Chemical Thermodynamics of Hydrogen Containing Systems

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In This Presentation …

Background

- Why hydrogen?
- Why is hydrogen flow metering important?
- From hydrogen production to its storage with thermophysical properties

Composition ?

T ?

P ?

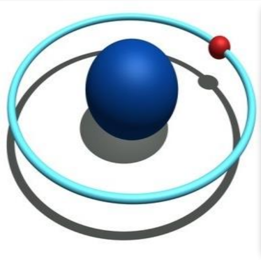
Thermodynamics

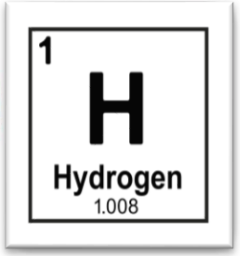
Here we used the adequate equation of sate and model to accurately predict the properties of H_2 containing streams

Summary/Potential Applications

Determination of hydrogen streams properties can enable us to select the secure hydrogen storage sites and precisely measure flow rates …

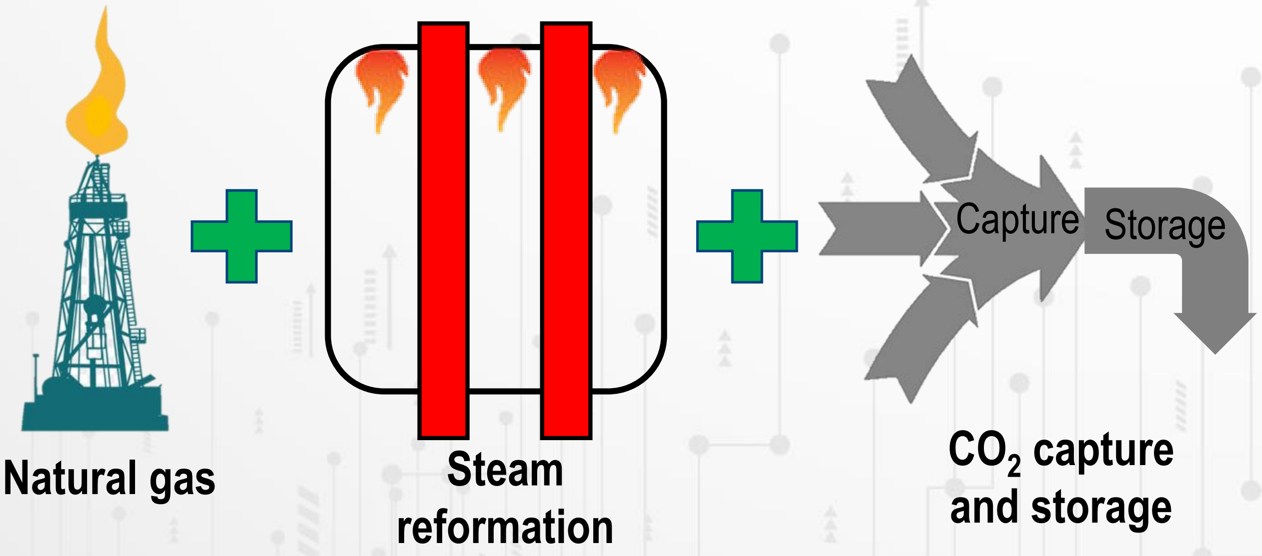
Why Study H_2 Properties?





- To touch net-zero targets, the emissions from fossil fuels must be reduced and the energy mix transition to low carbon energy sources must be accelerated
- Hydrogen has the potential to aid decarbonisation across different industries; transport, heat, power…

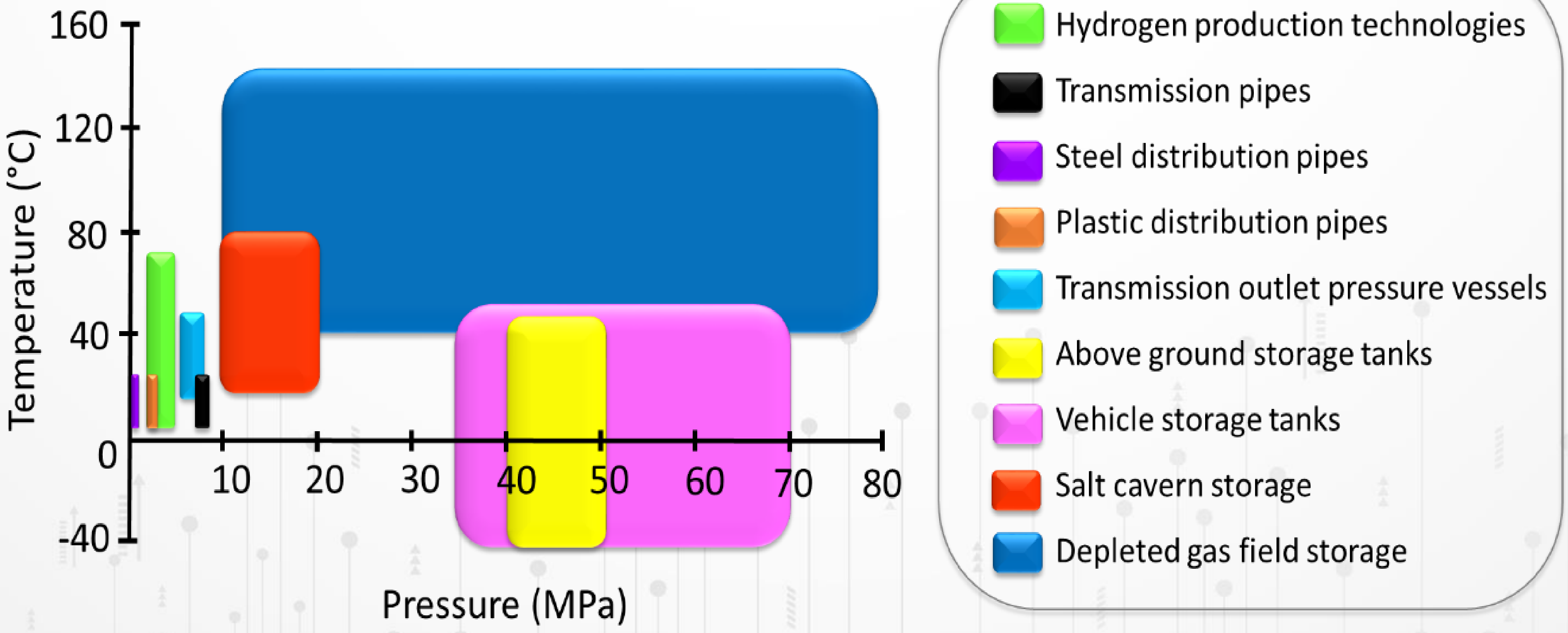
Hydrogen production; Composition?



