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

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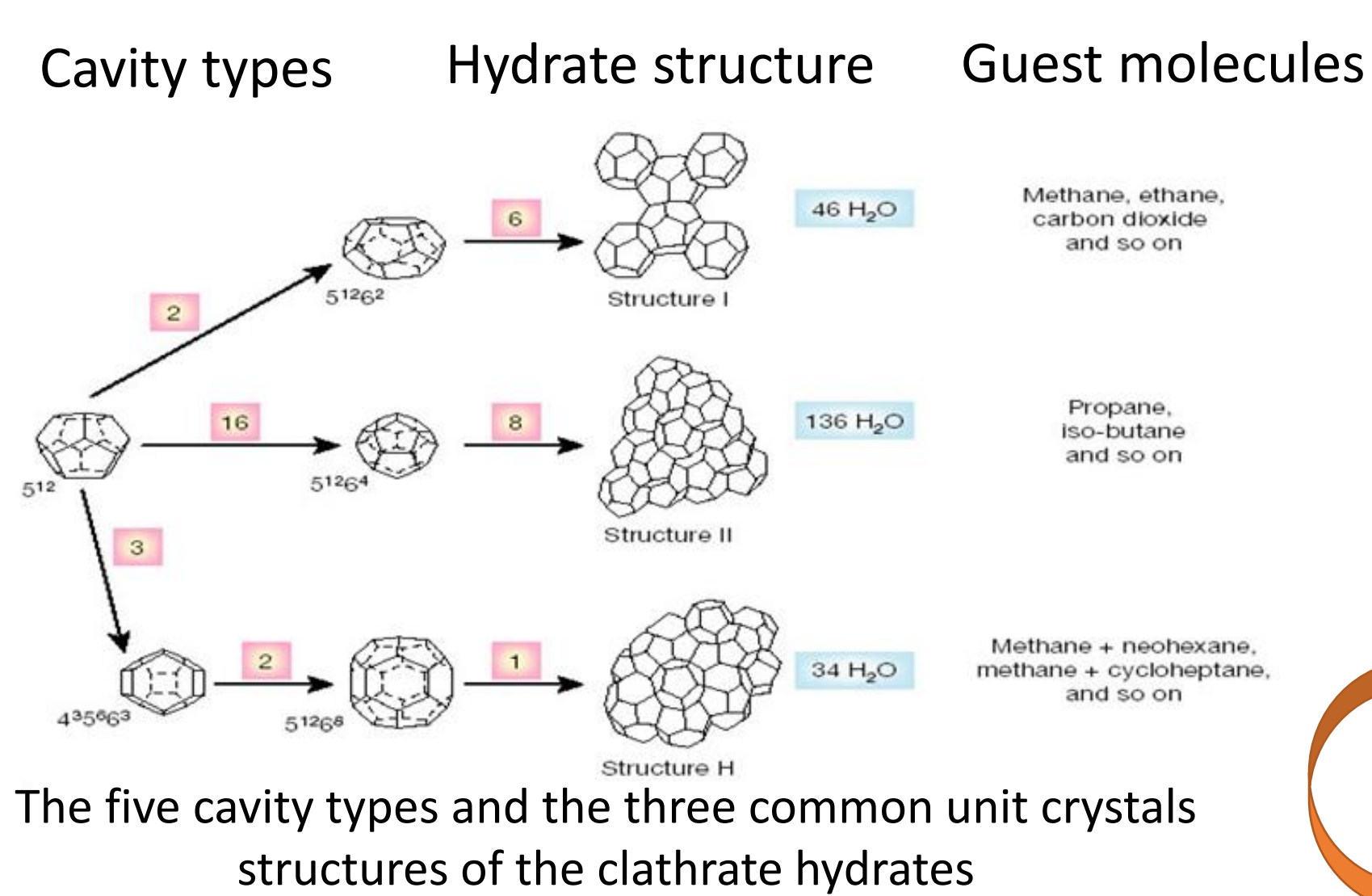
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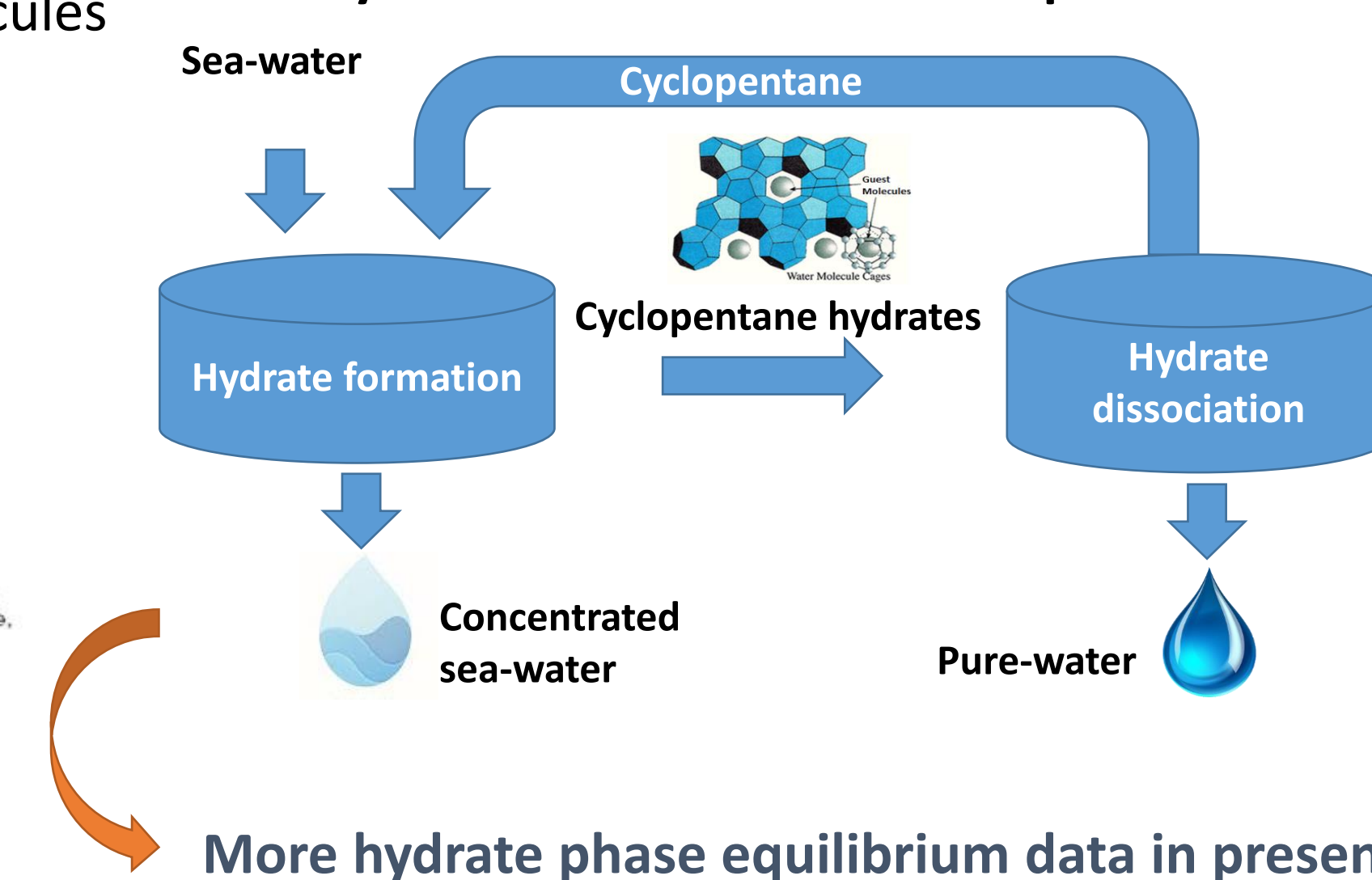
Introduction

