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Two-parameter equations of state like PR or SRK predict a universal critical compressibility, factor for pure compounds, being intrinsically unable to reasonably describe the PVT properties of different fluids and their asymmetric mixtures, which require at least three component specific parameters in the density dependence. In this paper, we have explored the capabilities of the Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) and the Simplified Perturbed Hard Chain Theory (SPHCT) equations of state to represent pure compound properties. Original parameters published by their respective authors overestimate critical temperatures, which is detrimental for the study and design of supercritical separation processes. Therefore, we have investigated here the performance of rescaled parameters for each model, i.e. those matching the experimental critical temperature and pressure of pure compounds. The rescaling of the size and energetic parameters as implemented in recent works in the literature was found to provide poor results, and instead a simple procedure to obtain optimized rescaled parameters from only T, P_c and the acentric factor is proposed. These parameters show a regular behaviour for n-alkanes with PC-SAFT and their performance is tested in this work also for carbon dioxide, using the recent equations by Span and Wagner as reference data. The proposed parameters reproduce vapour pressures with the same accuracy of PC-SAFT original parameters but assure an exact representation of the experimental critical pressure and temperature. However, this is achieved at the expense of underestimated liquid densities, this limitation being common to different models and becoming more pronounced for larger molecules. (c) 2005 Published by Elsevier B.V.

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