Comparison of Theoretically Calculated Thermal Conductivity Values of Dilute Water Vapor with Experimental Data and Possible Reasons for Their Differences

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The thermal conductivity of water vapor, even at low density, is difficult to measure accurately at elevated temperatures due to its highly corrosive impact on the experimental equipment. Most experimental data are characterized by relatively large uncertainties of ±(1.5-4)% estimated by the authors. The kinetic theory of gases is a very powerful tool to predict the transport properties of a gas directly from its intermolecular potential energy surface. Based on a classical mechanical description of the intermolecular collision process, transport properties of several molecular gases such as carbon dioxide, methane, and water vapor have been computed recently. The deviations from the best experimental data were generally smaller than ±1% for viscosity and thermal conductivity, except for the thermal conductivity of water vapor. The calculations for water vapor have been performed employing four recent potential energy hypersurfaces for water-water interactions. The resulting differences from the values of the IAPWS correlation, representing the best experimental thermal conductivity data for water vapor, are characterized by almost the same temperature dependence, with the best potential showing good agreement (within ±1%) between 300 K and 450 K. With increasing temperature the differences become larger and attain about -5% above 800 K. Two of the possible causes of these differences will be discussed in this contribution. One is failures of classical collision theory for so-called resonant and near-resonant collisions, vibrationally inelastic collisions, and general quantum effects. The other is insufficient consideration of radiation effects in the measurements. Particularly for water vapor, which is between a transparent and an opaque medium for the conditions of interest, a reasonable radiation correction is not only more important, but also more complex, than for most other common gases.