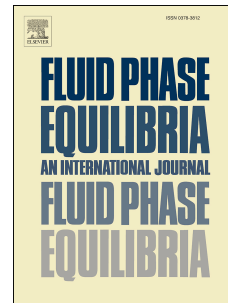


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Numerical aspects of classical Density Functional Theory for one-dimensional vapor-liquid interfaces

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Abstract

This study compares different algorithms for solving the equations of classical density functional theory for the one-dimensional vapor-liquid interface of real fluids: Picard iteration, Anderson mixing, a restarted quasi Newton method and two versions of the matrix-free inexact Newton method, one using analytic the other using numerically approximated derivatives. All algorithms converge to the same density profiles in all studied test cases. The calculation **time** of the slowest algorithm (Picard iteration), however, is up to twenty times longer than for the fastest algorithms (Anderson mixing and inexact Newton method with numerically approximated derivatives). Further, the computational speed-up of parallelization and of a convergence criterion based on the value of surface tension instead of the decrease of the norm of the residual are discussed. A Helmholtz energy functional consistent with the **perturbed-chain statistical associating fluid theory** (PC-SAFT) is applied which includes contributions due to hard-sphere repulsion, chain formation, dispersion as well as association. For the association term, we compare two widely used functionals.

Keywords: Classical density functional theory, **Surface tension**, PC-SAFT, Numerical methods, PETSc

1. Introduction

Classical density functional theory (DFT) is a versatile framework to study the properties of inhomogeneous systems and has been applied to many problems in chemical engineering and material science [1] [2] [3] [4]. It is based on a thermodynamic minimization principle: at equilibrium the grand potential Ω of a system consisting of N components at given values of temperature T , volume V and chemical potentials μ_i ($i = 1, \dots, N$) is minimal with respect to internal degrees of freedom. For inhomogeneous systems, the grand potential is a functional of the spatially varying density. The goal of DFT applications is to determine the equilibrium density profiles $\rho_i(\tilde{\mathbf{r}})$ as an internal degree of freedom iteratively until Ω has reached its minimum. The functional derivatives of Ω with respect to the density profiles are thus zero at equilibrium

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