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Predict C₂H₆ Concentration in Aqueous Solution Equilibrium with Its Hydrate in the Absence of Vapor

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A thermodynamics model is proposed to predict the concentration of C₂H₆ in pure water and NaCl solutions equilibrium with its hydrate in the absence of vapor. Van der Waals & Platteeuw model and Holder's model were used to calculate the chemical potential of components in hydrate and water, Pitzer's model was used to calculate the activity of water in the solution. C₂H₆ concentration in water (Table 1) along the H-Lw-V equilibrium curve (Figure 1), and at two-phase equilibrium of H-Lw in pure water from 5 bar to 1000 bar, and in NaCl solutions (m NaCl= 0.598 mol/kg) from 5 bar to 15 bar, from 273.15 K to 287.1 K were predicted (Figures 2, 3, 4). The results show that, in equilibrium with hydrate in the absence of vapor: (1) Concentration of C₂H₆ increases with increasing temperature and decreasing pressure (Figure 3), (2)

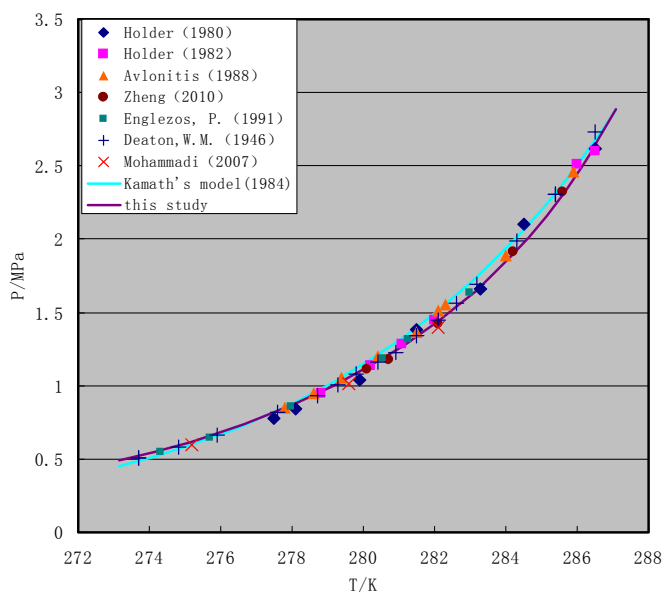


Fig. 1. Dissolution Pressure of Ethane Hydrate in Pure Water

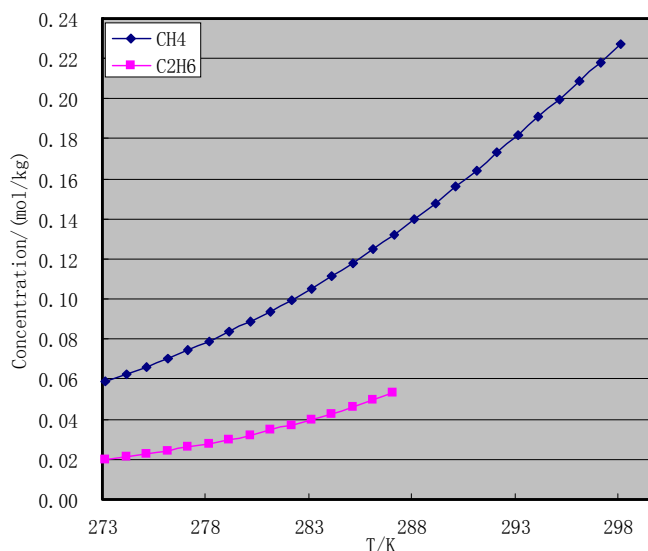


Fig. 2. Methane and Ethane Concentration in Pure Water along H-Lw-V curve

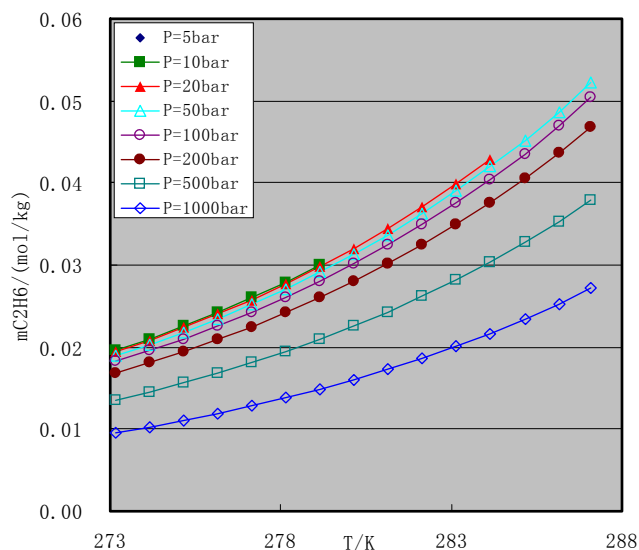


Fig. 3. Pressure Effects on the Concentration of Ethane in Pure Water Equilibrium with its Hydrate

