Specific Mixing Rules: Test and Application

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We start from the Helmholtz energy F being written as the sum $F = F_H + F_A + F_D$ where F_H is the hard-body contribution, F_A the attractive dispersion force contribution and F_D the dipolar contribution. In each of these terms some substance specific parameters like a characteristic density or a characteristic temperature occur. In the case of mixtures we need mixing rules for these parameters. If different sets of mixing rules are used in F_H, F_A and F_D we call them"specific mixing rules." A specific mixing rule for F_H was given by Boublik and Mansoori. Here, we discuss specific mixing rules for F_A and F_D. For F_A, several specific mixing rules will be tested for Lennard-Jones model mixtures by comparison with molecular simulation results. In particular, these tests are performed for vapor-liquid-phase-equilibria obtained with the NpT + test particle method. For F_D, we show again by comparison with simulation data that one mixing rule derived from perturbation theory works very well. Using these validated mixing rules, we enter the recently presented BACKONE family of equations of state and present thermodynamic properties including phase equilibria for the two binary mixtures methane + ethane and xenon + methylflouride. It is remarkable that only one state-independent parameter is needed for the description of each mixture.