Molecular simulation of fluid-fluid interfaces in reacting systems

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It has been proposed the study of the interfacial behaviour of a reacting system by molecular simulation techniques based on the Monte Carlo method [1,2]. The nature of the reactive processes at microscopic scale may be studied from the Statistical Mechanics point of view, and therefore, they can be subject to study of Molecular Simulation [1,2]. In a great deal of natural as well as industrial systems, reactive processes take place through fluid-fluid interfaces, as it generally happens in many atmospheric chemical processes. The approach employed to perform the simulation of a reacting system is based on the Reactive Monte Carlo method [3,6].

The reactive system subject to study is based on bidirectional reactions without electrostatic charges and follows the pattern $2A \rightleftarrows B$. This reaction is studied in inhomogeneous systems which present fluid-fluid interfaces. The molecules which form the system are modelled as components with spherical symmetry interacting through the Lennard-Jones intermolecular potential [1,2]. This potential is truncated at a cutoff distance, r_c, what allows to evaluate a finite number of interactions (each particle interacts only with those that are within a sphere centered in itself and whose radius is r_c). The remaining interactions by pairs with the rest of the molecules of the system are evaluated applying long-range corrections, which take into account the interactions between each atom with the rest of atoms which form the system, and located beyond the cutoff distance. In order to implement long-range corrections, the methodology, firstly developed by Janecek [17] and later modified by MacDowell and Blas [8] will be used. That allows a greater accuracy in the study of reactive equilibrium. Special attention is paid to the fluid-fluid interfacial tension, therefore methods based on techniques for the pertubation of the interfacial area [9] are employed, specially the Test-Area method [10].

Since the chemical behaviour of a reactive system is determined by environmental factors, it is important to study the effect of interfaces over the chemical equilibria, as well as the effect of these equilibria over the interfacial properties. In summary, there are three lines which are presented in this work: 1) study of the equilibrium in reactions following the pattern $2A \rightleftarrows B$ in inhomogeneous systems, by employing the Reactive Monte Carlo method; 2) implementation of the long-range corrections (MacDowell & Blas); 3) study of the fluid-fluid interfacial properties in reactive systems.

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