- 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.



Hydrate - based desalination process

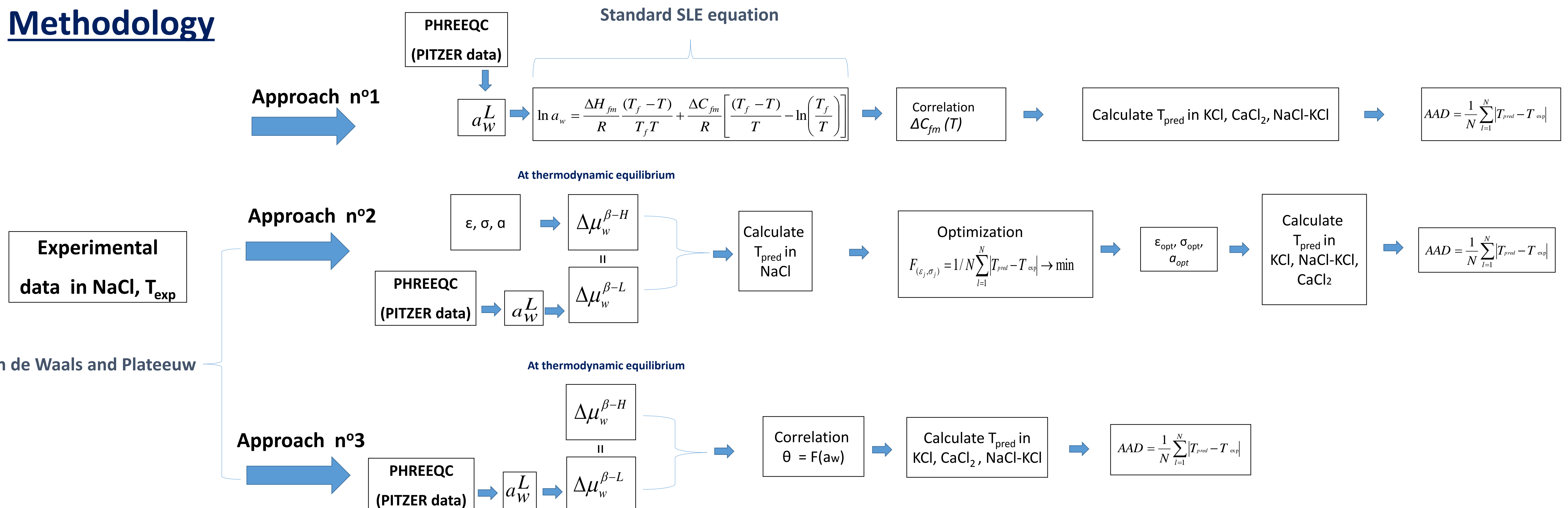


More hydrate phase equilibrium data in presence of salts are needed

Objective

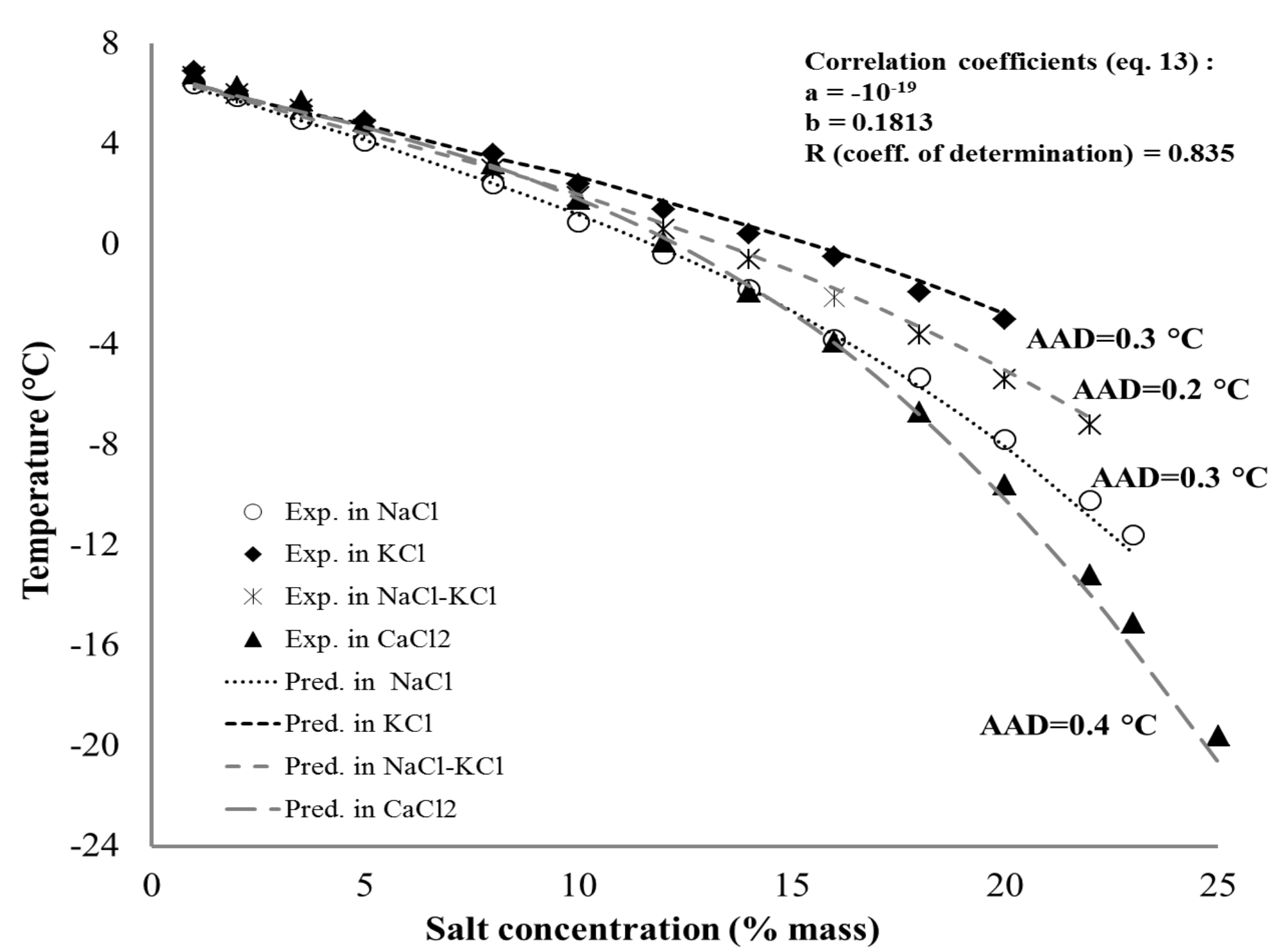
Model the equilibria of cyclopentane hydrates in the presence of salts (NaCl, KCl, NaCl-KCl, CaCl₂).