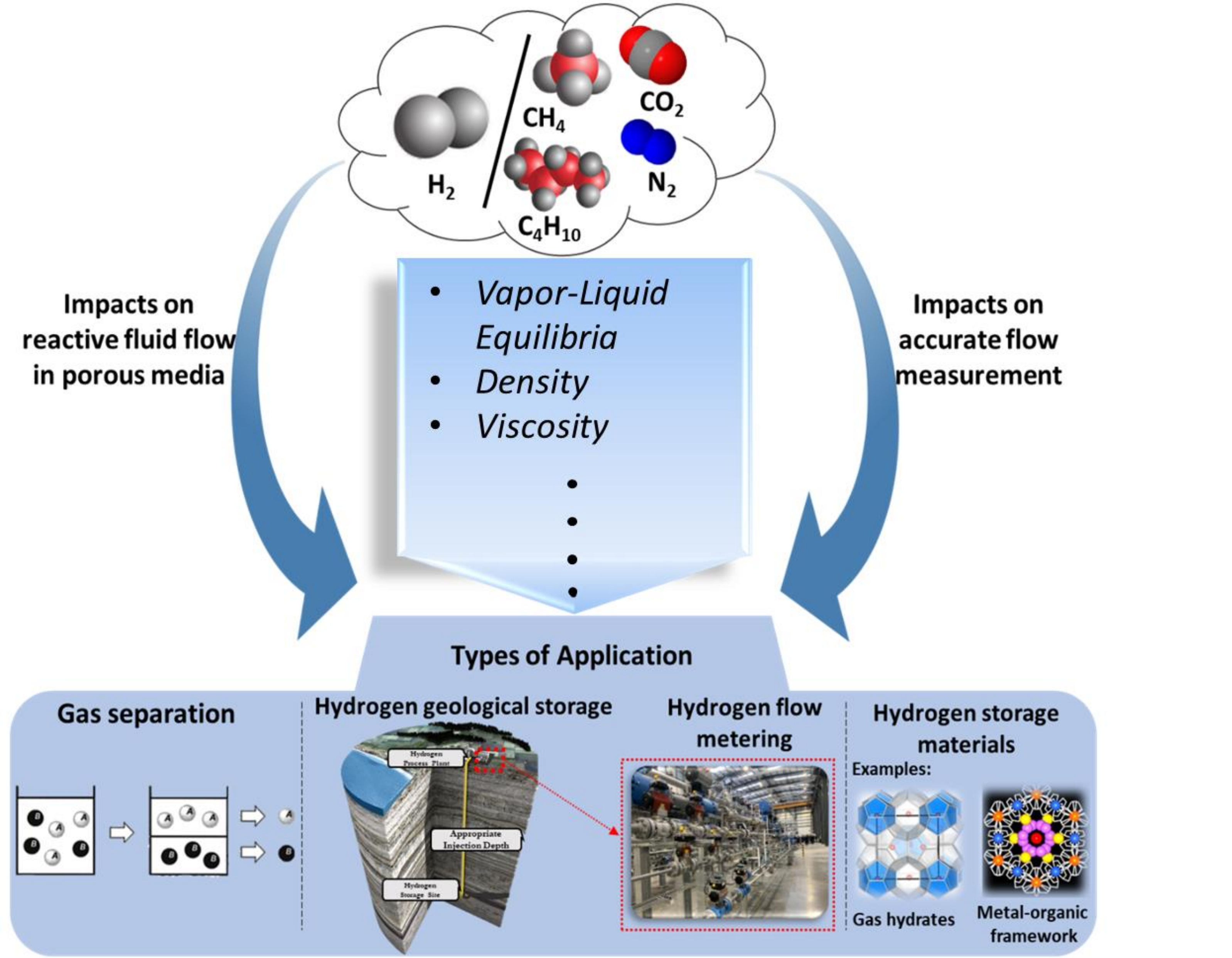
- 96% hydrogen currently produced through methane steam reformation which is called Blue Hydrogen.
- 7kg CO2 for 1kg hydrogen; Carbon capture and storage (CCS) process is essential to be low carbon blue hydrogen.

CH_4, CO_2, Natural gas; During the injection/production/transportation cycles, mixing of the mentioned gas components is inevitable

What are the Operating Conditions; P & T?



Which Properties?



Thermodynamic Models

GERG-2008 Equation of State (EoS) + *SuperTRAPP Model* = *Thermophysical properties*

Dimensionless Helmholtz energy: $\alpha(\delta,\tau,x) = \alpha^{o}(\rho,T,x) + \alpha^{r}(\delta,\tau,x)$

$\tau = T/T_r$ $\delta = \rho/\rho_r$ *x is the molar composition*

$$\mu(T,\rho) = \mu^{*}(T) + \Delta\mu_0(T_0,\rho_0)F_{\mu}(T,\rho)$$

** refers to dilute gas and **0** refers to a reference fluid*

Ideal-gas contribution: $\alpha^{o}(\rho,T,x) = \sum_{i=1}^{N} x_i[\alpha^{o}_{0i}(\rho,T) + \ln x_i]$

N: *number of mixture components*

x_i: *The mole fraction of each component i*

The residual part of Helmholtz energy: $\alpha^{r}(\delta,\tau,x) = \sum_{i=1}^{N} x_i\,\alpha^{r}_{0i}(\delta,\tau) + \Delta\,\alpha^{r}(\delta,\tau,x)$

