Fundamental Equation of State for Hydrogen Chloride

Monika Thol [C, S]
Thermodynamics, Ruhr-Universität Bochum, Bochum, Germany
m.thol@thermo.rub.de

Lorenzo Piazza
Ferchau Engineering GmbH, Kiel, Germany

Roland Span
Thermodynamics, Ruhr-Universität Bochum, Bochum, Germany

Designing thermodynamic processes in an efficient and energetically optimal way requires exact knowledge of thermodynamic properties of the applied fluids. Therefore, special algorithms were devised to develop technical equations of state. For many fluids that are interesting for industry and science only few experimental data sets are available. Thus, functional forms developed by simultaneous optimization are used. Those functional forms are not optimized for one special fluid, but for a group of fluids, and are based on fluids out of this group that are well investigated. In this way the accuracy can be increased, and the extrapolation behavior as well as the behavior in regions with few experimental data is improved. The simultaneously optimized functional form can be used to fit the fluid specific parameters for fluids that are less well investigated. The resulting equations of state are numerically stable and quite accurate. This approach was applied for polar and weakly associating fluids. Because of challenging fluid properties (e.g., toxicity, corrosion, acid formation when being in contact with water, etc.) it is quite difficult to measure properties of hydrogen chloride. Only few experimental data are available. Hence a new functional form for polar and weakly associating fluids was developed by the help of the simultaneous optimization established by Span and Wagner[1]. It was based on ammonia and methylene fluoride, because both fluids are well investigated and reference equations of state are available[2,3]. Dimethyl ether, diethyl ether, hydrogen sulfide, hydrogen chloride, methyl chloride, and methyl fluoride were included in the simultaneous optimization process as well. In this way an equation of state for hydrogen chloride was developed. It is valid for temperatures T = 155 – 330 K and pressures up to p = 20 MPa. In general, the uncertainties of calculated properties match the required standards for advanced technical equations of state in the given range of validity and the extrapolation behavior is reasonable.

[1] Span R., Wagner W., *Int. J. Therm. Physics*, 2003, 24:1, 491-500
[2] Tillner-Roth R., Harms-Watzenberg F., Baehr H. D., *DKV Tagungsbericht*, 1993, 20, 167-181
[3] Tillner-Roth R., Yokozeki A., *Chem. Ref. Data*, 1997, 26:6, 1273-1328