Final Report: DOE-EPSCoR

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DOE Patent Clearance Granted

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Office of Intellectual Property Law

DOE Chicago Operations Office

A number of graduate students are involved at various level of research in this project. We investigate the basic issues in materials using Monte Carlo simulations with specific interest in heterogeneous materials. Attempts have been made to seek collaborations with the DOE laboratories. Following are specific details.

Graduate students:

Following graduate students have been involved in this project: A. Balasubramaniam, Frank Bentrem, Luise Para Cueva, Xiaoli Huan, V. Mandula, A Rajendran, V. Ramanujam, Jun Xie, and Shurong Zheng. Bentrem and Xie are advanced graduate students who are studying the interface growth in polymer deposition at an impenetrable substrate. Ramanujam and Rajendran were helping visualizing the growth process. Cueva is trying to model the transport properties of heterogeneous media using interacting lattice gas with the help of Monte Carlo simulations. Balasubramaniam, Huan, Mandula, and Zheng were helping with the role of random numbers in these simulations.

Progress and Outcome:

This project has been very productive and helped students in their education. we have found many interesting results which are presented in the following:

(A) Interface growth:

Monte Carlo simulations are performed to study the interface growth and roughness in electrophoretic deposition of polymer chains in three dimensional lattice. A coarse grained model of polymer chain is used where a chain of length N is generated on the trail of a random walk of N steps with excluded volume constraints. Chains are released from one end of the sample and driven by a field E toward the substrate at the opposite end. Kink-Jump (K), crank-shaft (C), and reptation (R) segmental dynamics are used to move chains with a Metropolis algorithm. We address the questions, how does the interface grow? How does the steady-state interface width scale with the parameters such as temperature (T), field (E), molecular weight?

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In a continuous deposition process, the interface width (W) is found to grow with power-laws in time before saturating to a steady-state value (W_s). Several interesting scaling laws are observed [1,2]. While the steady-state width (W_s) decreases (de-roughens) with the field, it increases (roughens) linearly with the temperature. The steady-state interface width increases monotonically with the molecular weight (N).

Relaxing the interface by stop releasing new polymer chains into the system while continuing the segmental movements leads to a much lower relaxed interface width (W_r). Scaling of the relaxed interface width (W_r) with the temperature depends on the type of segmental dynamics and the range of temperature. With the slow (short range (K)) segmental dynamics, W_r increases with the temperature. Adding faster modes of segmental motion (C, R) leads to a non-monotonic temperature dependence - a decay of W_r with T at low temperature regime is followed by an increase at high temperatures. In contrast to steady-state interface width W_s [3], the relaxed interface width (W_r) shows a stretched exponential decay with the molecular weight. Faster segmental dynamics such as crank-shaft and reptation are essential to achieve equilibrium for both density profile and interface width [3,4] within the course of our simulations.

(B) Aggregation, segregation, and flow at the surface:

Aggregation, segregation, and flow of polymer chains on a heterogeneous surface are studied in presence of a field E with a hybrid Monte Carlo simulation [5]. The hybrid method involves a large-scale global stirring or equilibration to accelerate the simulation followed by a small-scale local mixing or equilibration to capture the details of the system. Several interesting observations are made. In general, effects of field, heterogeneity (i.e. the impurity or barrier concentration), and temperature on aggregation and desegregation of chains with low molecular weight are found to be different from that with high molecular weight. For example, at low molecular weight polymer, the impurity barriers act as seeds for pinning the growth of molecular aggregates that lead to larger aggregates at lower impurity concentration at low temperature. At high temperature, in contrast, larger aggregates appear at higher impurity concentration where pinning of aggregates is augmented by cluster of clustering. Dynamics of polymer chains varies from drift-like motion for short chains to strongly subdiffusive for long chains in various impurity concentration and field regimes. Linear and non-linear response of the flow rate are also identified in these regimes.

(C) Permeability of the granular heterogeneous media:

Attempts are made to study the flow of fluid through porous media formed by sediments in geomarine environment. Using an interacting lattice gas model for fluid, we study the fluid flow through such media by Monte Carlo methods [6,7]. In particular, we are studying the effect of temperature and pressure gradients on the flow rate response and evaluate the permeability. Very recently, we have examined the effect of porosity on the permeability of miscible fluid mixture and found that the permeability scales with a power law near pore percolation threshold [8].

References:

- [1] Electrophoretic deposition of polymer chains: a Monte Carlo study of density profile and conformation, G.M. Foo and R.B. Pandey, *Biomacromolecules*, 1, 407 (2000).
- [2] Roughening, deroughening, and nonuniversal scaling of the interface width in electrophoretic deposition of polymer chains, Frank W. Bentrem, R.B. Pandey, and F. Family, *Phys. Rev. E* 62, 914 (2000).
- [3] Interface relaxation in electrophoretic deposition of polymer chains: Effects of segmental dynamics, molecular weight, and field, F.W. Bentrem, June Xie, and R.B. Pandey, *Phys. Rev. E* 65, xxx (2002).
- [4] Density and conformation with relaxed substrate, bulk, and interface in electrophoretic deposition of polymer chains, F.W. Bentrem, June Xie, and R.B. Pandey, *J. Molecular Structure (THEOCHEM)* (2002, in press).
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- [6] A monte carlo simulation of thermal driven fluid: flux rate and density profile, R.B. Pandey and J.F. Gettrust, *Physica A* 293, 93 (2001).
- [7] Concentration gradient, diffusion, and flow through open porous medium near percolation threshold via computer simulations, R.B. Pandey, J.F. Gettrust, and D. Stauffer, *Physica A* 300, 1 (2001).
- [8] Density Profile and Flow of Miscible Fluid with Dissimilar Constituent Masses, R.B. Pandey, D. Stauffer, R. Seyfarth, Luis A. Cueva, J.F. Gettrust, and Warren Wood, *Physica A* (2002, in press)

Efforts to collaborate with DOE laboratories:

Attempts are made to identify research groups at DOE laboratories with overlapping research interests: Oak Ridge National laboratory and Lawrence Berkeley laboratory. A visit is made at the ORNL on May 16, 2000 with the research group of Dr. Hank D. Cochran, Leader, Fluid Structure and Properties Group Chemical Technology Division. A talk was given on our on going research and prospect of collaboration was discussed. The DOE workshop at the LBNL was attended and attempts were made to identify research groups from the DOE participants, i.e., we are interacted with the research group of Dr. Horst D. Simon at the National Energy Research Scientific Computing (NERSC), LBNL.

Expenditure of the Budget:

Our finance office will submit the details of expenditure.