterations of the phenomenon. It is also found that the critical time for a single period depends on the flow characteristics. For the given porosity and velocity field was found to be 1120 sec, while higher velocities or lower porosities will lead to longer time periods.

Conclusions

In the present work, the S_γ concept has been applied to predict the microstructure formation in a mixture flowing in a homogeneous porous medium. This microstructure formation process is

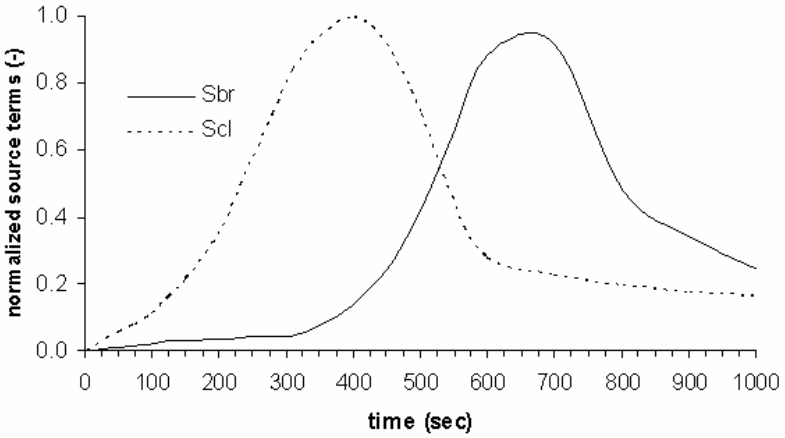

Figure 4: Relative significance of source terms

governed by the competition between the hydrodynamic phenomena, i.e. break-up and coalescence. Coalescence dominates at the first half of the process leading in a significant increment of the droplets' size. Since break-up becomes competitive at the late stage of the phenomenon, that size decreases up to a value almost equivalent to this of the initial conditions.

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