$\Delta\alpha^{r}$: Departure function

Density

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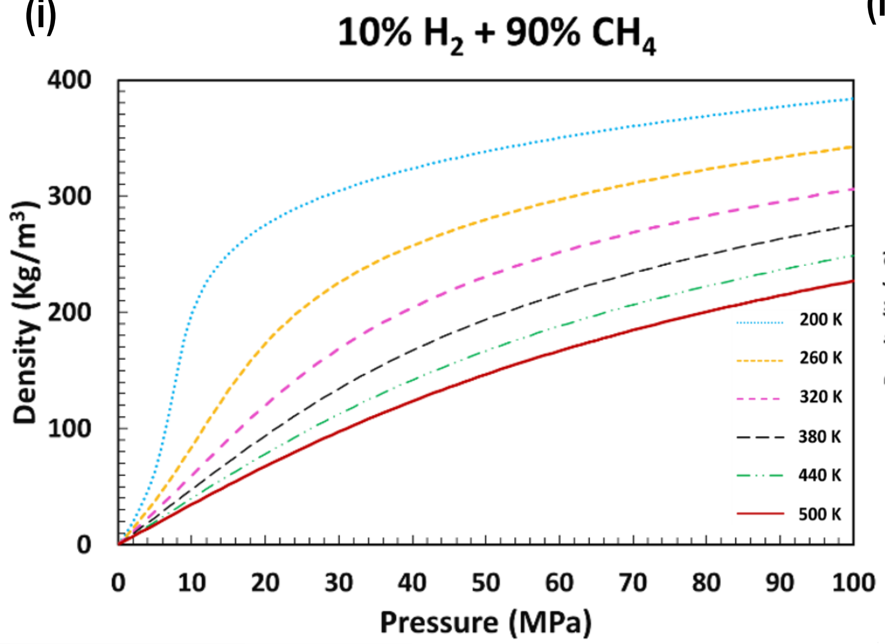
measuring for the energy transition

(i)



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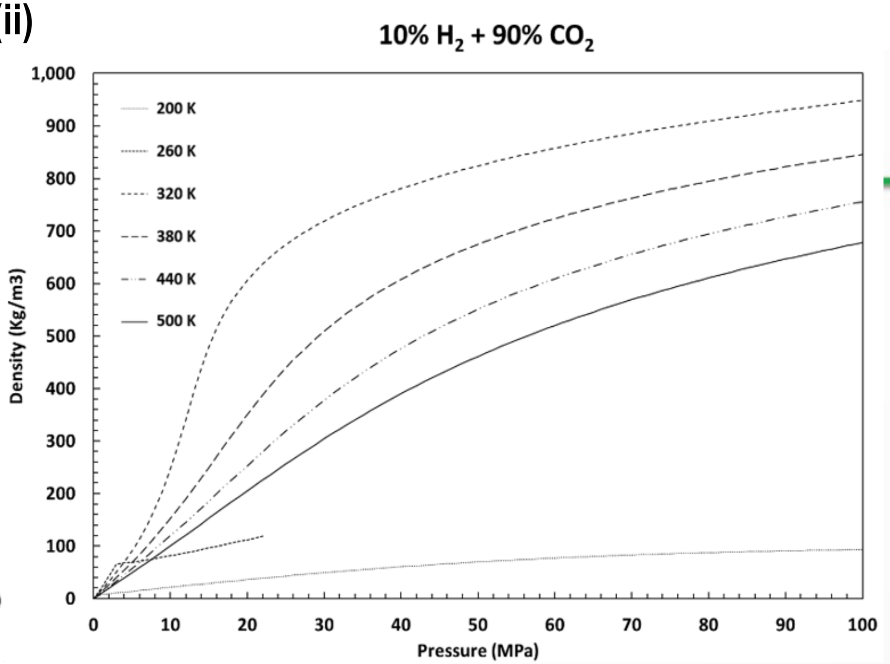
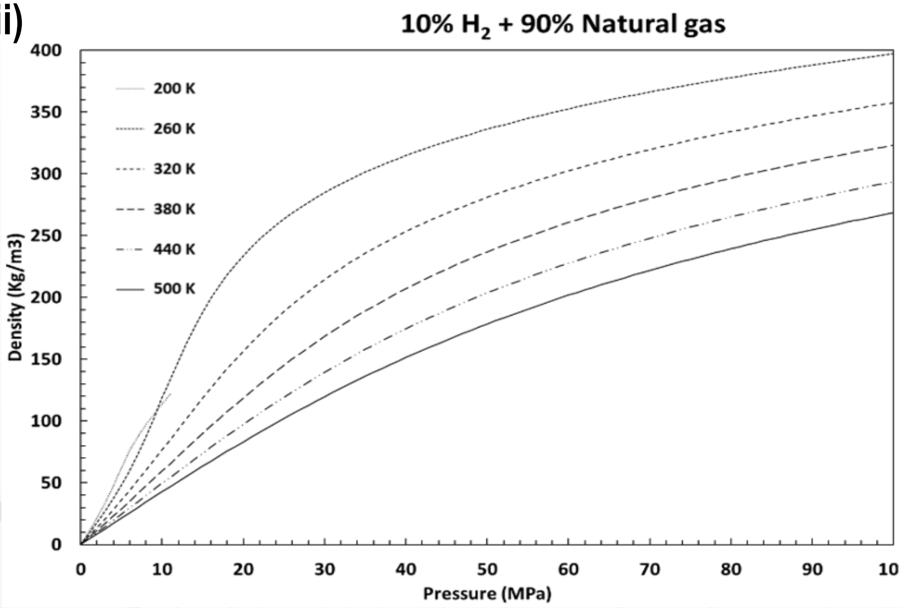


North-Sea Natural gas Composition

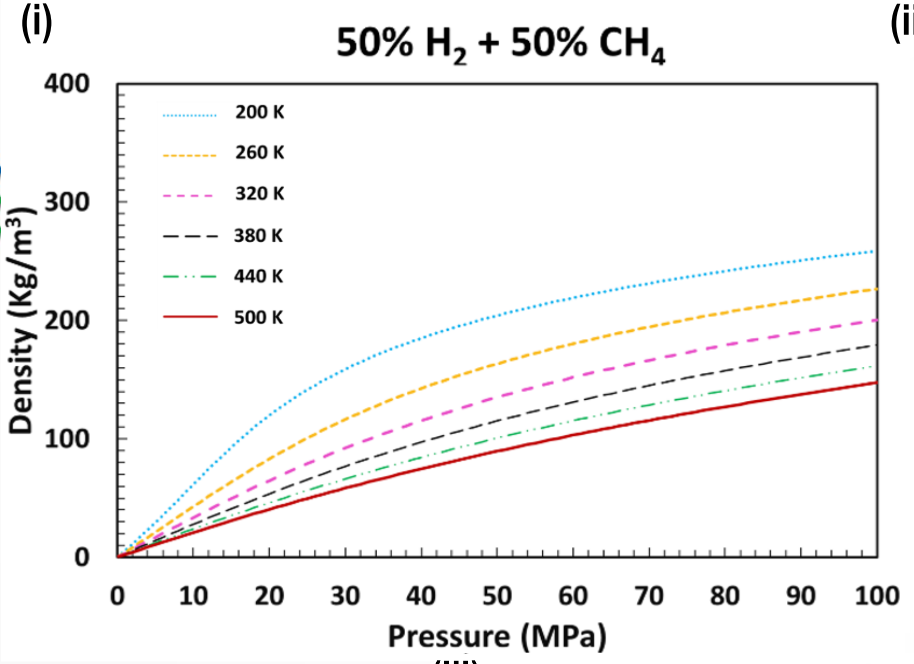
Component	Mole%
CH_4	83.60
C_2H_4	7.48
C_3H_8	3.92
n-C_4	0.81
i-C_4	0.81
n-C_5	0.15
i-C_5	0.14
N_2	1.95
CO_2	1.14

