

**DESCRIPTION OF EQUILIBRIUM LIQUID INTERFACES  
IN NONIONIC FLUIDS BY MULTILAYER QUASICHEMICAL APPROACH***Sorina P.O., Victorov A.I.*

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Planar and curved liquid interfaces occur in many different systems such as micellar solutions, mixtures of oil with water, microemulsions and other partially miscible liquids. The interfacial properties of such systems play crucial role in many fields, including oil-recovery, drug delivery, micellar catalysis, etc. Engineering applications of these spatially nonuniform systems need understanding of thermodynamic behavior that requires knowledge of the structural details of the interfacial boundaries. Most theoretical approaches proposed for such systems are limited to weakly interacting functional groups of molecules, as they do not take into account the correlations between interacting species [1, 2]. For nonuniform fluids that contain chainlike and associating species, most powerful instruments to predict structural details are computer simulations and iSAFT [3]; however, their application is rather involved computationally.

In this work, the description of local structure for liquid interfaces is performed with the aid of the multilayer quasichemical model (MQuM) [4, 5]. The model takes into account specific interactions between functional groups and connectivity of chainlike molecules. Correlations between interacting groups are described within the Guggenheim quasichemical approximation. The local structure of the interface is presented by the concentration profiles of the molecular segments, the profiles of orientations of the functional groups and chemical bonds of molecular chains in three directions. Within the model, we calculate the profiles of normal and tangential pressure and the interfacial tension for amphiphile-oil-water, alcohol-water, alkane-water and other organic-water systems. We also demonstrate the effect of chain branching on the structure and thermodynamic properties of fluid interfaces.

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