Measurement of CO\textsubscript{2} + freon phase equilibria and extension of the predictive E-PPR78 equation of state to freon-containing systems

Jean-Noël Jaubert\textsuperscript{1*}, Romain Privat\textsuperscript{1}, Jun-Wei Qian\textsuperscript{1}, Niramol Juntarachat\textsuperscript{1} and Christophe Coquelet\textsuperscript{2}

\textsuperscript{1}Université de Lorraine, ENSIC (Ecole Nationale Supérieure des Industries Chimiques), LRGP (Laboratoire Réactions et Génie des Procédés), 1 rue Grandville, 54000 Nancy, France.

\textsuperscript{2}Centre Thermodynamique des Procédés (CTP), Département Énergétique et Procédés, Mines ParisTech – Armines, 35 rue Saint Honoré 77305 Fontainebleau Cedex, France.

\texttt{jean-noel.jaubert@univ-lorraine.fr}

Scientific topic: 2 (equations of state)

Keywords: Freons, predictive equation of state, group-contribution concept, binary interaction parameter

Abstract
Chlorofluorocarbons (CFCs) and hydrochlorofluorocarbons (HCFCs) have a high ozone depletion potential (ODP) and hydrofluorocarbons (HFCs) are high global warming potential (GWP) refrigerants. Consequently, refrigeration and airconditioning industries carry out extensive researches to find highly efficient alternative refrigerants with zero ODP and GWP lower than 150.
The search for next-generation refrigerants requires the preselection of good candidate likely to exhibit low environmental impact and leading to high thermodynamic cycle efficiency.
To do so, disposing of powerful predictive thermodynamic models is a necessary prerequisite. In this work, the well established E-PPR78 predictive equation of state was extended to systems containing freons. Therefore, 6 different groups were added to the 21 already-existing groups: group 22: CF\textsubscript{3}-CF\textsubscript{3} (R116), group 23: -CF\textsubscript{3}, group 24: -CF\textsubscript{2}, group 25: =CF\textsubscript{2} =CF-, group 26: CHF\textsubscript{2}-CH\textsubscript{3} (R152a), group 27: CF\textsubscript{3}-CH\textsubscript{2}F (R134a). All the experimental data available in the open literature were then selected to estimate the various group interaction parameters between the 6 new groups and the 21 previously defined.
To complete the study, vapor-liquid equilibrium and critical data for the CO\textsubscript{2} + R1234yf and CO\textsubscript{2} + R1234ze(E) systems – deemed as promising alternative refrigerant mixtures – were measured and correlated.
The E-PPR78 equation of state finally shows a good ability to model the large variety of phase behaviors encountered in this class of fluids (criticality, azeotropy, liquid-liquid equilibria, vapor-liquid-liquid equilibria etc.) and consequently.