Modeling and Calculations of Liquid-Vapor Interfacial Properties

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Due to very low thickness of interfacial region in vapor-liquid or liquid-liquid equilibrium systems, it is extremely difficult or even impossible in practice to obtain thermophysical properties of the system at this region. Computer simulations have been done using different approaches of molecular dynamics or Monte-Carlo methods. In spite of obtaining exact simulation results with powerful and fast processors, the required cpu time for convergence is a challenge in the area. To overcome the difficulty another approach has been proposed based on mathematical manipulations of thermodynamic relations to obtain a consistent system of equations which leads to find exact and reliable results in the shortest possible time by fewer calculation compared to the simulation methods. From equilibrium thermophysical properties, determination of interfacial surface tension, interfacial region thickness and density profile at this region have especial importance. Surface tension is a macroscopic thermophysical property of fluids that can describe lots of natural phenomena applicable in industry. This property influences on the processes such as boiling heat transfer, condensation, fluid flow in micro channels, electronic circuit cooling systems, inkjet printers and many other applications. Study of mass, heat, and momentum transfer phenomena between two phases at vapor-liquid equilibrium is possible by determining interfacial region thickness of phases. In the present work thermophysical properties are obtained using thermodynamical modeling approach based on the van der Waals mean field theory of capillarity. Van der Waals classical mean field theory has been applied for modeling and calculation of liquid-vapor interfacial properties of 25 systems using Redlich-Kwong (RK), Soave-Redlich-Kwong (SRK), and Peng-Robinson (PR) equations of state. Volume shift correction as well as the critical pressure correction methods were successfully applied in this work to obtain better agreement between experimental and calculated data. The proposed formulation based on the RK equation of state showed the best agreement between experimental and calculated values of interfacial tension.