# Rational Design of Low-GWP Drop-in Replacements Through a 4E Analysis Using Robust Thermodynamic Models

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In light of the F-gases emission prospects in the near future, the Kigali Amendment has pledged to limit the production and distribution of high global warming potential (GWP) third-generation refrigerants in contemporary refrigeration and air conditioning systems (RAC). Significantly, approximately 20% of current RAC units employing hydrofluorocarbons (HFCs) are expected to undergo complete replacement in the coming years, aligning with eco-conscious European directives [1,2]. To address this concern, the polar soft-SAFT molecular-based equation of state (EoS) has been predictively employed for the identification and development of alternative low-GWP fluorinated refrigerants as direct drop-ins for prevalent HFC refrigerants in today's RAC systems, specifically R134a (GWP=1300) and R410A (GWP=1924) [3]. A comprehensive and precise thermodynamic model has been developed for this purpose, accurately simulating the properties of refrigerants, including vapor-liquid equilibrium, thermophysical, and derivative properties, in addition to binary mixtures at a coarse-grain level [4]. The modeling framework is systematically applied to evaluate the suitability of alternative refrigerants, ensuring retrofitting criteria based on a multi-dimensional analysis (4E) encompassing energy, exergy, environmental, and economic characteristics, along with a detailed assessment of safety and technical considerations. Furthermore, Artificial Neural Network (ANN) techniques, in conjunction with SAFT models, are integrated to predict the thermophysical and thermodynamic properties of newly formulated blends where experimental data is lacking, showcasing the innovative application of artificial intelligence in the search for low-GWP refrigerants without the need of further experiments. This comprehensive methodology is proven effective across various operational conditions and system designs, highlighting its applicability, transferability and accuracy. Additional analysis of environmental impact and projected cost is included to quantify the impact associated with their use and emissions, aiding in the identification of appropriate substitutes from a techno-environmental-economic perspective. The compatibility KPIs are also reproduced for R513A (GWP=608), R450A (GWP=682), and R32 (GWP=675), which are well-recognized alternatives for R134a and R410A in domestic and commercial settings nowadays, providing a detailed comparison among mid- to low-GWP cooling agents.

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