(iii)



Density (Cont'd)

(i)



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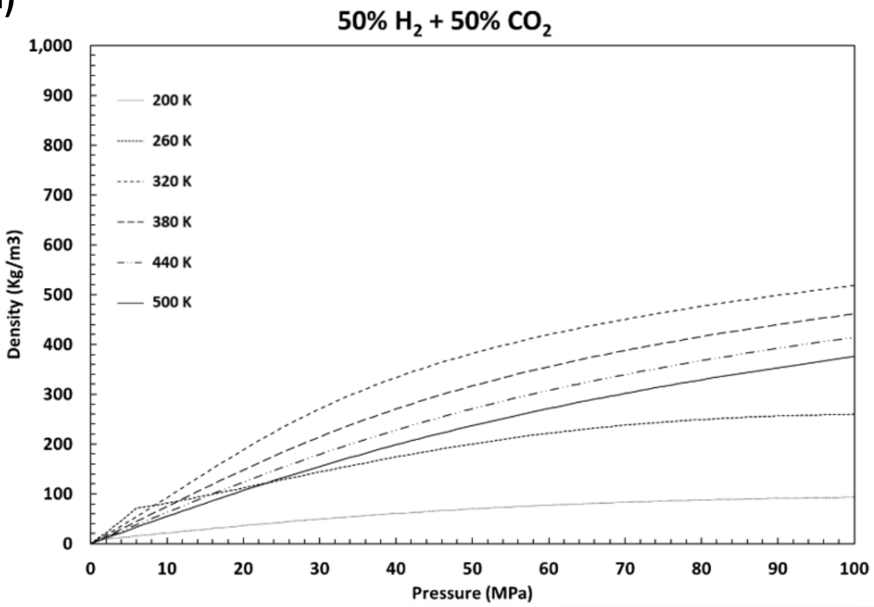

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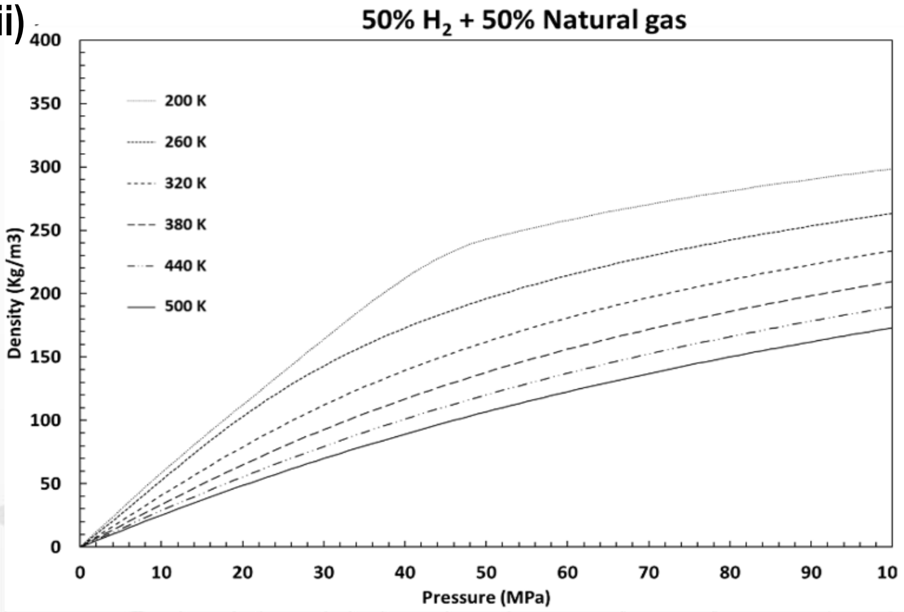
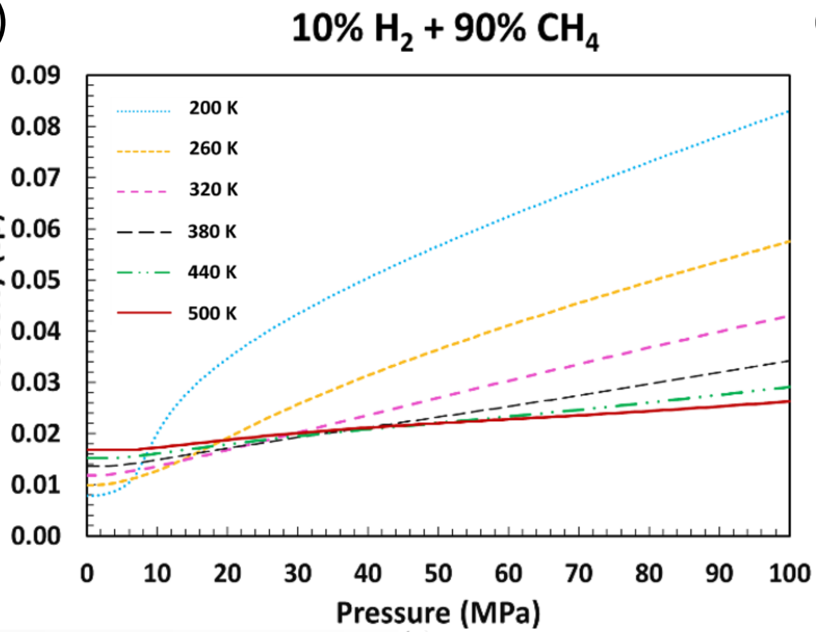


