Analytical approximation of thermal and calorific real-gas equations of state within wide ranges of density and temperature for internal ballistics applications

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For the improvement of operation process in chemical propulsion units, CFD methods are becoming more and more important. Predictability can only be reached with detailed physical and chemical submodels. The basis for state-of-the-art CFD codes is still the assumption of ideal gas properties. The assumption of ideal gas behavior is known to be valid for low-density gases, when interaction of molecules is negligible. However, thermodynamic conditions in modern propulsion units can be out of the range of validity of the ideal gas approximation, in particular, in local regions with high pressure and low temperature. At these conditions, real gas effects must be taken into account. In this paper, analytical thermal and calorific real-gas equations of state for main chemical species (H2O, CO2, CO, H2, N2, O2, and n-alkanes) relevant to combustion detonation, propulsion, and internal ballistics problems have been derived. The equations contain only 7 parameters and provide the error less than 1% (in average) at temperatures from 500 to 2000–2500 K and densities up to the critical density.