Application of Molecular Modeling Tools for the Rationale Design of New Low Global Warming Potential Refrigerants

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The use of hydrofluorocarbons (HFCs) as alternative non-ozone depleting refrigerants for chlorofluorocarbons (CFCs) and hydrochlorofluorocarbons (HCFCs) has grown during the last couple of decades. Owing to their considerable global warming potential (GWP), a global deal was reached in year 2016 to limit the production and consumption of HFCs. The latter creates an urgent demand for developing and theoretically modeling new low GWP fourth generation refrigerants that would replace the currently used ones. Among the required properties, knowing vapor-liquid equilibria, critical properties, viscosities, thermal conductivities, heat capacities, speed of sound, and interfacial properties of these compounds is of great importance for the rational design of new refrigerants, as they need to be benchmarked with the current ones in use for the same applications. The statistical associating fluid theory (SAFT) coupled with the density gradient theory (DGT) and Rosenfeld's excess entropy scaling were used to accurately predict the thermophysical, interfacial and transport properties of HFC and hydrofluoroolefin (HFO) based commercial refrigerants. Molecular analyses of the results show that the presence or absence of an azeotrope in HFC binary systems is strongly dependent on the fluorine number of mixed components. It was also found that azeotropic binary mixtures of HFC/HFO + alkanes exhibit an unusual "aneotropic" behavior at the interface characterized by the presence of a minimum in surface tension as a function of mixture composition. Molecular simulations were also performed to further study molecular interactions leading to this unusual behavior and validate interfacial density profiles determined by the theory. We believe that this work proves the applicability of using SAFT as a tool for rationally designing new low GWP refrigerants and for making accurate predictions at conditions where experimental data does not exist. In addition, molecular simulations provide molecular details of the behavior at the interface, complementing results obtained by the theory.