Advanced Property Models for Processing, Transport and Storage of Gas Mixtures Containing H_2

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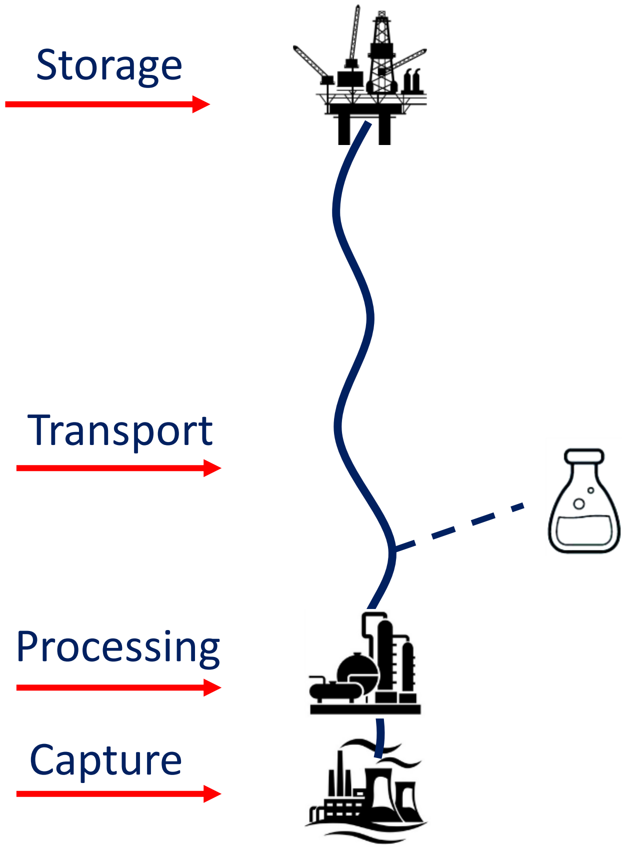
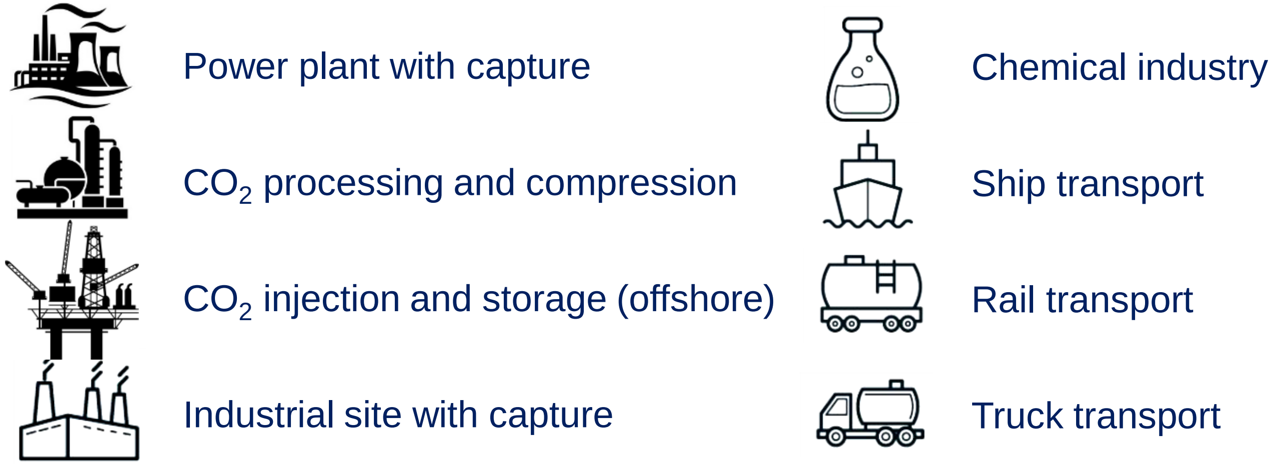
Requirements on Property Models – Transport as an Example



What we discussed so far:

- Power plant close to base load as CO_2 source
- One fuel, one capture process
- ➢ Essentially a constant CO_2 stream with constant composition

