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Letter to the Editor

Comments on "PVTxy properties of CO_2 mixtures relevant for CO_2 capture, transport and storage: Review of available experimental data and theoretical models"

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ABSTRACT

In a recent paper, Li et al. conducted an exhaustive literature survey of the available experimental data of mixtures containing CO_2 in order to design industrial processes dealing with CO_2 capture, CO_2 storage and CO_2 transport. The present letter to the editor is devoted (i) to make some comments on what Li et al. wrote about our work and which we feel might lack of accuracy, (ii) to give some more information about three binary systems of interest for the aforementioned applications with CO_2.

In a recent paper [1], Li et al. conducted an exhaustive literature survey of the available experimental data of mixtures containing CO_2 in order to design industrial processes dealing with CO_2 capture, CO_2 storage and CO_2 transport. In addition, an extensive set of thermodynamic models usable to correlate these data is presented and analyzed by these authors. Among them, the PPR78 equation of state [2–10] (named PPR by the authors) is briefly described.

The work developed by Li et al. is of the highest interest for the chemical engineering community because it makes the point about the impact of the impurities on the design and operation of carbon capture and storage (CCS) processes.

The present letter is devoted (i) to make some comments on what Li et al. wrote about our work and which we feel might lack of accuracy, (ii) to give some more information about three binary systems of interest for the aforementioned applications with CO_2.

- First of all, we would like to mention that in our article dedicated to the prediction of fluid phase behavior of mixtures containing CO_2 [5], not only the systems CO_2 + n-alkanes are considered but also many other ones such as CO_2 + branched alkanes, CO_2 + aromatic compounds and CO_2 + cycloalkanes. The sentence "*The predictive-PR (PPR) EOS was evaluated by Vitu* et al. [87] *regarding the phase equilibria of CO_2 + n-alkanes*" written by Li et al. thus appears a bit restrictive.
- We also would like to state that contrary to what is written by Li et al., we never claimed that our PPR78 equation of state led to better results than models like SAFT-VR, PC-SAFT, soft-SAFT or PRSV-WS. The only comparison we made is brought up in the following sentence (written in [5]): "*When compared to other predictive models like PSRK, LCVM or GC-SAFT, the proposed PPR78 model always leads to better results*". It is important to point out that we only compared PPR78 to three different predictive models (PSRK, LCVM and GC-SAFT) and never to non-predictive models such as SAFT-VR, PC-SAFT, soft-SAFT and PRSV-WS (note that the adjective non-predictive means that the model requires the fitting of some parameters on experimental data before being used).
- Li et al. summarize and evaluate the available experimental data and investigate the theoretical models that have been proposed in the literature to estimate the properties of CO_2 mixtures containing impurities like N_2 and H_2S. They however never make mention of our modeling works dealing with these systems. The capability of the PPR78 equation of state to represent the phase behavior of both these binary systems (CO_2 + N_2 and CO_2 + H_2S) is discussed and illustrated in two papers, one about the prediction of systems containing nitrogen [6], and another one about the prediction of systems involving hydrogen sulfide [8].
- Li et al. are right when they explain that we did not give any specific detail regarding our calculations for the system CH_4 + CO_2 in our previous paper [5]. Indeed, this paper only

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