Abstract Submitted for the MAR05 Meeting of The American Physical Society

Phase equilibrium predicted by the Soave-Redlich-Kwong equation at low temperatures KIMBERLY WADELTON, Sweet Briar College, MICHAEL MISOVICH, Hope College — This study developed vapor-liquid equilibrium relationships for vapor pressure and liquid density predicted by the Soave-Redlich-Kwong cubic equation of state (SRK) in the low temperature limit. Dimensionless variables were defined to simplify calculations. One, reduced density, was defined by dividing the actual density by density in the zero temperature limit. During this process, a useful form of the SRK equation was developed. Vapor pressures and phase densities were calculated numerically using a regula-falsi procedure. The method gave efficient calculations for reduced temperatures from approximately 0.0002 to approximately 0.9999. By manipulating the numerical data for reduced pressure and reduced temperature, functional relationships were suggested and verified analytically. Results of the predictive equations for reduced pressure were compared to the numerical results and differed at worst within one order of magnitude over the temperature range from zero to the critical point. Further modeling of the difference between the predictive equations and the actual SRK results is suggested.

> Kimberly Wadelton Sweet Briar College

Date submitted: 29 Nov 2004

Electronic form version 1.4