Thermodynamic Quantities of Square-Well Gases at Isobaric Process

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The thermodynamic functions for square-well gases evaluated till the third virial coefficient are investigated at an isobaric process. Some thermodynamic functions are analytically expressed as functions of intensive variables, temperature, and pressure. Some thermodynamic quantities for H_2O are calculated numerically and drawn graphically. In critical states, the heat capacity, thermal expansivity, and isothermal compressibility diverge to infinity at the critical point while the Gibbs free energy, volume, enthalpy, and entropy are continuous at the critical point. In the coexistence of two phases, the boiling temperatures and the enthalpy changes of vaporization are obtained by numerical calculations for 16 substances. The Gibbs free energy indicates a polygonal line; entropy, volume, and enthalpy jump from the liquid to the gaseous phase at the boiling point. The heat capacity does not diverge to infinity but shows a finite discrepancy at boiling point. This suggests that a first-order phase transition at the boiling point and a second-order phase transition at the critical point may occur.

Key words: Square-Well Potential; Gibbs Free Energy; Isobaric Process; Critical Constants; Enthalpy Changes of Vaporization; First- and Second-Order Phase Transition.