Methodology

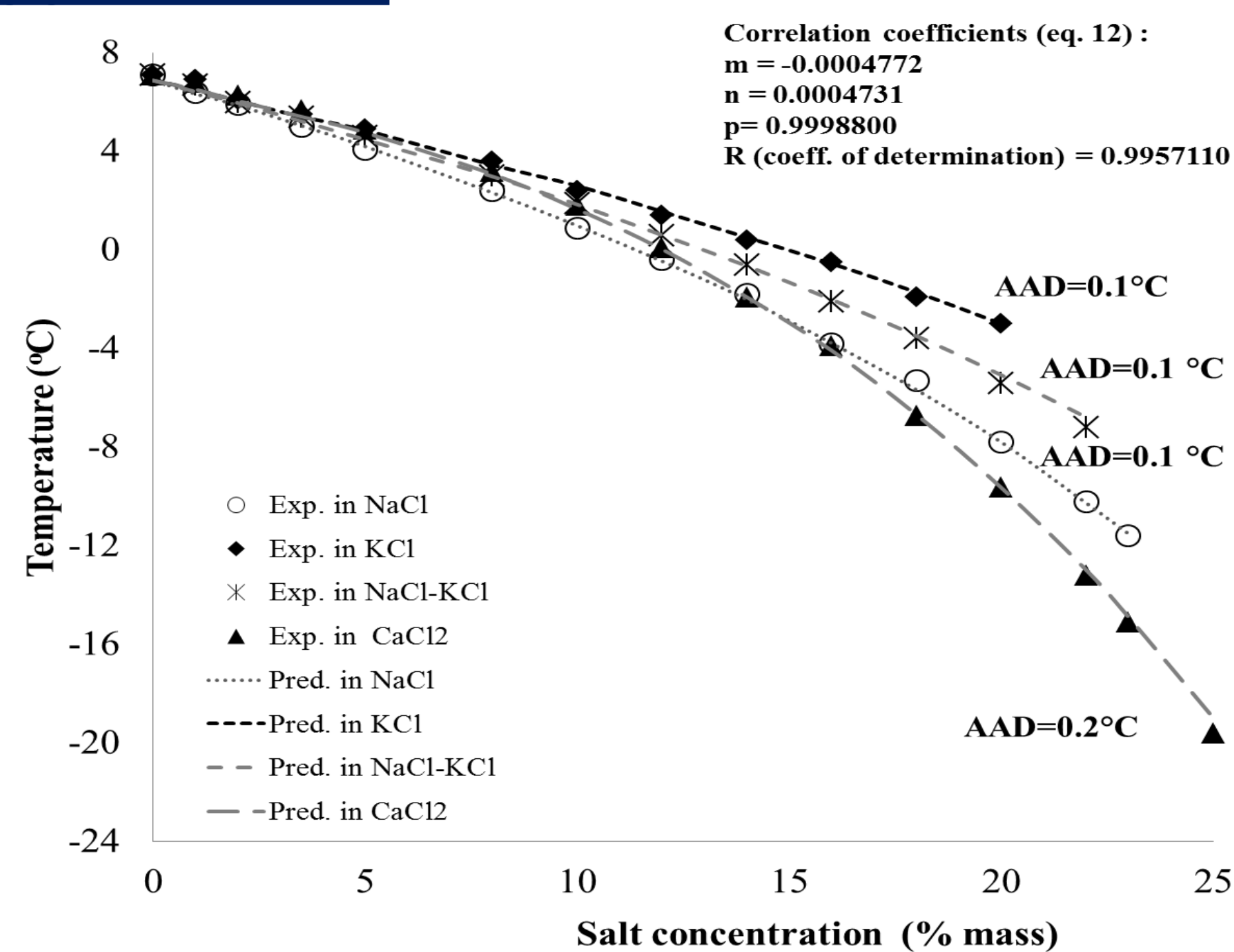


Modelling results

