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# THERMODYNAMICS OF CYCLOPENTANE HYDRATES FORMATION FROM BRINE: EXPERIMENTAL AND MODELLING STUDY

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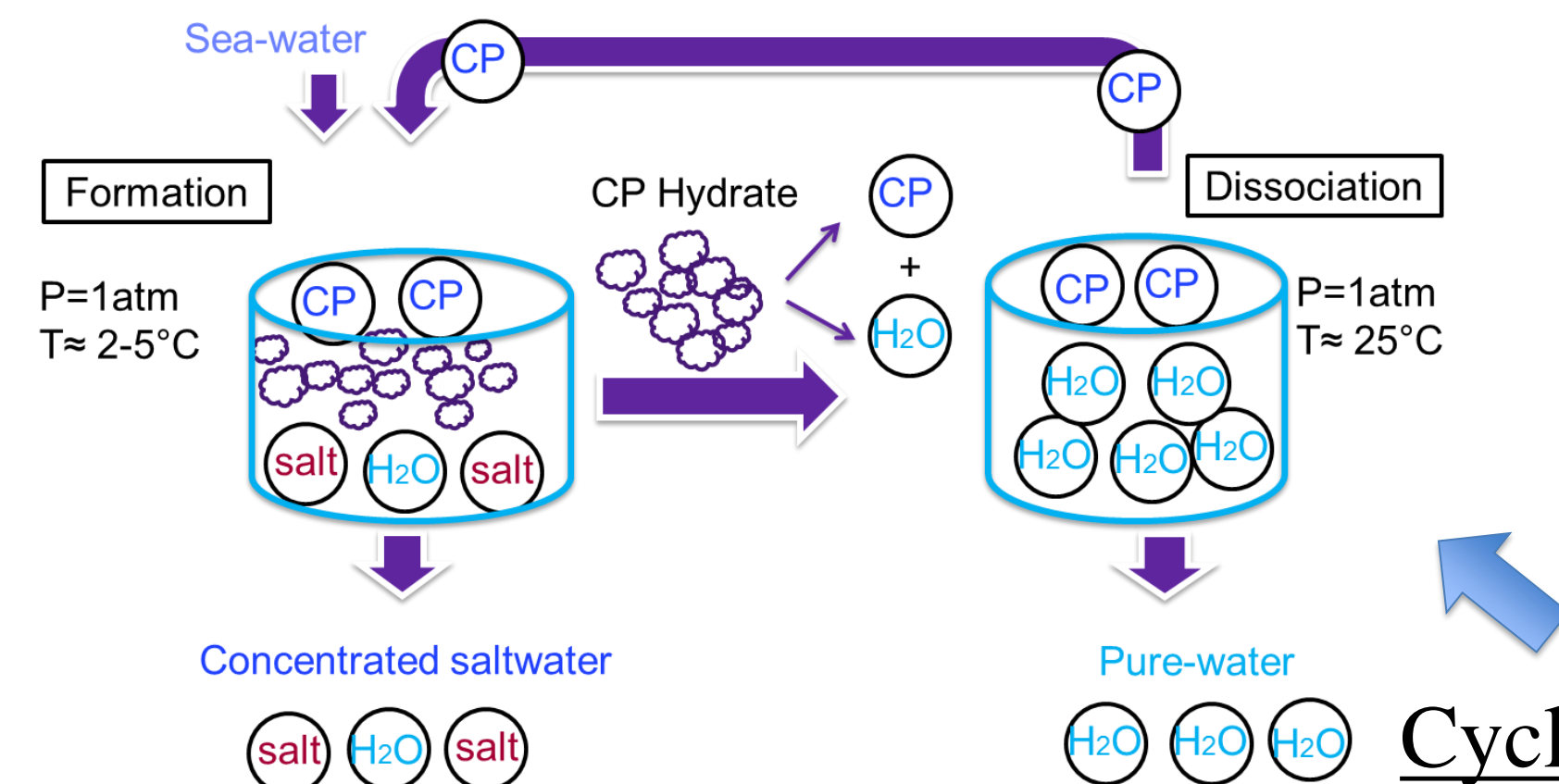
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## Introduction

