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Thermodynamic modelling of cyclopentane hydrates equilibria with NaCl, KCl, CaCl2 or NaCl-KCl present

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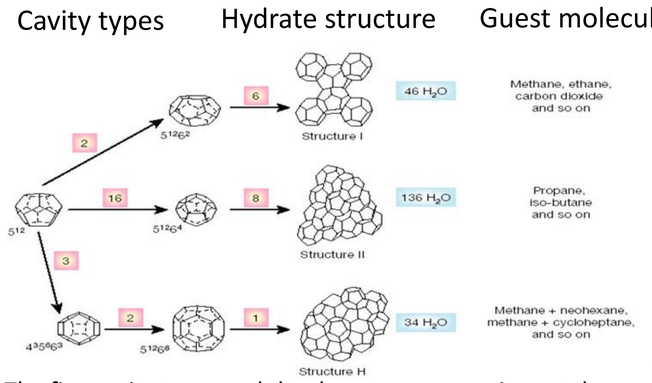
CODEGEPRA 2017

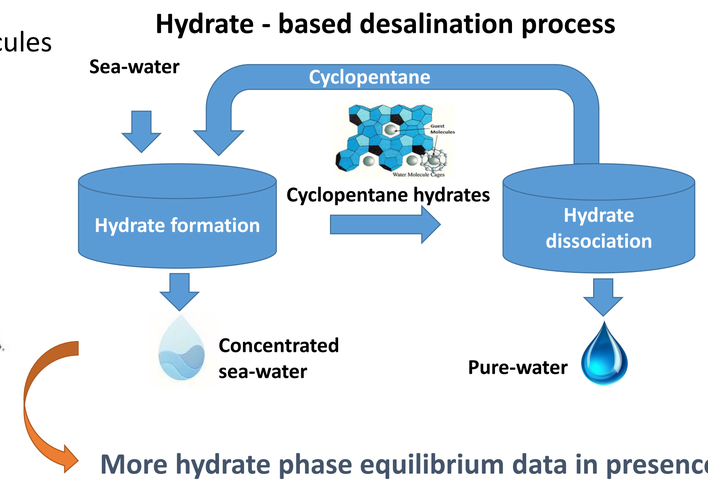
Introduction

- Clathrate hydrates are ice-like crystalline compounds consisting of cage-like structures formed by hydrogen-bonded water molecules that enclose guest molecules stabilizing the lattice structure.

E. Dendy Sloan, Jr, 2003.



The five cavity types and the three common unit crystals structures of the clathrate hydrates