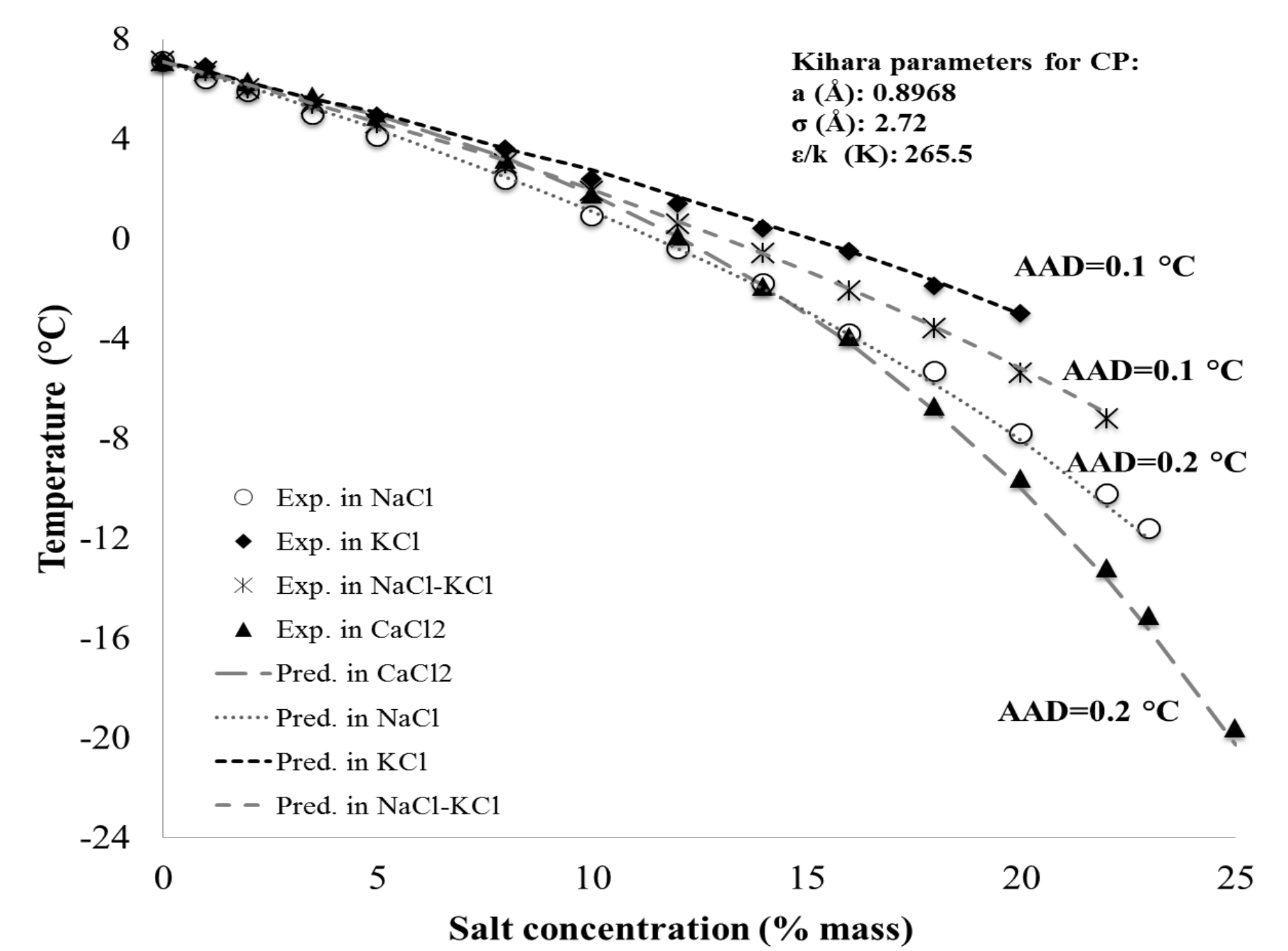
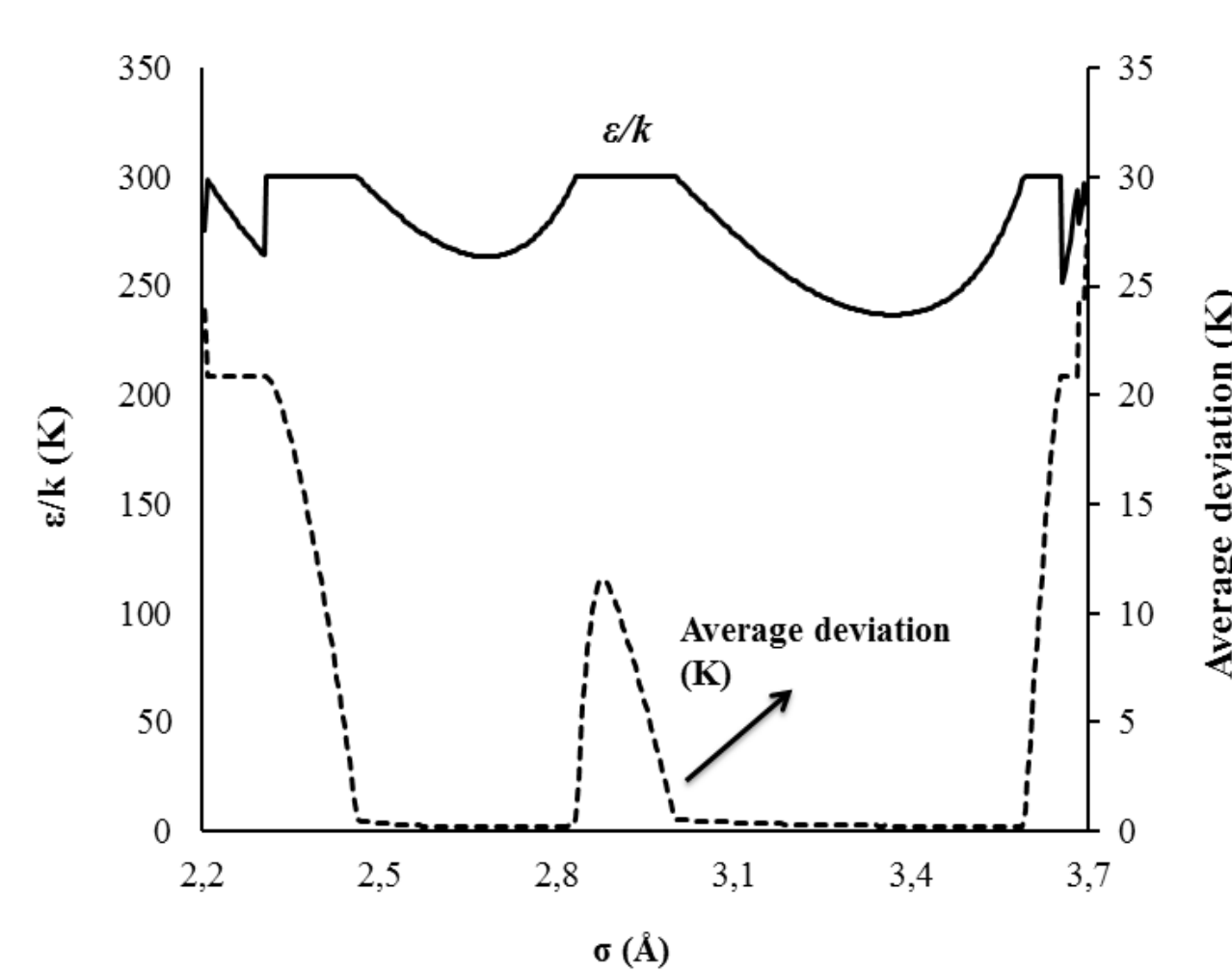
