Generalized calculation of pure saturation properties using cubic equations of state

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Abstract

Little attention has been given to the bubble temperature problem of a pure component in academic field. A robust methodology for solving the pure saturation temperature (vapor temperature) is proposed by using cubic equations of state. The methodology is based on a Newton-Raphson iterative technique for solving phase equilibrium criteria, coupled with initialization procedures. This methodology is free of numerical pitfalls from the critical point to very low reduced pressure. The fact that the given pressure is equal to the pressure at the inflection point of the initial temperature isotherm yields an automatic initialization of the calculations inside a region of convergence where the EOS can always predict vapor temperatures. In addition, the initialization method can also be used to calculate vapor pressures. Examples for vdW, RK, SRK and PR EOS show that the methodology can give perfect predictions for saturation properties even at very low reduced pressure and temperature.

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