# Thermophysical Behaviour of Fluorinated Blends Using Molecular Dynamics Simulations Combined with Soft-Saft

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While the use of alternative refrigerants such as hydrofluorocarbons (HFCs) seemed a permanent solution to substitute previous ozone-depleting substances, their use is now progressively decreased following the Kigali Amendment application in 2016 due to their high global warming potential (GWP). Unsaturated HFCs such as hydrofluoroolefins (HFOs) are considered feasible alternatives due to their high reaction rates with atmospheric OH and low atmospheric lifetimes, resulting in very low GWP[1]. However, even with an increasing amount of new experimental data for these systems, the available information is still limited. In this regard, computational tools are useful to understand the physicochemical behavior of these systems and characterize them, completing the information provided by experiments.

In this work, two different molecular modeling tools: molecular dynamics simulations and the molecular-based soft-SAFT equation of state are combined to compute the coexistence densities, vapor pressures, heat capacities, and dynamic viscosities of several alternative refrigerant blends, including ternary mixtures like R407-F, in a wide temperature range. Two different all-atom force fields[2,3], successfully employed in previous molecular simulations of hydrofluoroolefins and hydrofluoroalkanes, have been used. The obtained results are compared with a soft-SAFT model, where the capacities of the polar version are discussed. Agreement between both methods and data correlations (when available) was met, validating both simulation tools' predictive capability.

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