Development of an Empirical Multiparameter Equation of State for the Reactive NO_2+N_2O_4 System

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The information about fluid properties are crucial for the development, control and simulation of current and new energy technologies. Today's standard in accurately calculating these properties is through the use of multiparameter equations of state in terms of the Helmholtz energy. For many fluids in industrial processes, these empirically based equations are used along with combination rules that enable the computation of mixture properties. However, not all substances occur in a pure state, instead, they exist in chemical equilibria with other substances, where the equilibrium composition depends on temperature and pressure. One of these reactive mixtures is the NO_2+N_2O_4 system. Due to the presence of NO_2 in flue gases and its impact on Earth's atmosphere, it is an important component in combustion related technologies, such as CCS processes. Whereas, N_2O_4 presents a commonly used oxidizer for rocket fuels. Considering their importance in technical applications, a new equation of state for the equilibrium of N_2O_4 and NO_2 is under development. As a first fundamental equation of state for a reactive mixture, multiple enhancements had to be implemented in order to fit this functional form. These included the computation of the equilibrium composition as a function of temperature and pressure, which implies a changing molar mass and requires the calculation of the isobaric heat capacity from the enthalpy of reaction. The current status of the present equation describes the whole fluid area at temperatures of 262 K ≤ T ≤ 835 K and pressures of p ≤ 60 MPa. While the equation yields reasonable results for densities, the calculation of the speed of sound and heat capacities exhibits shortcomings due to a second decomposition of NO_2 into NO and O_2, which still has to be investigated.