1 Modification of the Density Model for CO$_2$ Solutions

Hu et al. (2007) made systematic assessment of experimental pressure-volume-temperature-composition (PVTx) data of the CO$_2$-H$_2$O and CO$_2$-H$_2$O-NaCl systems published before 2006, where the most accurate data were used by Duan et al. (2008) to develop a density model (abbreviated here as DH08) for the CO$_2$ solutions. The model was successfully extended to the aqueous solutions in the CO$_2$-H$_2$O-NaCl system without using any additional parameters. Recently, Yu et al. (2013) assessed some new PVTx data of the CO$_2$-H$_2$O system published since 2006, as well as some data published before 2006 but not assessed in the past. Compared with the data used to fit the DH08 model, these data cover a wider P-x range, and some of them are in the intermediate to high temperature region not covered by the past data. The DH08 model cannot reproduce these data with an accuracy close to that in reproducing the data used in the model fitting. In order to adapt to more extensive data, the DH08 model is modified by adding quadratic terms of pressure and concentration in the perturbation part:

\[
V = V_w [1 + (A_i + A_2P + B_1P^2) x + B_2x^2]
\]

where \(V\), \(V_w\) and \(x\) are the molar volume of solution, molar volume of water and the mole fraction of CO$_2$, respectively, \(A_i\) and \(B_i\) are functions of temperature, \(V_w\) is calculated with the IAPWS-IF97 model (Wagner et al., 2000).

2 Fit and Test of the New Model

The new model is fitted with only the most accurate data available, i.e. those in Table 1 and few data of Capobianco et al. (2013). The new and DH08 models are compared with the data in Table 1, where AD and MD are the average and maximum deviations, respectively. The two models are also compared with the data of Kojima et al. (2001), Capobianco et al. (2013) and Blencoe et al. (2001). The deviations of the two models and their correlations with P-T-x conditions show that the new model is obviously superior to the DH08 model in most cases, particularly at high temperatures, pressures or concentrations.

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References