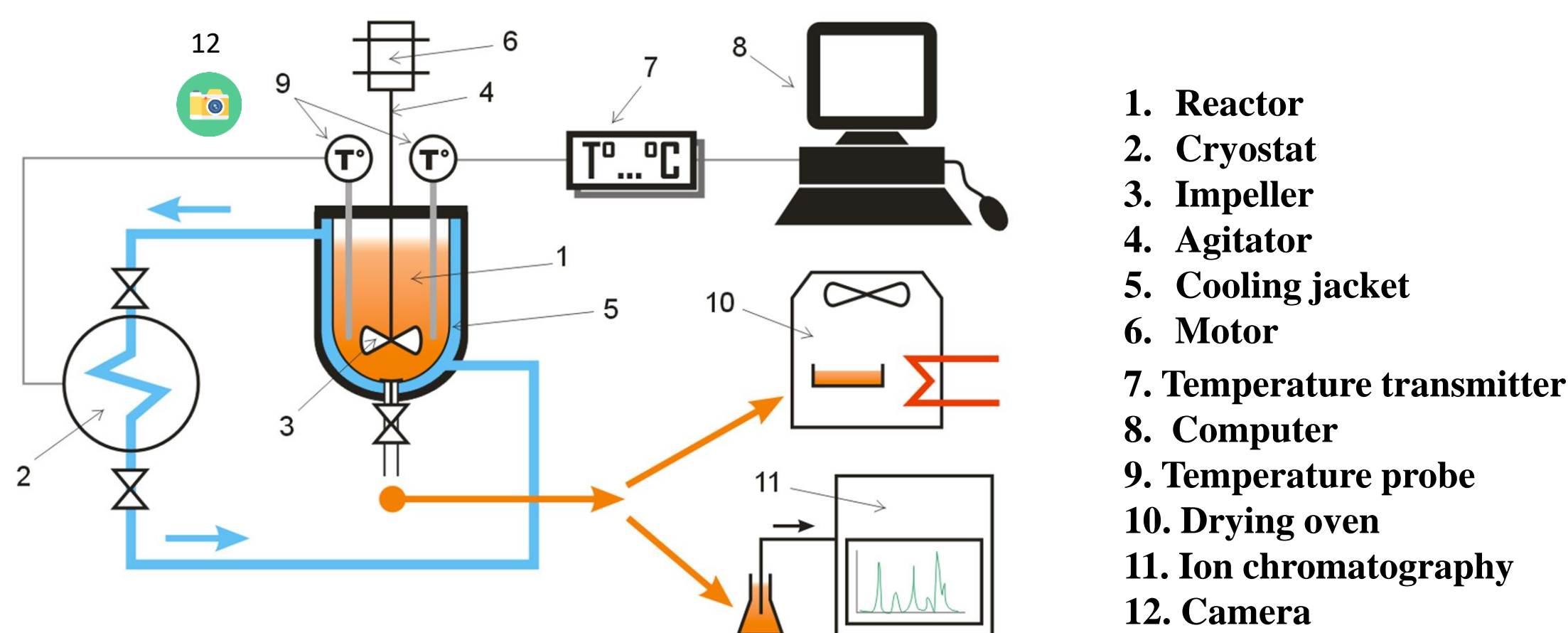
Hydrates can be used to remove salt from saline water or to clean water as a purification method