- Possibly use of part of the CO_2 as feedstock



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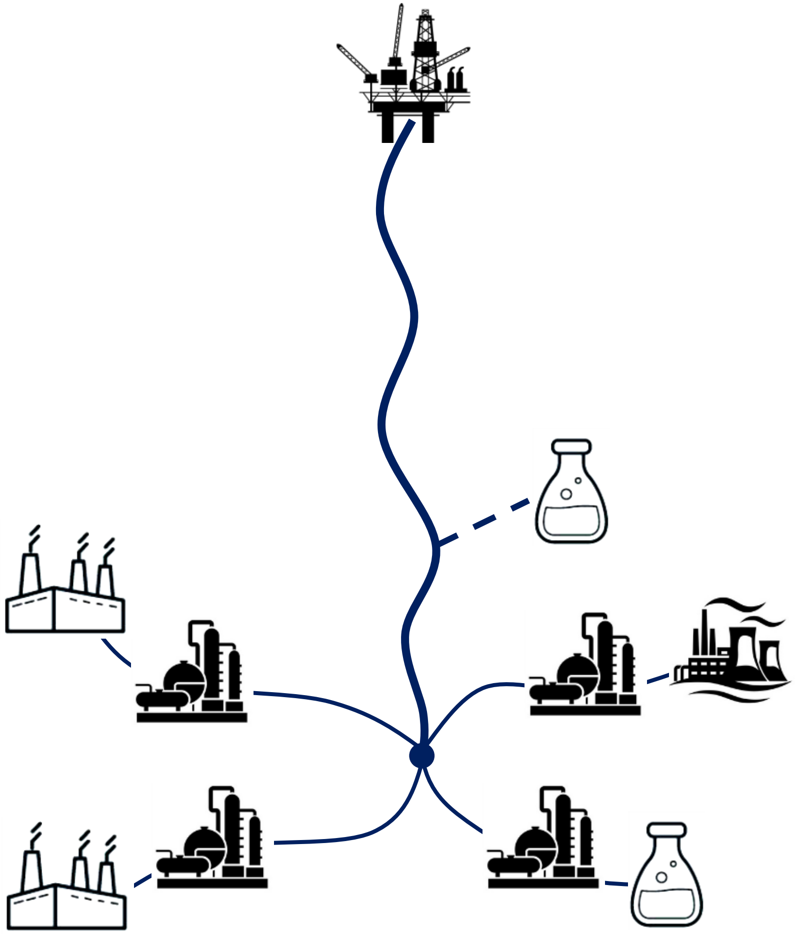
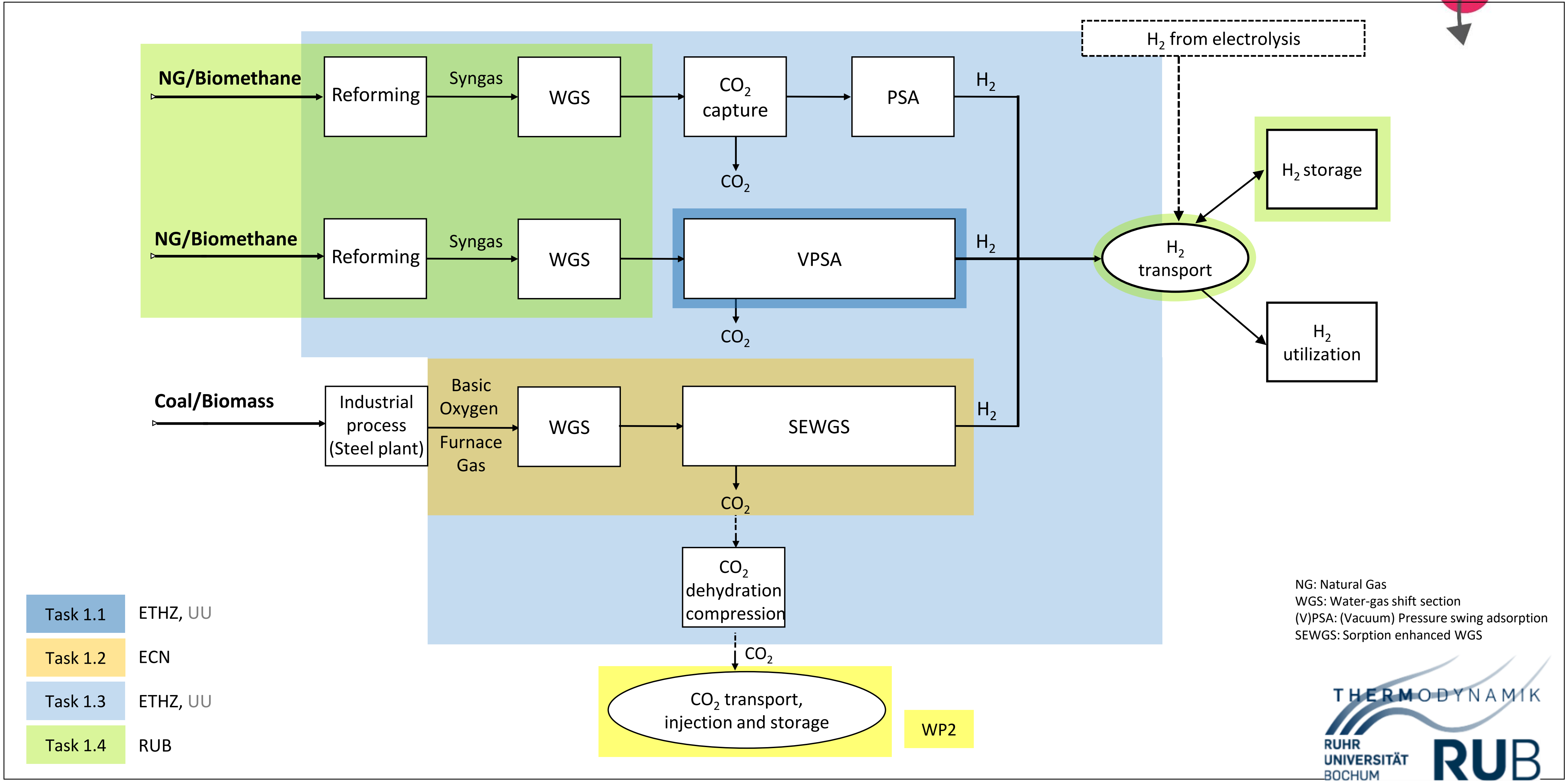


