Short Fundamental Equations of State for Industrial Fluids

E.W. Lemmon [C, S]
Physical and Chemical Properties Division, National Institute of Standards and Technology, Boulder, CO, U.S.A.

R. Span
Thermodynamik und Energietechnik, Universität Paderborn, Paderborn, Germany

In a preceding project, functional forms for "short" Helmholtz equations of state for typical non- and weakly polar fluids and for typical polar fluids were developed by simultaneous optimization. The coefficients of these equations of state were fitted to data sets of 15 non- and weakly polar fluids and of 12 typical polar fluids, which were mostly used in the simultaneous optimization procedure; see [1–3].

In this project, equations of state have been developed for the fluids carbon monoxide, carbonyl sulfide, decane, hydrogen sulfide, krypton, nitrous oxide, nonane, sulfur dioxide, toluene, xenon, R-116, R-141b, R-142b, R-218, R-227ea, R-23, and R-41. The functional forms used are identical with those described above – only the 12 coefficients of the equations of state were fitted to substance specific data sets, while the simultaneously optimized functional forms (the combination of polynomial and exponential terms with the temperature and density exponents) were left unchanged. The results prove that simultaneously optimized functional forms can be applied to other fluids out of the class of fluids for which they were optimized without significant loss of accuracy. The high numerical stability of the functional forms resulted in fits which could not be described previously by accurate empirical equations of state. Typical uncertainties of properties calculated using the new equations are 0.2% in density at pressures up to 30 MPa, 0.5% at higher pressures, 1% to 2% in heat capacities, and 0.2% in vapor pressure. Deviations in the critical region are higher for all properties except vapor pressure.

References:

[1] R. Span and W. Wagner, Equations of state for technical applications. I. Simultaneously optimized functional forms for nonpolar and polar fluids, Int. J. Thermophys., in press.

[2] R. Span and W. Wagner, Equations of state for technical applications. II. Results for nonpolar fluids, Int. J. Thermophys., in press.

[3] R. Span and W. Wagner, Equations of state for technical applications. III. Results for Polar fluids, Int. J. Thermophys., in press.