

Development of Computational Design Tools for Refrigerant Fluids

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Recently, the concerns of climate change initiated the search for new refrigerants with low Global Warming Potential (GWP). Specifically, the use of hydrofluoroolefins (HFOs) is presently considered. Due to the presence of double bond(s) and, consequently, high reaction rates with atmospheric OH, HFOs have much lower atmospheric lifetime than the HFC-based refrigerants presently in use. However, a more systematic search for new classes of refrigerants that, in addition to having low GWP, would also satisfy performance and safety requirements, has not been attempted. Also of interest are the potential trade-offs between these different requirements that may guide practical design decisions. In this work, we present our efforts on development computational tools for screening of potential candidates for refrigerant fluids. Various screening criteria (GWP, flammability, cycle performance) are estimated based on the candidate's molecular structure. Screening examples using large diverse sets of molecules will be presented.