Industrial Clusters and Hubs:

- Different CO_2 sources
- Some at base load, some fluctuating
- Different origins of the CO_2
- **Different capture technologies**

➢ **Different impurities** – in ELEGANCY including **hydrogen**

Different CO_2 Sources and Capture Technologies



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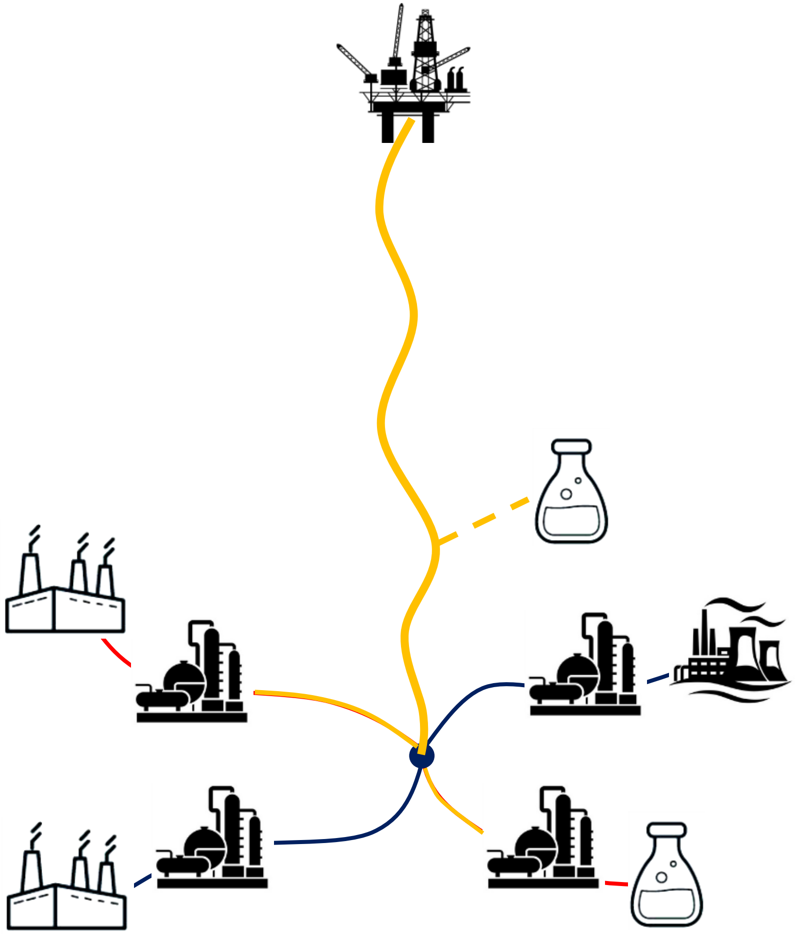