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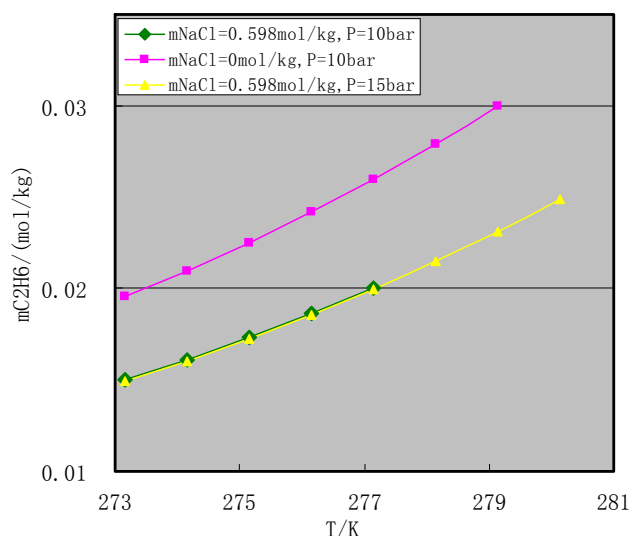


Fig. 4. Salt Effects on the Concentration of Ethane in aqueous Solution Equilibrium with its Hydrate

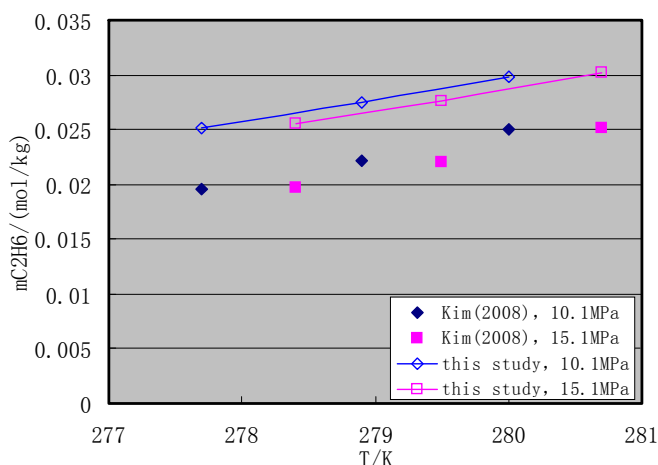


Fig. 5. Concentration of Ethane in Pure Water Equilibrium with its Hydrate Calculated from this Model Compared with Experimental Data

Table 1 Concentration of Ethane Equilibrium with its Hydrate Calculated from this Model Compared with VLE Concentration at H-Lw-V Equilibrium condition

T/K	P/bar	$m_{C_2H_6}^a$ (mol/kg)	$m_{C_2H_6}^b$ (mol/kg)
273.15	4.87900	0.019623	0.019623
274.15	5.48700	0.021049	0.021049
275.15	6.17372	0.022586	0.022585
276.15	6.95051	0.024240	0.024239
277.15	7.83024	0.026021	0.026020
278.15	8.82941	0.027939	0.027938
279.15	9.96698	0.030005	0.030004
280.15	11.26662	0.032230	0.032228
281.15	12.75686	0.034625	0.034623
282.15	14.47539	0.037203	0.037200
283.15	16.47007	0.039976	0.039974
284.15	18.80547	0.042957	0.042954
285.15	21.57557	0.046159	0.046155
286.15	24.92565	0.049594	0.049591
287.10	28.87617	0.053077	0.053073

Note :a-VLE,calculated from Duan's online model, <http://www.geochem-model.org>; b-HLVE,this study

Concentration decreases with increasing concentration of electrolyte at same temperature and pressure (Figure 4), (3) Previous experimental work might under estimated the ethane concentration in aqueous solution equilibrium with its hydrate (Figure 5), more accurate measurements need to be done in the future.

Key words: Hydrate, concentration, ethane, thermodynamics model

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