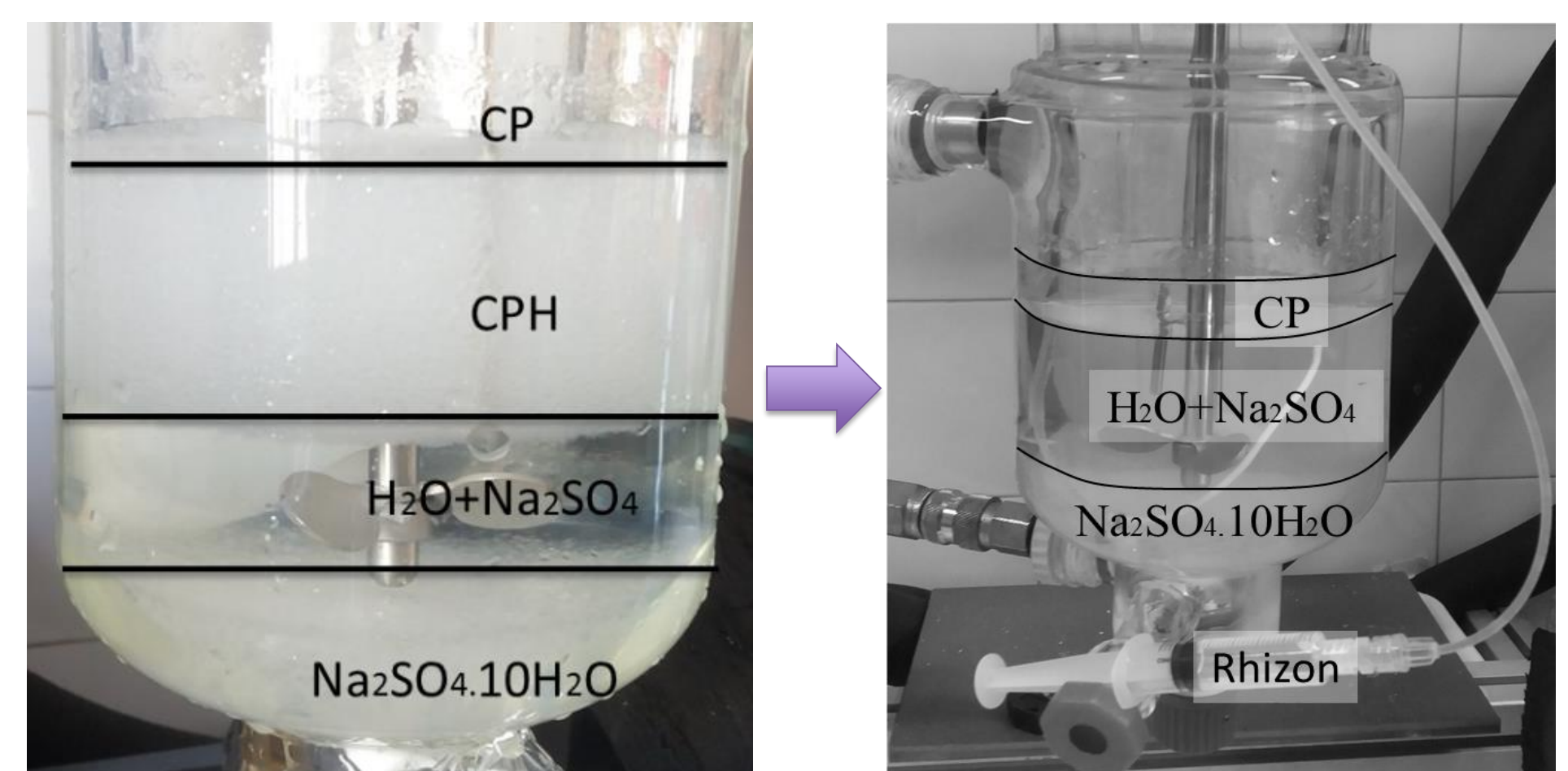
## Objective

- ❖ NaCl, KCl, NaCl-KCl, CaCl<sub>2</sub>, Na<sub>2</sub>SO<sub>4</sub>, MgCl<sub>2</sub>, MgCl<sub>2</sub>-NaCl, MgCl<sub>2</sub>-NaCl-KCl at different concentrations
- ❖ Develop four models based on Standard Freezing Point Depression (SFPD) equation, Hu-Lee-Sum (HLS) correlation, Kihara and Activity-Based Occupancy Correlation (ABOC) to predict the equilibrium conditions.