What we need to know:

- **Phase behaviour** needs to be known for varying composition, pressure, temperature
- **Density** needs to be known accurately for custody transfer, to avoid allocation errors
- **Speed of sound** for flow measurement, dynamic models
- Small amounts of hydrogen in transport, hydrogen rich mixtures in separation and processing

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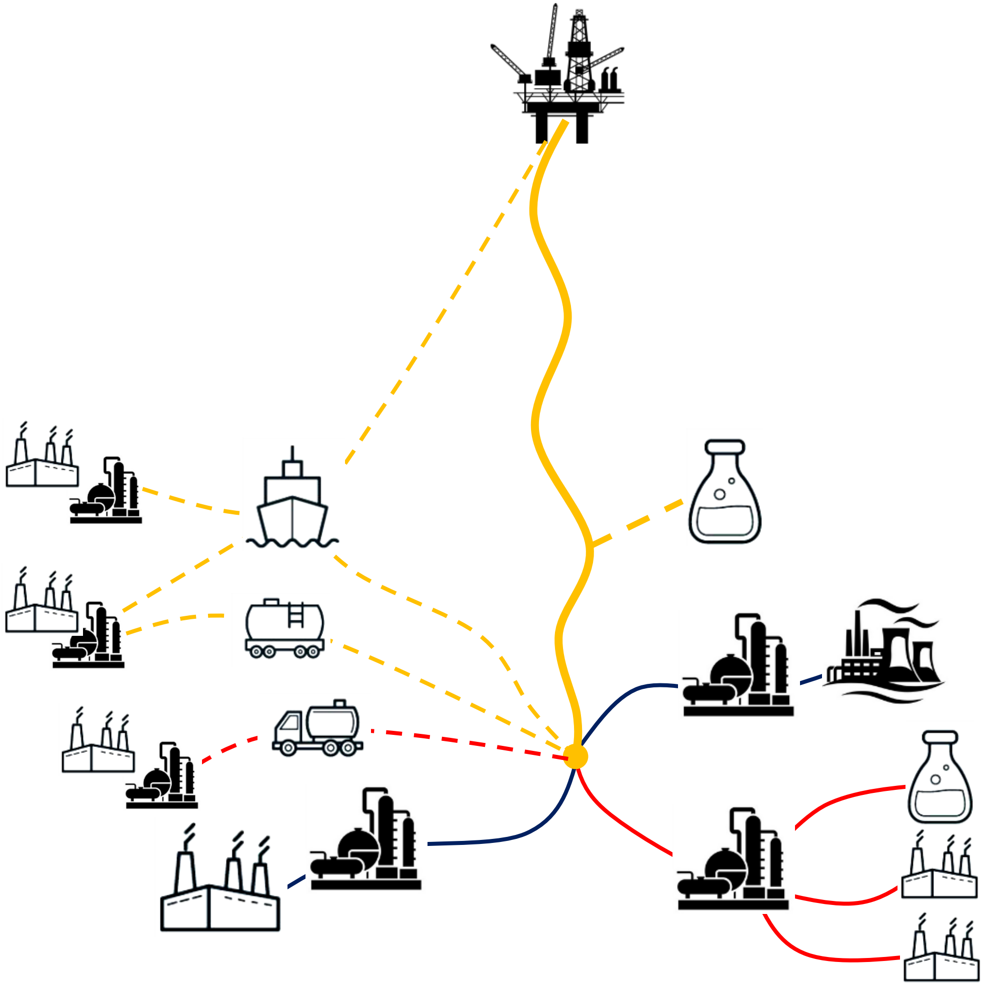

