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ΕΡΕΥΝΗΤΙΚΟ ΙΝΣΤΙΤΟΥΤΟ ΧΗΜΙΚΗΣ ΜΗΧΑΝΙΚΗΣ
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ΦΡΟΝΤΙΣΤΗΡΙΟ - ΣΕΜΙΝΑΡΙΟ

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Διευθυντής ΙΤΕ/ΕΙΧΗΜΥΘ

ΘΕΜΑ: **1. Network of grains-in-cell model for swarms and beds of grains. Formulation and application to creeping flow and convective mass transfer processes**
2. Hierarchical simulator of the growth of biofilms and prediction of their effective permeability and diffusion coefficient

ΤΟΠΟΣ: Αίθουσα Σεμιναρίων ΙΤΕ/ΕΙΧΗΜΥΘ

ΗΜΕΡΟΜΗΝΙΑ: Τετάρτη, 24 Νοεμβρίου 2004

ΩΡΑ: 17:00

ΠΕΡΙΛΗΨΗ

1. A new model consisting of a 3-D network of hydraulic resistors is developed for the representation of granular porous materials and swarms of grains. A grain-in-cell model with appropriately distributed dimensions is used for the calculation of the conductivity of each resistor of the network. In the past, unit cell models have been used to model transport processes in homogeneous, loosely packed assemblages of uniform particles. However, randomly packed beds have a considerable degree of inhomogeneity in the local porosity and interconnectivity, even when they consist of monosized grains. These phenomena are accentuated in the case of multisized grains. Swarms, such as fluidized beds, display an even stronger degree of inhomogeneity, including extensive clustering and channeling features, because of the mobility of the grains. These inhomogeneities have strong effects on the *local* permeability and mass transfer coefficient, as well as on the corresponding macroscopic (effective) values.

The new model is designed to account for assemblage inhomogeneities and network-wide interactions. The size distribution of the grains, the distribution of the local porosity, the distribution of the local connectivity, and the various types and degrees of correlation among these distributions are taken into account explicitly, and the flow and mass transfer problems are solved on a network-wide basis, thus accounting for mesoscopic cooperative effects. This approach provides effective modeling of transport processes in heterogeneous grain beds and swarms

2. A new simulator is developed for the prediction of the rate and pattern of growth of biofilms, as well as the local and effective values of transport properties, notably of the hydraulic permeability and the diffusion coefficient. The simulator is based upon the concept that a typical biofilm constitutes a *hierarchical porous material*. This concept stems from the fact that biofilm contains pores with characteristic size ranging from a few hundreds of nanometers, in the tightly bound extracellular polymeric substances (EPS) matrix surrounding the cell membrane, to several tens of micrometers, in the water conduits traversing the overall biofilm structure. The structural hierarchy of a biofilm exhibits at least four structural levels: a macroscopic level (several tens of μm to few mm) which includes the entire structure of the biofilm, a mesoscopic level (few μm to several tens of μm) which includes a few cells and the surrounding EPS matrix, a microscopic level (several hundreds of nm to few μm) which contains a single microbial cell and, finally, a sub-microscopic level (several nm to few hundreds of nm) which refers to the polymeric fibers which constitute the EPS matrix and to various cellular organelles with emphasis on the cellular membrane. In the approach presented here, an appropriate structure representation model is developed and the creeping flow and passive diffusion problems are solved at all the appropriate structural levels.