## Apparatus



## Experimental observation



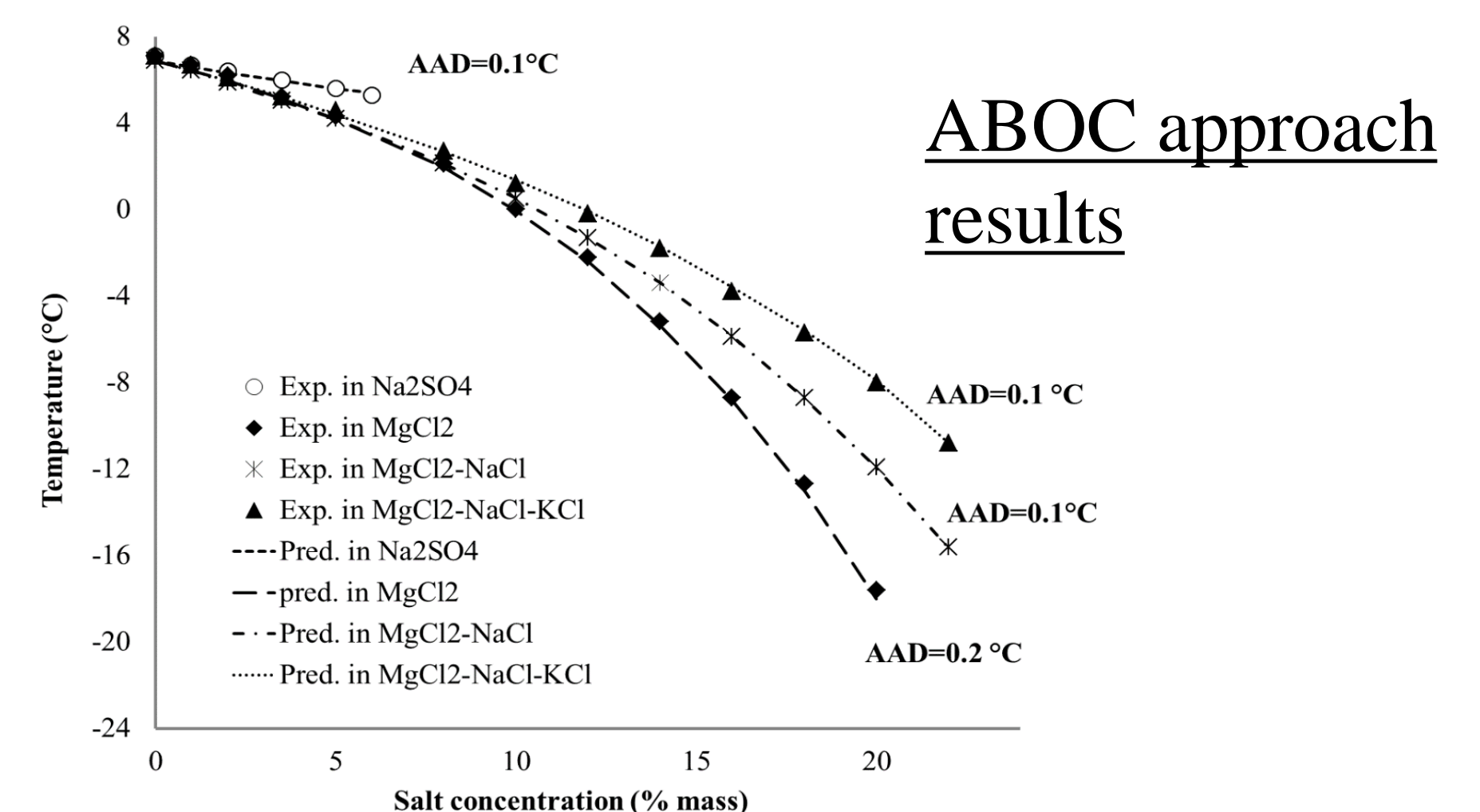
Up to eutectic point and salt co-precipitation !

## Thermodynamic data and Modelling

- ❖ 4 thermodynamic approaches:
  - Standard Freezing Point Depression (SFPD)
  - Hu-Lee-Sum correlation
  - Kihara approach
  - Activity-Based Occupancy Correlation (ABOC)

$\theta(a_w) = m \times (a_w^2) + n \times (a_w) + p$   
occupancy of cavities correlated to water activity

Model.	Na <sub>2</sub> SO <sub>4</sub>	MgCl <sub>2</sub>	MgCl <sub>2</sub> - NaCl	MgCl <sub>2</sub> - NaCl-KCl	NaCl	KCl	NaCl-KCl	CaCl <sub>2</sub>
SFPD	0.1	0.5	0.4	0.3	0.3	0.3	0.2	0.4
Hu-Lee-Sum	0.3	0.7	0.4	0.2	0.5	0.3	0.3	0.5
Kihara	0.2	0.5	0.2	0.1	0.2	0.1	0.1	0.2
ABOC	0.1	0.2	0.1	0.1	0.1	0.1	0.1	0.2



## Conclusions

- ❖ Phase equilibrium data of CP hydrates in saline systems were determined.
- ❖ Simulated results agree well with the experimental equilibrium data
- ❖ Model predictions within 0.2°C accuracy

Ho-Van, S. et al., AIChE Journal 64(6) (2018)

Ho-Van, S. et al., Industrial & Engineering Chemistry Research 57(43) (2018)