Viscosity

(i)



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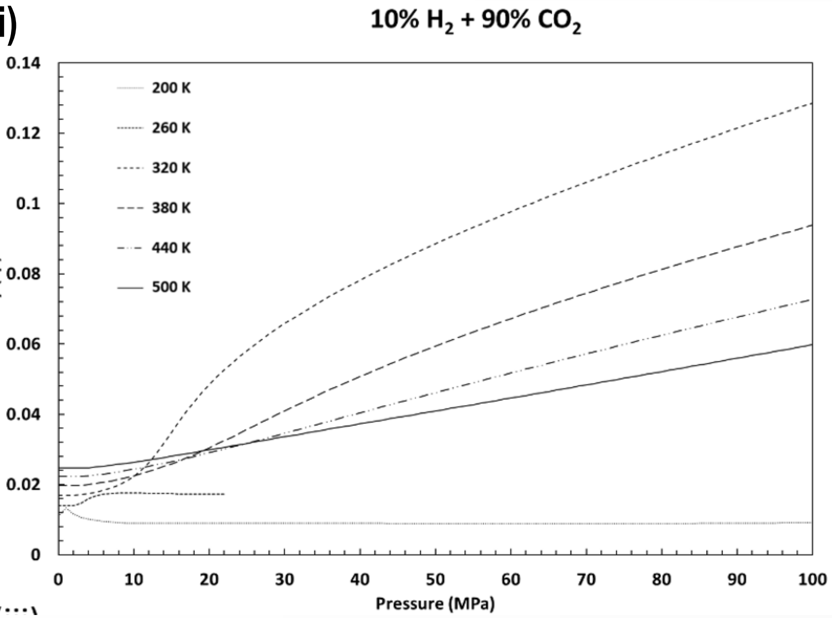

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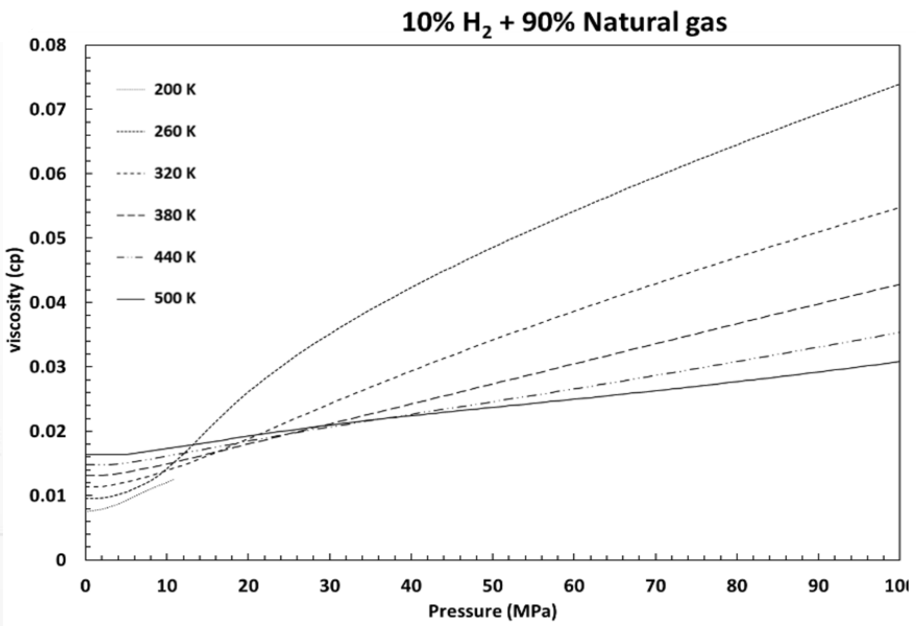

Viscosity (Cont'd)

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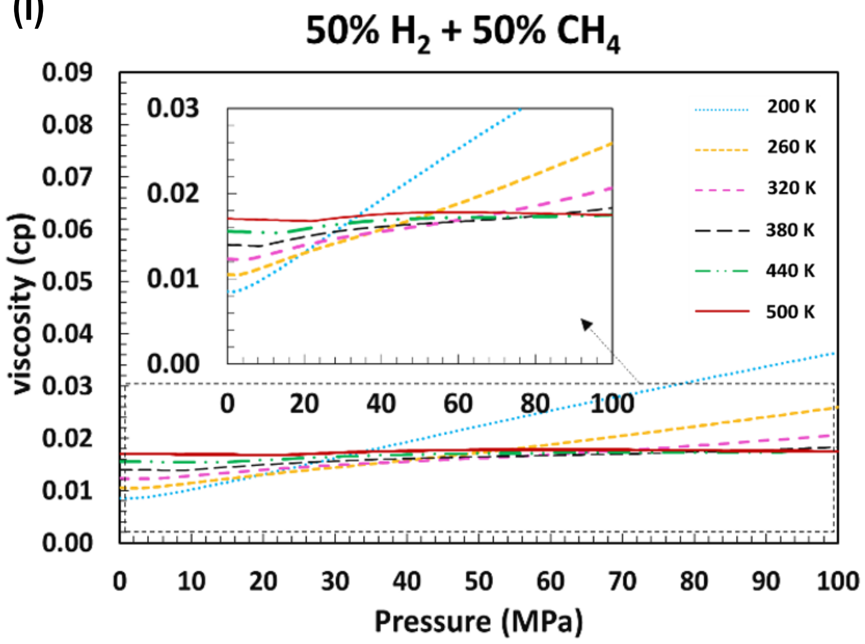