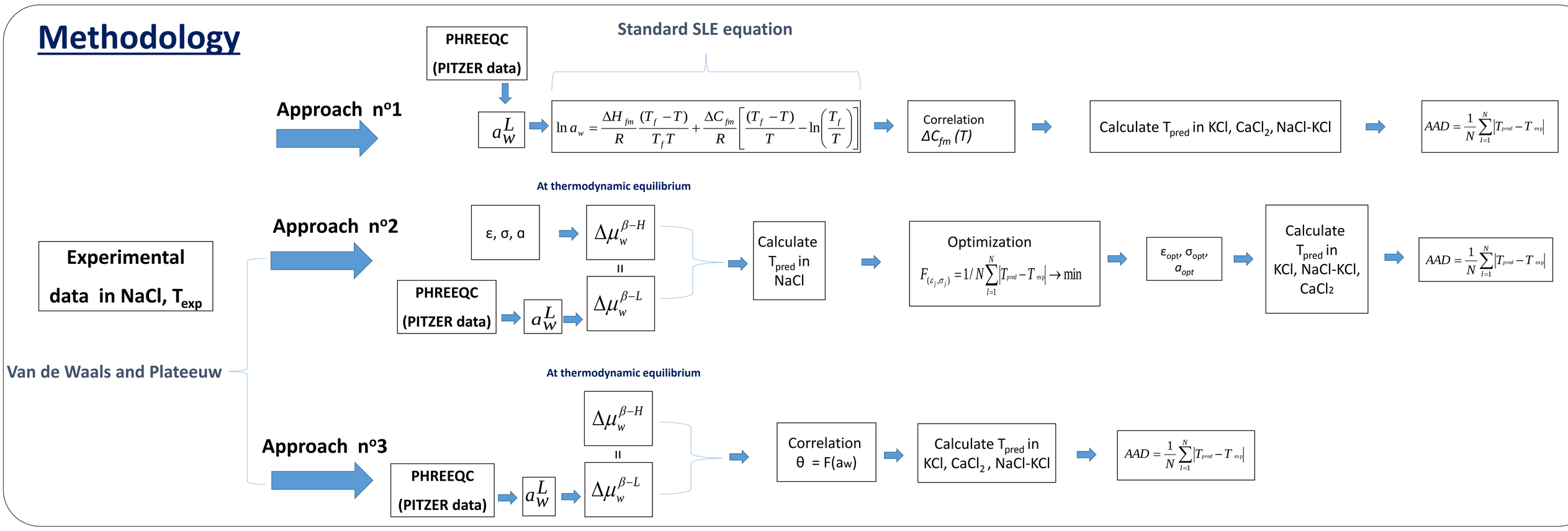


More hydrate phase equilibrium data in presence of salts are needed

Objective

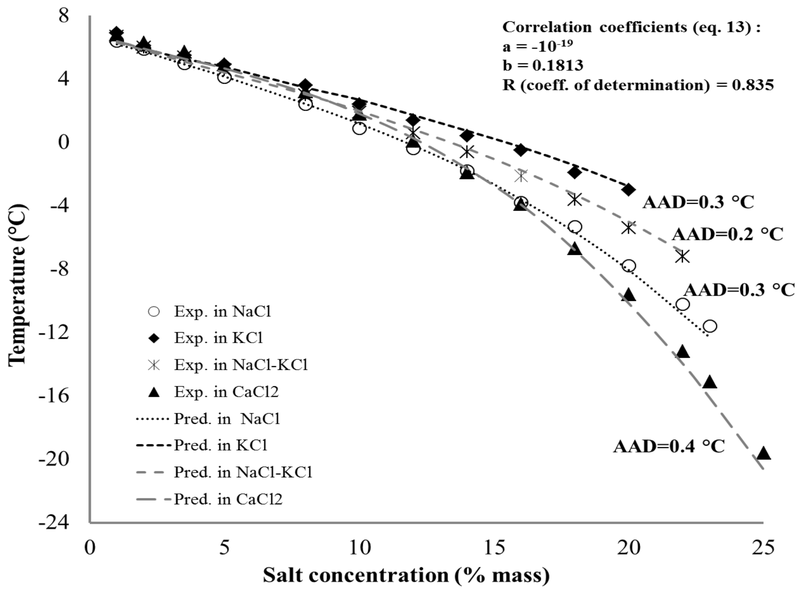
Model the equilibria of cyclopentane hydrates in the presence of salts (NaCl, KCl, NaCl-KCl, $CaCl_2$).

