

## Association Equation of State for Ethanol

J.F. Estela-Urbe<sup>C, S</sup>

*Facultad de Ingeniería, Pontificia Universidad Javeriana Cali, Cali, Columbia*

*jfe@javerianacali.edu.co*

The objective of this work is to present a recent fundamental equation of state for ethanol derived from the Schroeder, Penoncello, and Schroeder equation of 2014 but with the addition of an association term to account explicitly for the association effects of ethanol. Thus, the new equation comprises three terms: one is the ideal-gas part of the Helmholtz energy, the second is a multiparameter function representing the residual part of the Helmholtz energy, and the third is the association term from SAFT. As a result, the functional form of the multiparameter term was reduced from 25 to 23 adjustable coefficients. The association term of the new equation made it possible to calculate the fractions of free sites of saturated-liquid ethanol at temperatures between 275 and 500 K in very good agreement with the Luck data of 1980. In addition, the calculated percentage average absolute deviations in thermodynamic properties were 0.336 for  $ppT$ , 0.815 for vapor pressures, 3.363 for saturated-liquid densities, 11.96 for saturated-vapor densities, 11.32 for isochoric heat capacities, 2.791 for isobaric heat capacities, and 0.591 for speeds of sound; for second virial coefficients the average absolute deviation was  $112 \text{ cm}^3 \cdot \text{mol}^{-1}$ . Those results showed that, apart from saturated liquid densities, the new equation improved on the accuracy of the abovementioned equation of state. The equation also proved to behave well under extreme extrapolation.