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Solid Phase I of Carbon Dioxide: A New Gibbs Free Energy Equation of State and its Application for the Calculation of the Solubility of CO_2 in different solvents

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Carbon dioxide (CO_2) freeze-out is a very common issue encountered in liquefaction of gases (like air components, methane, hydrogen) because of its high triple-point temperature. This phenomenon is rather problematic in liquefaction facilities as it can cause fouling in heat exchanger tubes that leads to unscheduled plant shutdowns. Nevertheless, CO_2 freeze-out can also be a useful separation technique, making it possible to remove CO_2 from industrial plant emissions [1] or purification units like in biogas upgrading [2] through the cryogenic carbon capture process. Consequently, an accurate prediction of low-temperature phase equilibria involving solid CO_2 is necessary.

In this work, a new Gibbs free energy Equation of State (EoS) with temperature and pressure as the independent variables was developped to describe the solid phase I of carbon dioxide ("dry ice"), continuing the work carried out by Stringari et al. on the modeling of solid methane [3] and solid benzene [4]. The model for the solid phase has been coupled with the reference equation of state for the fluid phases developed by Span and Wagner [5] in order to reproduce analytically the equality of Gibbs free energy, the experimental volume change, and the experimental enthalpy change at the triple point. The EoS for the solid phase has a validity range from 2 to 800 K in temperature and up to 12 GPa in pressure.

The new EoS, alongside two different EoSs developed for phase I of solid CO_2 [6,7] and the Classical Approach [8] were coupled in turn to the GERG-2008 EoS [9] as implemented on REFPROP v10 [10] to predict the solubility of CO_2 in different solvents (like N_2, CH_4, and H_2).

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