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Fluids under Confinement: A Computer Simulation Study

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It is well known that when fluids are confined in small pores, their properties change from those in bulk. The thermodynamics, for instance is modified; the phase diagram is strongly affected by the pore size and by the interaction of the fluid with the pore surface. Moreover, the coexistence lines of the fluids are shifted respect to the bulk as a result of the confinement. They might be shifted towards higher or lower temperatures depending on the fluid and the pore characteristics. On the other hand, the dynamics and the structure of the fluids can also be modified in narrow pores.

By small geometries, we mean pores of sizes comparable with the dimension of the fluid molecular--diameter, i.e., from few to dozen of molecular diameters. In this case, the wall--geometry and the interactions between the fluid and the pore--walls play an important role.

What is the nature of the new phase transitions? Are there well defined triple or critical points in these systems? Is the structure of the confined fluid the same as in bulk? How are the transport properties of the fluid affected by confinement (i.e. diffusion coefficients, viscosity, etc.)? Those are important questions that will help us to understand or much better describe processes in tribology, chemical engineering, adsorption, oil extraction, catalysis, etc.

Therefore, the phenomena have been studied from different perspectives. From theoretical approximations, people for instance have used density functional theories to study capillary condensation by minimization of the Grand potential functional. From the experimental perspective, people have used different techniques such as mass and volumetric adsorption, optical, ultrasonic velocity and attenuation, differential scanning calorimetry, heat capacity, neutron scattering and surface force apparatus to investigate confined fluids.

However, over the last years, computer simulations became an important tool to study such interfacial systems from a microscopic point of view. Particularly, the study of confined fluids has been conducted by two classical computer simulations approaches: Molecular Dynamics and Monte Carlo. The major advantage of computer techniques is the possibility to obtain more information of dynamical, thermodynamical and structural properties of confined fluids from a molecular level, which sometimes are not easy to obtain from real experiments. For instance, computer simulations allow us to investigate fluids at high pressures or at low temperatures in experimental conditions that are difficult to reach. Certainly, computer simulations have also limitations and people should carefully analyze the results especially if they want to compare them with experimental data. Classical computer simulations need information about the potential interactions of all molecules in the system, so in order to have a realistic approximation, it is necessary to have an adequate force field of the system which can be complicated to obtain. Nevertheless, I believe computer simulations are a different alternative to carry out these kinds of investigations with good results.

Finally, it is important to mention that traditionally there were only two major approaches to address problems in science and engineering: theory and experiments. However, with the invention and rapid growth of the computers, computer simulations have become of crucial importance in the study of different processes. They are not theory neither experiments, although, people with theoretical background consider them as experiments and people with experimental background consider them as theory. In fact, from my point of view, they complement our investigations and they should be considered as a practical, different and independent way to study scientific and technological problems.

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