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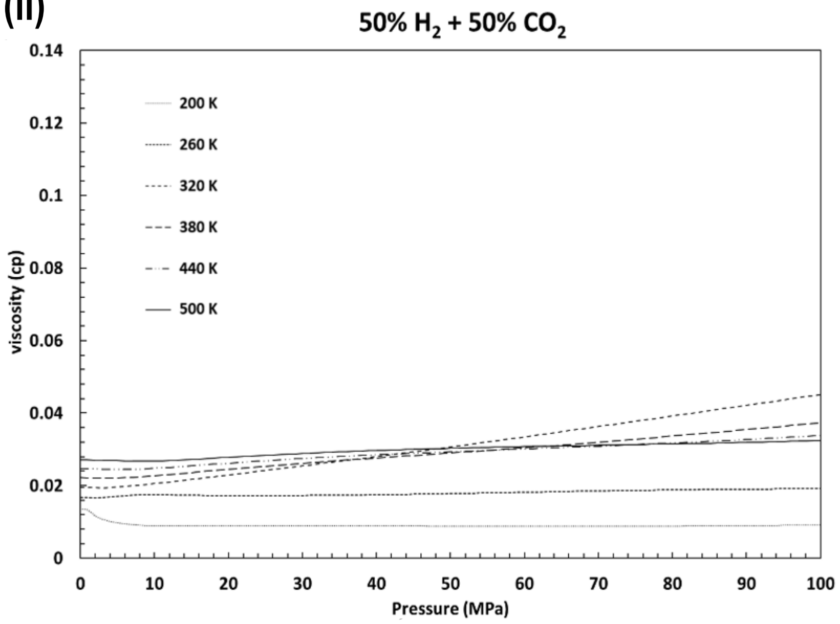

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