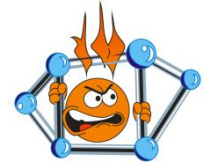


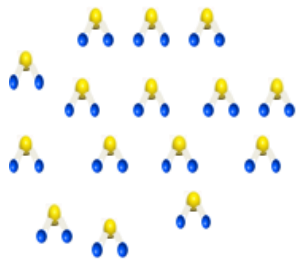
ÉCOLE NATIONALE SUPÉRIEURE DES MINES

# Crystallization of mixed gas hydrates under equilibrium and non-equilibrium conditions: PVT<sub>x</sub> measurements and thermodynamic modeling

MAGHSOODLOO S., BOUILLOT B., DOUZET J.,  
HO-VAN S., HERRI J.M.



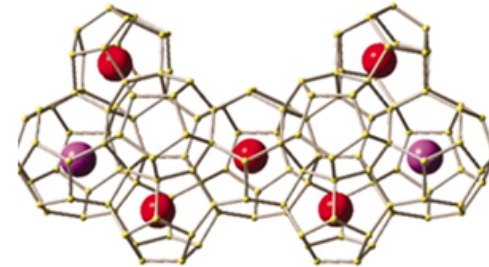
## What are gas hydrates?



0-10°C



10-100 bar



**Water and gas molecules**

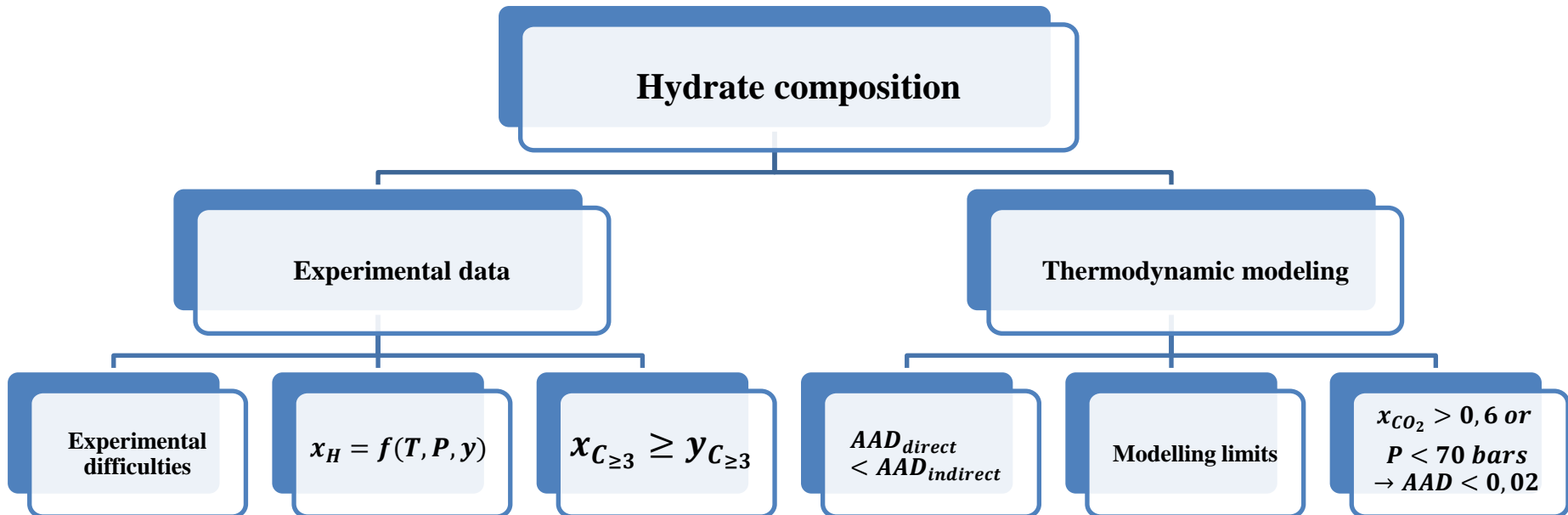
**Clathrate gas hydrate**

Hydrate composition and volume

Effects of crystallization rate

The capability of thermodynamic modeling

# Hydrate composition

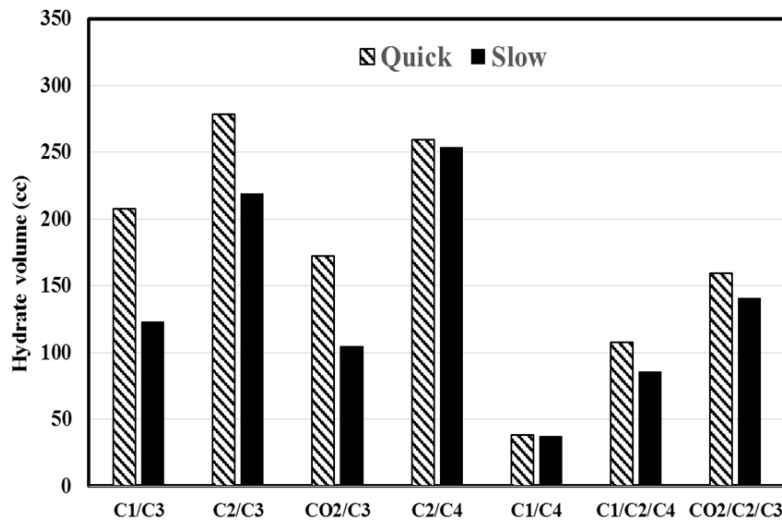


Maghsoodloo et al., Fluid phase equilibria. 472 (2018). 22-38.