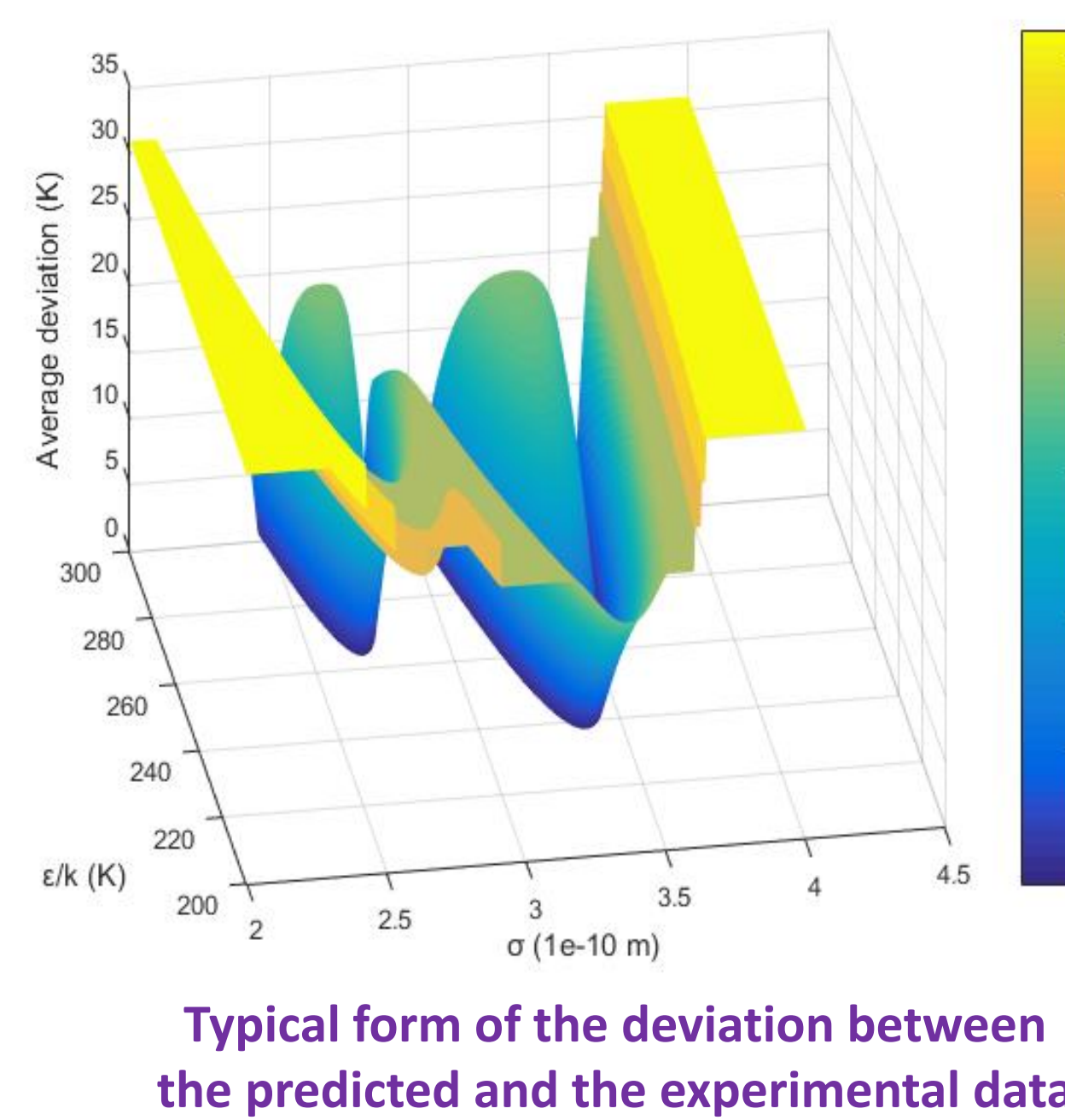
Approach n°1



Approach n°3



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 approaches 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