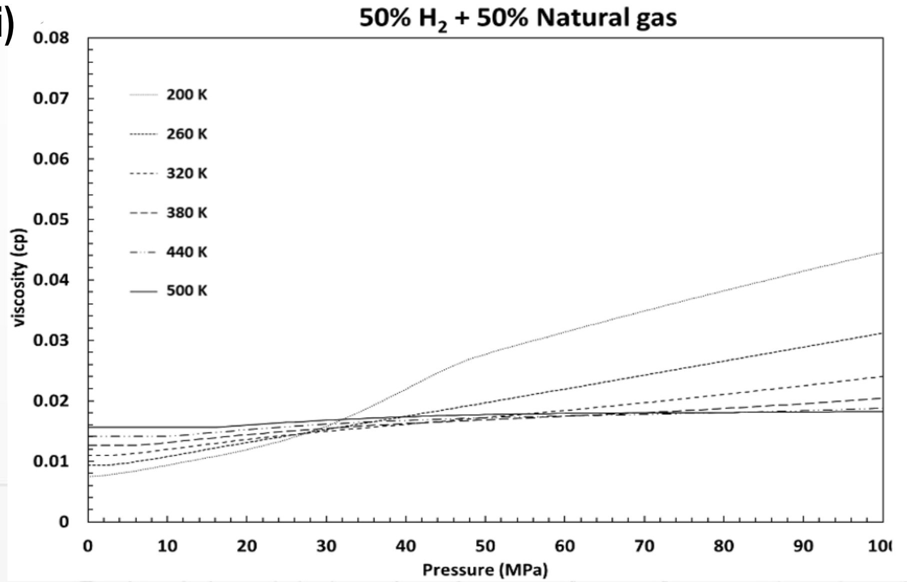
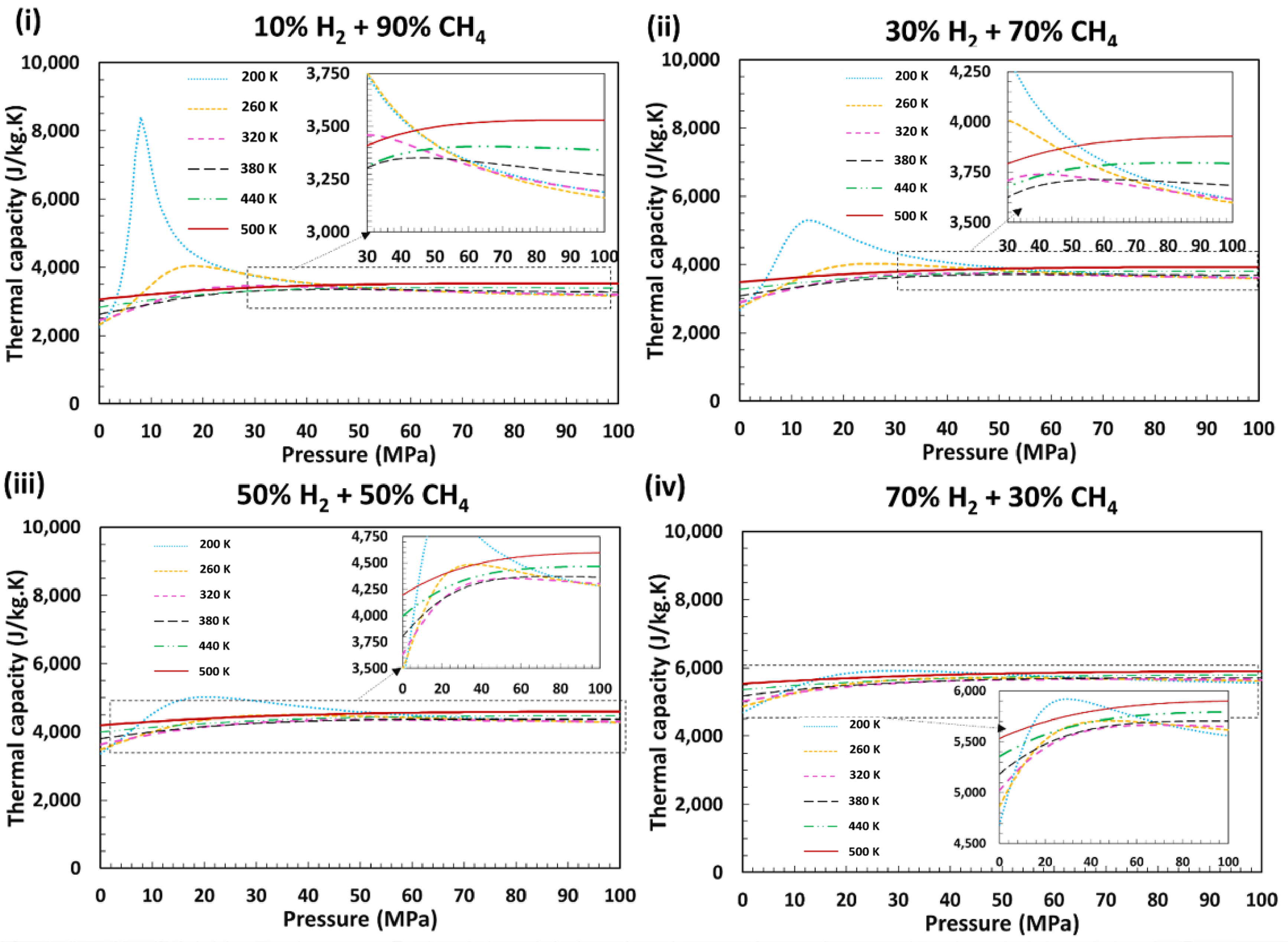
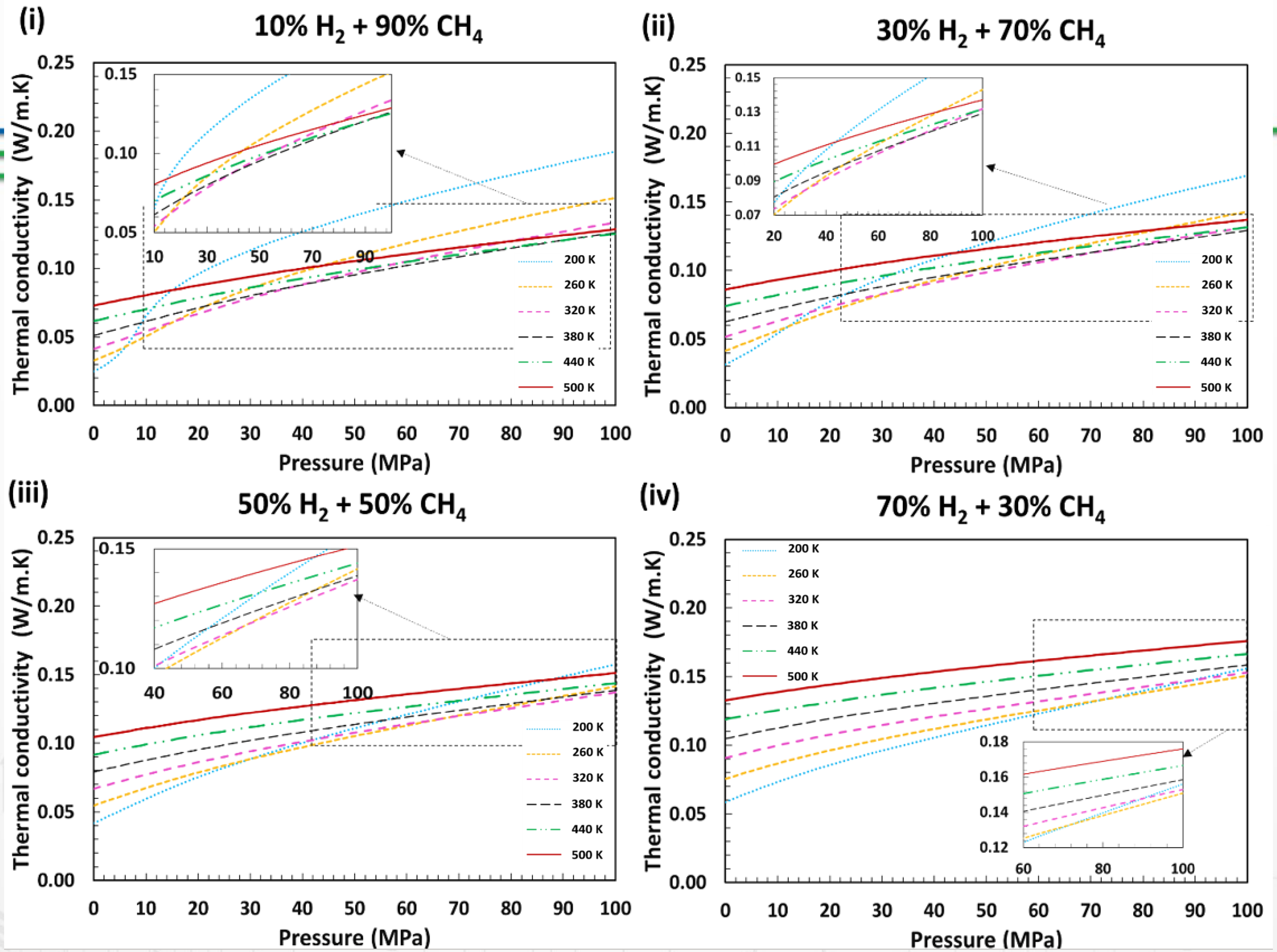


