Calculation of Heat Capacity for Supercritical Fluids

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The equation of state of a substance can be employed to estimate heat capacity. The values of the constants appearing in equations are based on the behavior of the pressure, temperature and specific volume of fluids. The equation of state obtained in above method can represent accurately the behavior of the pressure, temperature and specific volume. But it is not suitable to use the equation of state to calculate the heat capacity because the deviation is enlarged by the second derivatives. The calculation deviation of heat capacity can be reduced by using the constants appearing in equations based on behavior of the heat capacity, temperature and specific volume. The function, which was applied to calculate the heat capacity of supercritical fluids in this paper, was based on the Modified Benedict-Webb-Rubin (MBWR) equation of state. The constants appearing in the function were determined by the actual behavior of the heat capacity, temperature and specific volume. The residual function method and modified item was used in the MBWR equation of state to calculate heat capacity for a supercritical fluid. The results compared with literature data show that the function is applicable to the prediction of heat capacity for supercritical fluids. A simple function also was developed to predict heat capacity for a supercritical fluid based on the above research. It is simple and convenient for the calculation of heat capacity. The new simple function has deviations similar to those of the complicated function.