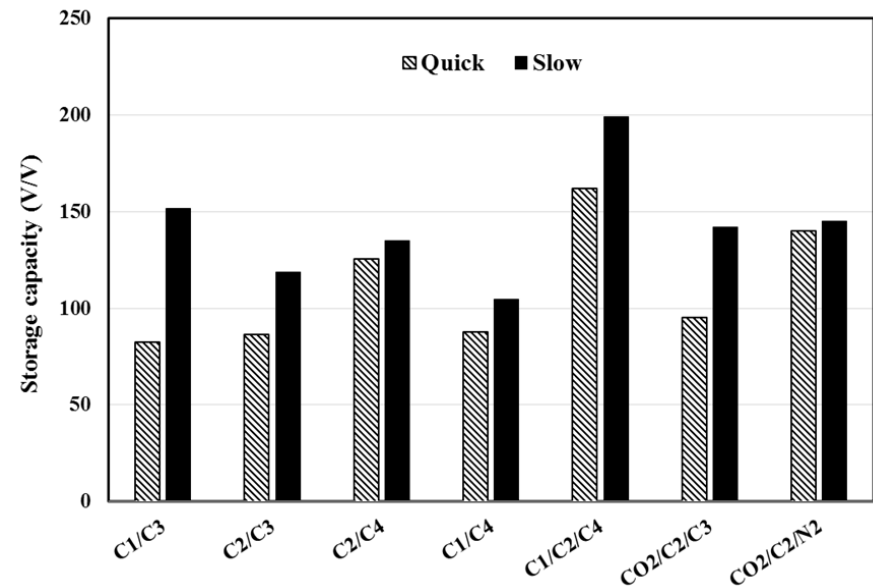
## Effects of crystallization rate

### Different hydrate composition and pressure at final state

Hydrate volume



Storage capacity

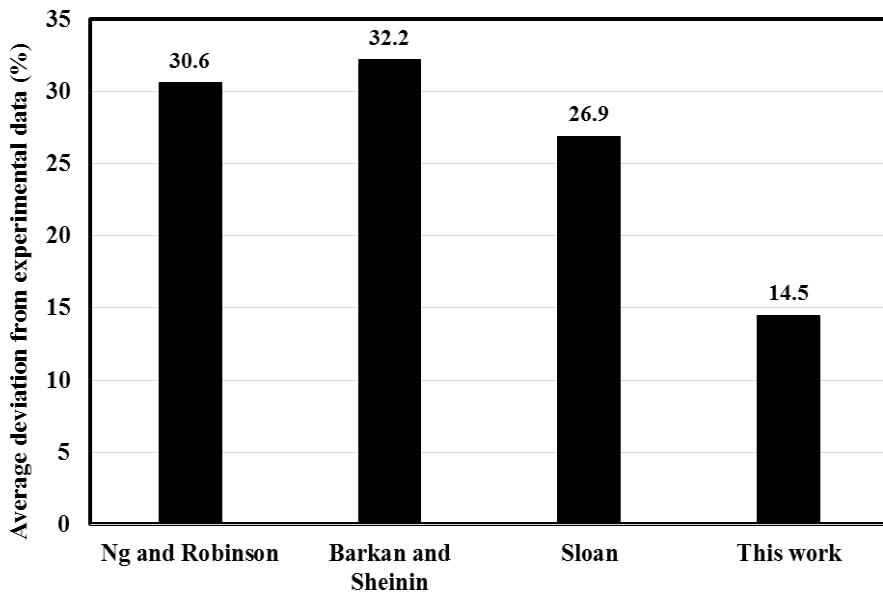


Maghsoodloo et al., J. Chemical Thermodynamics. 122 (2018). 73-84.

# Thermodynamic Modeling (vdW approach and Kihara Potential)

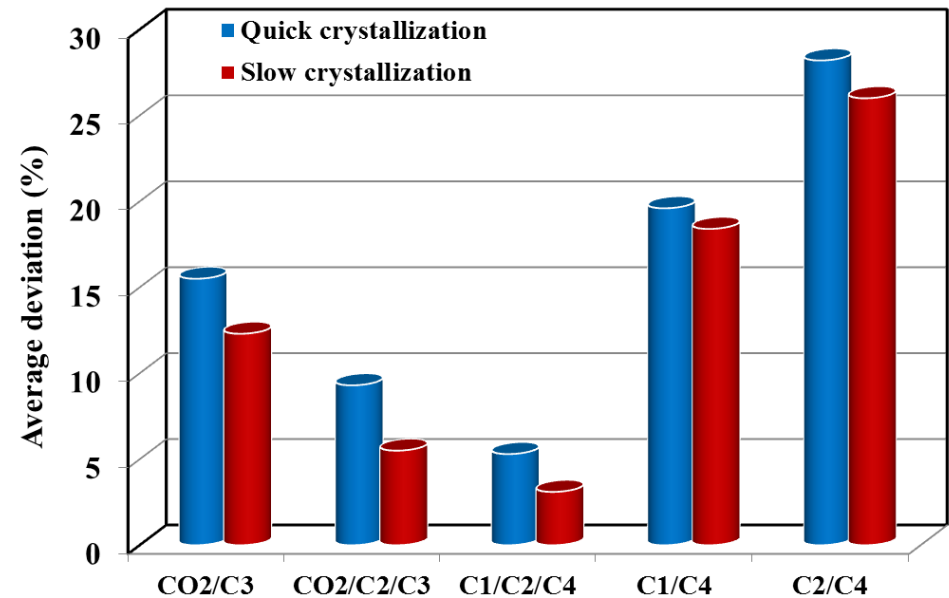
Kihara parameters optimization for propane in mixtures

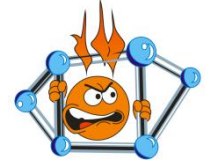
$$\varepsilon=195.0 \quad \sigma=3.34 \quad a=0.6502$$



Kihara parameters of propane from different references

Thermodynamic model simulation, equilibrium pressure





## Conclusion

- Different crystallization rate → Different hydrate phase properties
- Mixed gas hydrate crystallization seems to be driven by kinetics (high driving force)

Slow crystallization

Less kinetic effects

Thermodynamic  
equilibrium

These elucidations could have a significant impact on clathrate hydrate applications which thermodynamic equilibrium is essentially taken into account such as energy storage and transportation or CCS.



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# THANKS FOR YOUR ATTENTION

