Development of a Molecular Model for the Prediction of Phase Equilibria and Thermodynamic Properties of Hydrofluorocarbons (HFC) and Their Mixtures

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The low boiling point of hydrofluorocarbons (HFCs), combined with other physicochemical properties, promote their use as refrigerants and as blowing agents in polymer formulations. These substances represent an alternative to traditional compounds used in these applications, such as chlorofluorocarbons (CFCs), suspected of causing the destruction of the stratospheric ozone. A deep knowledge of their properties is needed before they can finally be put into use. In fact, modeling of HFCs has been an active research field for some decades, since the nonideal behavior of these mixtures poses a challenge to any modeling approach [1].

The objective of this work is to provide a molecular model based on the soft-SAFT EoS [2] for the description of the vapor-liquid equilibria of HFCs, of their mixtures, and of their mixtures with other types of compounds. The final goal is not only to obtain good agreement with the available experimental data, but also to search for trends in the parameters, seeking the transferability of the method for prediction purposes. The advantage of using a SAFT-type equation is its solid Statistical Mechanics basis. It is possible to quantify the different microscopic contributions governing the macroscopic behavior of the system. HFCs are modeled here as Lennard-Jones chains composed of m segments, with the dipole moment considered through an associating term. Five molecular parameters are needed in total.

The model has been applied to 14 HFCs (R41, R32, R23, R152a, R143a, R134a, R125, R245fa, R245ca, R236fa, R236ea, R227ea, R365mfc, and R338mccq), providing correlations of the molecular parameters with the molecular weights of the compounds. Soft-SAFT is able to provide quantitative results for densities and pressures of pure fluids and their mixtures. These results encourage the development of these types of models for predicting properties of HFCs for their final applications.

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[2] F.J. Blas and L.F. Vega, *Ind. Eng. Chem. Res.* **37**, 660 (1998).