Methodology



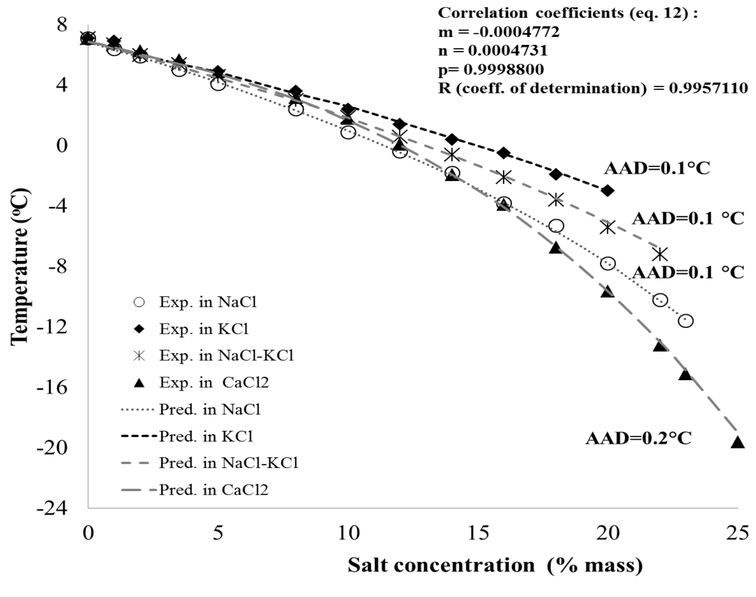
Modelling results

Approach n°1



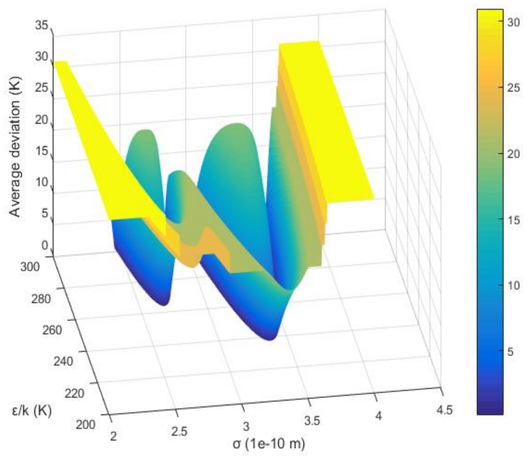
Predicted and experimental equilibrium temperatures: Approach n°1

Approach n°3

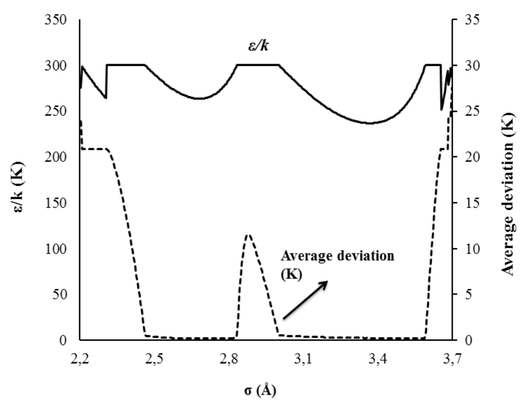


Predicted and experimental equilibrium temperatures: Approach n°3

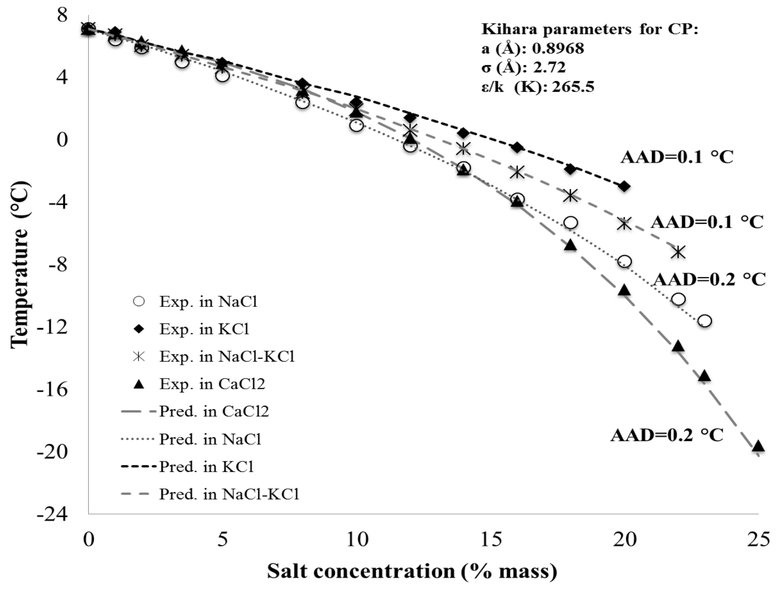
Approach n°2



Typical form of the deviation between the predicted and the experimental data



ε/k versus σ at the minimum deviation with experimental data



Predicted and experimental equilibrium temperatures: Approach n°2

Summary : AAD (°C or K) of three approaches

	NaCl	KCl	NaCl-KCl	$CaCl_2$
Approach n°1	0.3	0.3	0.2	0.4
Approach n°2	0.2	0.1	0.1	0.2
Approach n°3	**0.1**	**0.1**	**0.1**	**0.2**

Conclusion

1. All approches are capable of predicting the equilibrium temperatures of cyclopentane hydrates in brine with the average deviation less than, or equal to 0.4 K in all cases.

2. The new correlation between occupancy factor and water activity (approach n°3) is probably the best to obtain quick, consistent, and accurate dissociation temperature of cyclopentane hydrates in brine