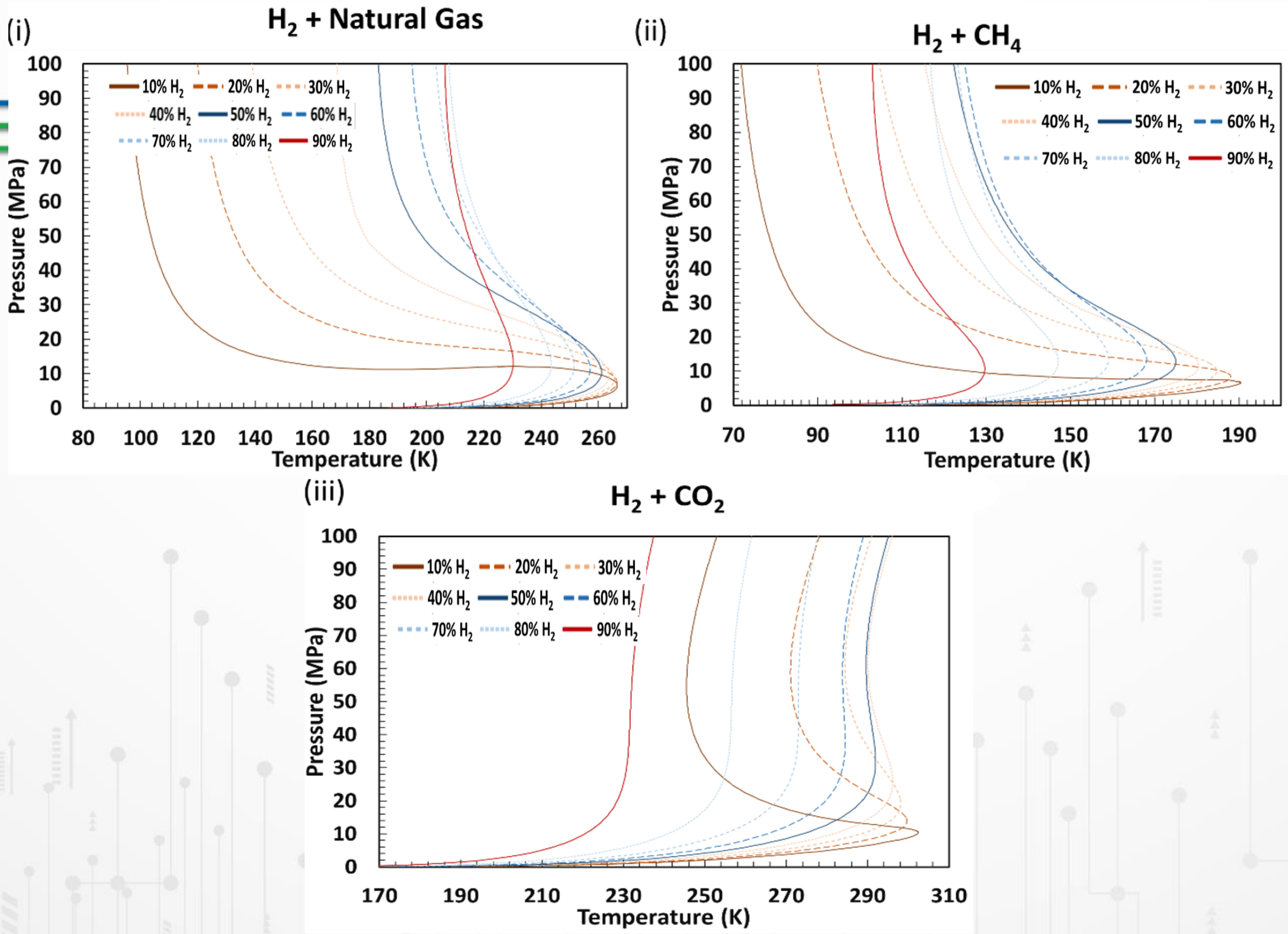
Thermal Capacity



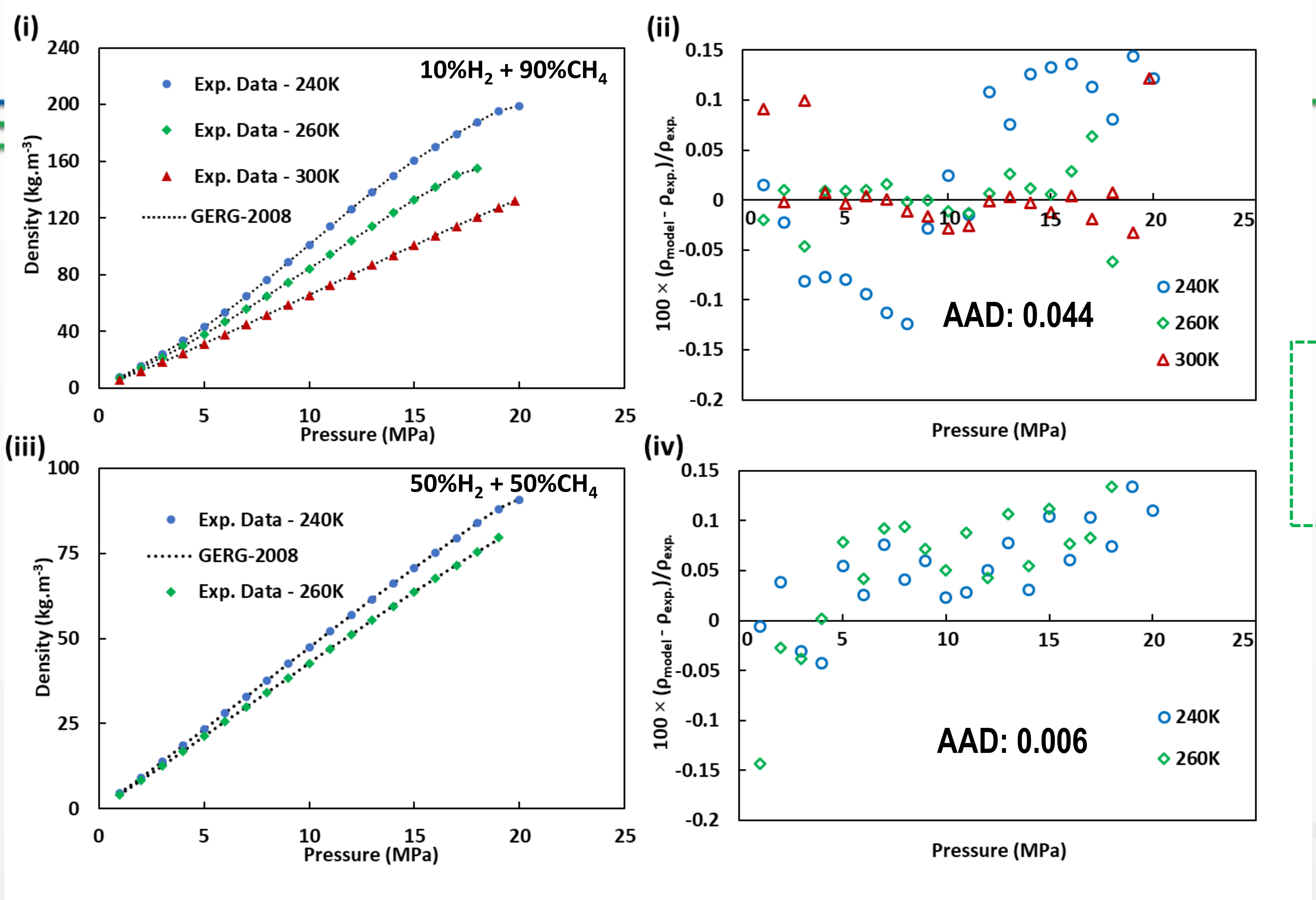
Thermal Conductivity



Vapour Liquid Equilibria (VLE)



Thermodynamic Modelling vs Experimental Results



- ✓ The high accuracy of GERG-2008 EoS predictions with relatively low errors

Summary

- ✓ The GERG-2008 EoS and SuperTRAPP model can accurately predict density, viscosity, thermal capacity and conductivity of hydrogen when mixed with other gaseous species including CH_4, CO_2 and a typical North Sea natural gas.
- ✓ The model has been successfully applied to a wide range of pressures, temperatures, and gas mixture compositions which cover the temperature and pressure conditions experienced within the whole hydrogen-based energy system from production to storage in geological formations.
- ✓ The obtained results can be employed by a range of different stakeholders to effectually design and develop innovative infrastructure for the hydrogen economy.

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Thanks for your time and attention!

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