Parameter Estimation on Molecular Models of Complex Fluids by Stochastic Optimization Techniques

March 9, 2017

Abstract

With the rising of the study of some ionic liquids, many mathematical problems have appeared, as, for example, complex roots of nonlinear systems and the best parameters for fitting experimental data. This work presents a schematic way to solve these problems, but based on a thermodynamic model that has all of the mentioned obstacles. The scheme uses stochastic techniques as a central tool. The results by using these techniques allow to obtain good parameters that can predict some facts in the interaction of the ionic liquid with low concentrations of water. Another important fact of the present work is that by using this scheme, it is possible to save computational time and obtain results in a matter of hours.