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ΕΡΕΥΝΗΤΙΚΟ ΙΝΣΤΙΤΟΥΤΟ ΧΗΜΙΚΗΣ ΜΗΧΑΝΙΚΗΣ
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Διευθυντής ΙΤΕ/ΕΙΧΗΜΥΘ

ΘΕΜΑ:
1. **Brownian dynamics of aerosol particle aggregate**
   Δυναμική κίνηση κατά brown συσσωματωμάτων αεροκολλοειδών σωματιδίων
2. **Immiscible two-phase flow in porous media**
   Ροή δυο μη-αναμείξιμων φάσεων σε πορώδη μέσα

ΤΟΠΟΣ: Αίθουσα Σεμιναρίων ΙΤΕ/ΕΙΧΗΜΥΘ

ΗΜΕΡΟΜΗΝΙΑ: Τετάρτη, 15 Δεκεμβρίου 2004

ΩΡΑ: 17:00

ΠΕΡΙΛΗΨΗ

1. A new model of the translational and rotational motion of rigid aggregates of aerosol particles has been developed, taking into account the stochastic Brownian force, gravity, and the hydrodynamic drag as a function of the size and shape of the aggregate. The model is used to simulate the dynamics of aerosol aggregates of various sizes and shapes, in order to extract the corresponding diffusion coefficient values. The diffusion coefficient, which is a second order tensor, is shown to be a strong function of the number of particles forming the aggregate (N), as well as of the detailed shape of the aggregate. In the case of aggregates composed of many particles, the norm of the diffusion coefficient tensor is much smaller (by a factor of ca. 10 for N=30 to a factor of 100 for N=500) than the diffusion coefficient obtained using the equivalent mobility radius method and other similar methods. For any given value of N, the diffusion coefficient varies considerably as a function of the overall shape and the internal structure of the aggregate. A simple analytical correlation between the expected value of the effective diffusion coefficient and the number of particles in the aggregate, N, can be obtained. These results are expected to have important consequences in the simulation of aggregation and filtration processes.

2. A recently developed predictive model (DeProF) considers steady-state two-phase flow in porous media (SS2φPM) as a composition of two experimentally observed flow patterns, namely CPF (connected-oil pathway flow) and DOF (disconnected oil flow). The latter (DOF) includes the motion of ganglia as well as of droplets so that the total flow is decomposed in three prototype flows, namely CPF, GD (ganglion dynamics) and DTF (drop traffic flow).
The key difference between these prototype flow patterns is the degree of disconnection of the non-wetting phase ('oil') which, in turn, affects the relative magnitude of the rate of energy dissipation caused by capillary effects compared to that caused by viscous stresses. The observed flow is usually a mixture of the basic prototype flows. Each flow pattern prevails over mesoscopic-scale regions of the porous medium (ranging from a few to several hundred pores), whereas the macroscopic flow is homogeneous in the absence of macroscopic inhomogeneity.
Analytical functions that incorporate all the basic pore scale flow mechanisms are derived for each prototype flow. Disconnected-oil flow is 'homogenized' at the unit cell level, yielding a hydraulic

conductance that is a function of the local pore geometry, the local flow arrangement, and the local flow velocity. The length-scale gap between micro- and macroscopic flow is bridged using EMT (effective medium theory). Then, all physically admissible (internally constrained) combinations of the prototype flows are determined. Postulating that each physically admissible flow combination has the same probability of being 'visited', we can evaluate the mean macroscopic relative contribution of each pattern to the total flow, as well as the 'expected' flow arrangement, flowrates and power dissipation.

The new model accounts for the non-linearity of the flow as well as for the effects of all the system parameters. The quantitative and qualitative agreement between several existing sets of adequately documented data and the corresponding theoretical predictions of the new model is excellent. In order further to exploit the predictive capability of the DeProF model, several macroscopic interstitial physical quantities corresponding to each prototype flow, as well as to the total flow, are determined. These quantities are: the magnitude of the domain of physically admissible solutions, the interfacial area per unit volume, the mechanical power dissipation per unit volume, and the degree of disconnectedness of the non-wetting phase. The dependence of these characteristic quantities on the values of the flow system parameters is presented in graph form, and a tentative suggestion for their use in the proper macroscopic phenomenological description of two-phase flow in porous media is made.