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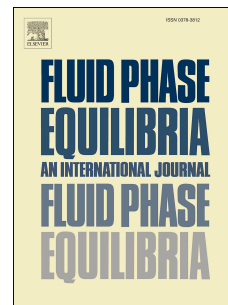
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Thermodynamic properties of dilute hydrogen in supercritical water

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Abstract

A thermodynamic model is developed to calculate the fugacity coefficients and partial molar volumes of hydrogen at infinite dilution in water at 647.1-2000 K and pure water densities between 0 and 1500 kg m⁻³. The model is based on the predicted values of DCFI (the dimensionless integral of the infinite dilution hydrogen - water direct correlation). Values of DCFI at low water densities are calculated from accurately known second cross virial coefficients; at high water densities predictions are based on the relations from the theory of a mixture of hard spheres; DCFI values at intermediate water densities are interpolated using a variant of corresponding-states correlation. Predicted values of the hydrogen fugacity coefficients at infinite dilution in water are compared with experimental data and results of the literature equations of state. The included Excel spreadsheet allows calculations provided that values of T , P , ρ_1^* , and κ_T for pure water are entered by a user.

Keywords: hydrogen; infinite dilution partial molar volume; fugacity coefficient;
thermodynamic model

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