

## Thermodynamic modelling of cyclopentane hydrates equilibria with NaCl, KCl, CaCl<sub>2</sub> or NaCl-KCl present

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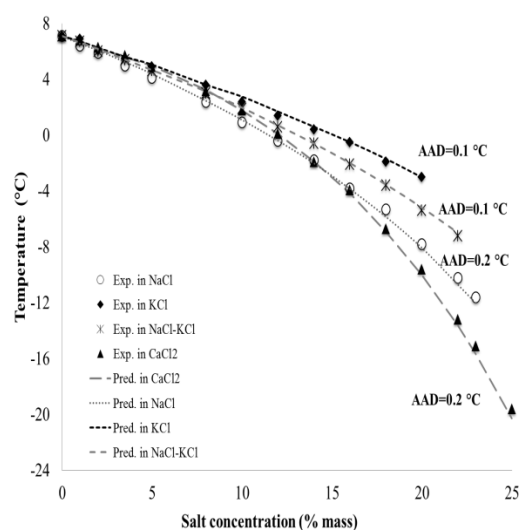
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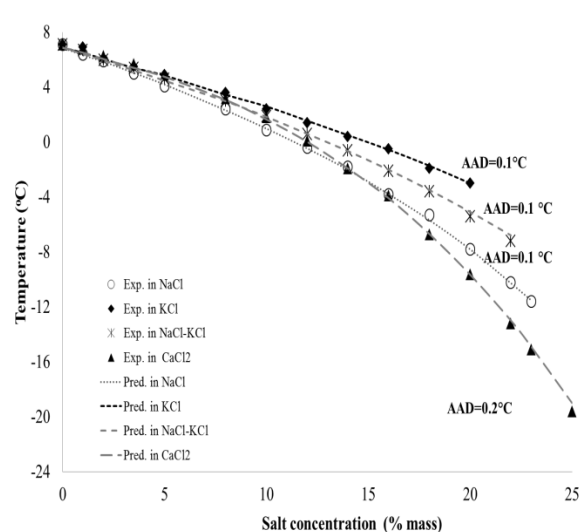
### Abstract

This study aims at modelling the equilibria of cyclopentane hydrates in the presence of salts. Three kinds of salts were considered: NaCl, KCl, and CaCl<sub>2</sub> with a wide range of concentration. Three different thermodynamic models were then used to predict the equilibrium conditions. The geochemical model PHREEQC was applied in all the three approaches to compute the water activity in salt solution using the PITZER database. The equilibrium data in the presence of NaCl were used in the all three models.

The first approach is based on the standard solid-liquid equation (Hildebrand and Scott) usually used for modelling solid-liquid equilibria of a pure solute in a solvent to obtain a new correlation of the heat capacity difference of cyclopentane hydrates and the freezing point. The two last approaches are both based on the van der Waals and Platteuw model by either optimizing the Kihara parameters or using a new correlation between the cage occupancy and water activity. The results of three modified models have a good accordance with the experimental data in the presence of whatever kinds of salts with the average absolute deviation equal or less than to 0.4°C. Whilst using the new Kihara parameter and the new correlation between the cage occupancy factor and water activity in van der Waals and Platteuw method can be a good suggestion as the deviation is almost zero for all kinds of salts, especially in the presence of KCl and a mixture of NaCl-KCl with the deviation around 0.1°C as presented in Figure 1.



a: Approach n°2



b: Approach n°3

Figure 1: Experimental and predicted dissociation temperature of cyclopentane hydrates in the presence of salt