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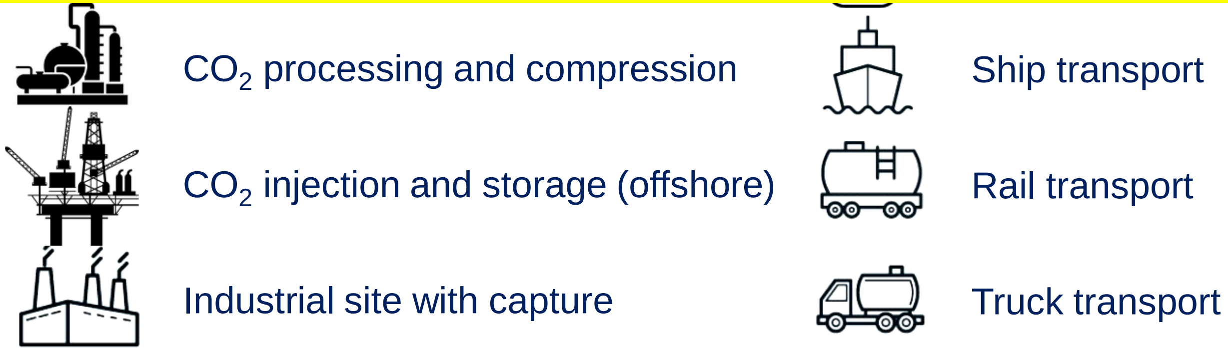
Different means of capture, processing and transport require property data in a broad range of compositions, temperatures, and pressures!



Helmholtz-Energy Based Multiparameter Mixture Models

- Mixtures are described based on the 1990's approach by Lemmon & Tillner-Roth
  - Pure fluid equations of state
  - Mixing rules for δ_m und τ_m with up to 4 adjustable parameters
  - "Departure function" for an improved description of well measured mixtures

$$\alpha(\delta,\tau,\bar{x}) = \sum_{i=1}^{N} x_i \left[\alpha^0_{oi}(\rho,T) + \ln x_i\right] + \sum_{i=1}^{N} x_i \alpha^\mathrm{r}_{oi}(\delta_\mathrm{m},\tau_\mathrm{m}) + \sum_{i=1}^{N-1}\sum_{j=i+1}^{N} x_i x_j F_{ij} \alpha^\mathrm{r}_{ij}(\delta_\mathrm{m},\tau_\mathrm{m})$$

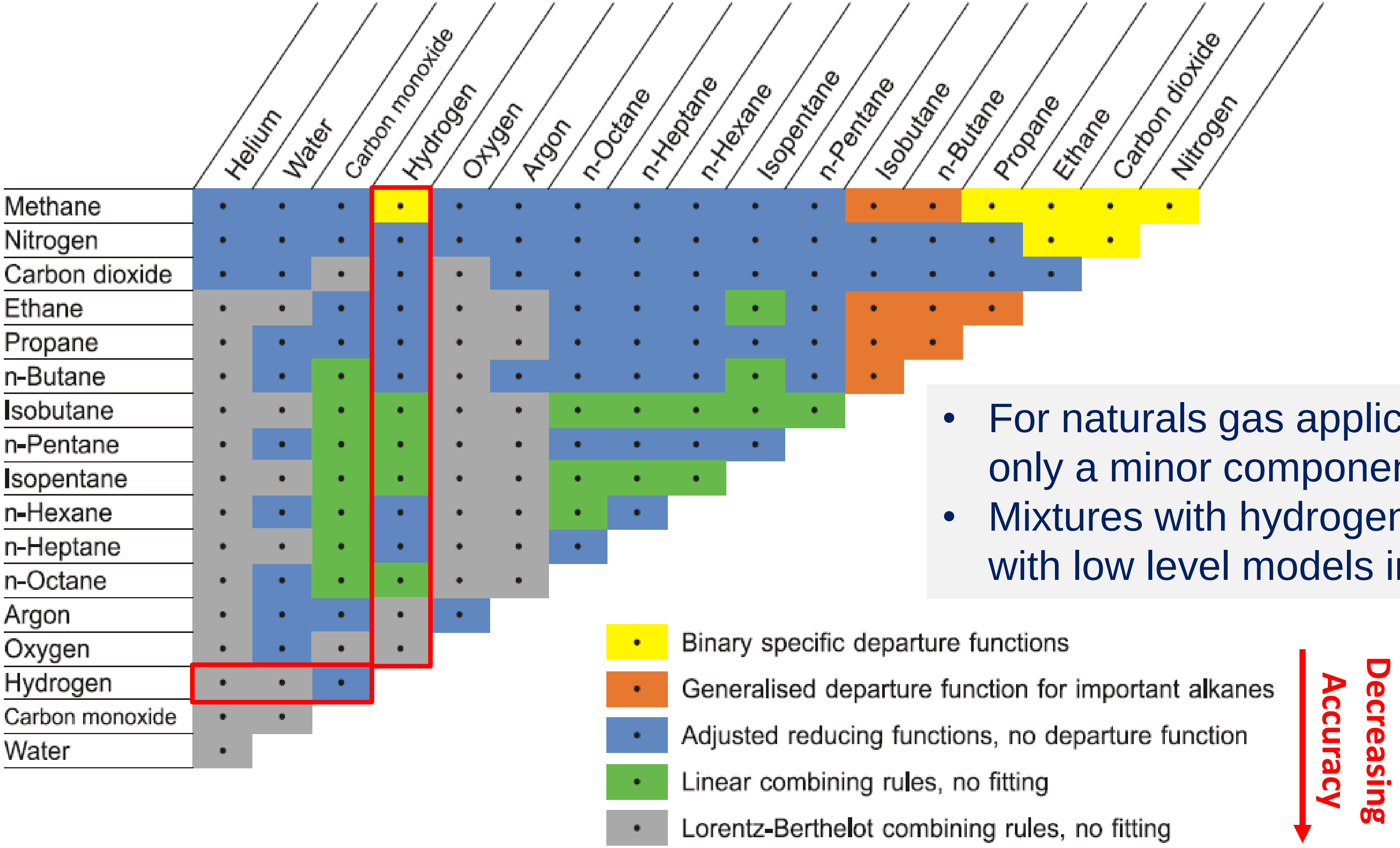
corresponding states with four parameters

