# Molecular Dynamics Simulations and Global Equation of State of Square-Well Fluids with Variable Well-Widths

S.B. Kiselev[C,S] and J.F. Ely
*Chemical Engineering Department, Colorado School of Mines, Golden, CO, U.S.A.*
*skiselev@mines.edu*

J.R. Elliot, Jr.
*Chemical Engineering Department, The University of Akron, Akron, OH, U.S.A.*

One of the fundamental problems in statistical mechanics is to calculate the thermodynamic and interfacial properties of fluids resulting from the interactions between their molecules. The square-well (SW) potential model is the simplest model that incorporates both repulsive and attractive interactions, and has been extensively studied over the last few decades by computer simulations. In this work, we present the results of extensive new molecular dynamic (MD) simulations in the one-phase region for square well fluids with well widths, L = 1.10, 1.15, 1.20, 1.25, 1.375, 1.50, 1.75, 1.90, 2.0, and 2.10. These data have been used in developing a crossover equation of state (CR EoS) for square-well fluids, with the well widths $1.1 < L < 2.1$, which incorporates non-analytic scaling laws in the critical region, and in the limit of low densities yields the exact second and third virial coefficients. Also, in the high-temperature region, it reproduces first-order perturbation theory results. The CR EoS was tested against our new MD simulations, and earlier MD and Monte-Carlo (MC) simulations obtained by other authors, as well. Excellent agreement between calculated values and simulation data for all SW fluids is observed. In combination with the density-functional theory, the CR EoS is also capable of reproducing surface tension simulations with high accuracy. Application of the CR EoS for solid-liquid equilibrium calculations, in combination with the Lennard-Jones and Devonshire cell model for the solid phase, is also discussed.