The Volume Translated Peng-Robinson Group Contribution Equation of State - Actual Stage of Development and Typical Applications

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For the development and design of industrial processes, reliable knowledge of the real behavior of pure compounds and their mixtures as a function of pressure, temperature, and composition, in particular phase equilibria, is most important. Assuming that 1000 components are of technical interest, vapor-liquid equilibrium data for approximately 500 000 binary systems are needed to fit all required binary interaction parameters. Due to the fact that the measurement of all needed properties is nearly impossible, the process engineer depends on factual data banks. Besides the different phase equilibria, the Dortmund Data Bank as a comprehensive factual data bank for thermophysical properties contains nearly all worldwide available pure component, excess, and transport properties. But unfortunately, only a very small part of the experimental data for fitting the required binary model parameters are available. Since the assumption of ideal behavior for the missing binary systems can be very erroneous, powerful predictive thermodynamic models have been developed. Group contribution methods allow the prediction of the required phase equilibrium data using only a limited number of group interaction parameters. To cover sub- and supercritical conditions, group contribution equations of state have to be applied. They automatically take into account both phases and can be used up to high pressures and supercritical conditions. This allows for example the calculation of phase envelopes. Furthermore, the introduction of Henry coefficients for gaseous compounds is not required. At the same time, enthalpies, heat capacities, densities and so on are directly accessible. Today, the most sophisticated group contribution equation of state is the volume translated Peng-Robinson group contribution equation of state VTPR. The limited range of applicability is currently being further developed within the UNIFAC consortium (www.unifac.org). We will present the current stage of development and demonstrate the suitability as a universal model in the area of process design.