Refrigeration Cycle Design By Molecular Simulation

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We describe a molecular simulation methodology to calculate the properties of a vapor-compression refrigeration cycle, and its coeffcient of performance, in the case when the refrigerant is a mixture. The methodology requires only a molecular force-field model for each refrigerant pure component and expressions for the vapor pressure curves of the pure components. The former is readily constructed, and the latter is available in the literature or may be estimated by empirical formulae. The approach involves a combination of several available computer simulation techniques for the individual processes of the cycle. We describe the methodology in the case of binary and ternary refrigerant mixtures. This extends our earlier work in cases when the refrigerant is a pure fluid. The simulations entail the calculation of bubble- and dew-point curves for refrigerant mixtures, for which we describe a new approach. We compare the results with those obtained from the Equation-of-State model used in the standard REFPROP software and available experimental data for the test case of refrigerant 507A, a 50 weight % mixture of R125 (CHF_2CF_3) and R1431 (CH_3CF_3).