pure fluid equations

departure function

- **In multicomponent mixtures models for all binary subsystems required**
- **Four Levels of accuracy:** (a) purely predictive description with combination rules, (b) fitting of the four corresponding states parameters, (c) generalized departure function, (d) binary specific departure function

GERG-2008 as Starting Point



- For naturals gas applications hydrogen is only a minor component
- Mixtures with hydrogen are described only with low level models in GERG-2008

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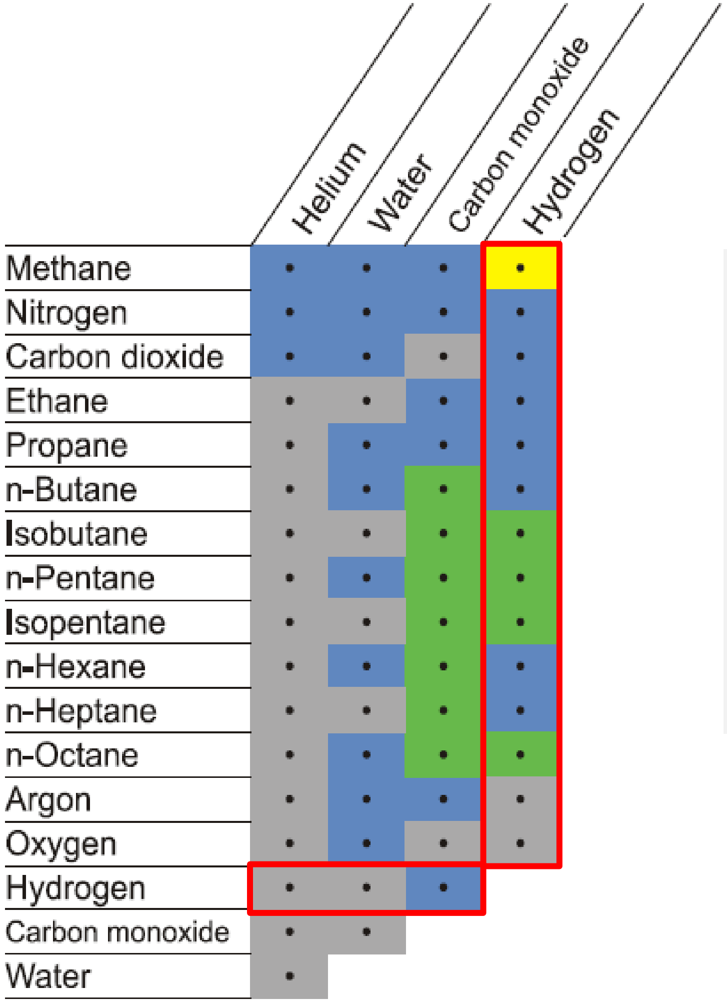
Improving GERG-2008 for Mixtures with Hydrogen



- Replace the GERG-2008 equation of state for pure hydrogen by the new international standard
- Develop mixture models for the most relevant binary subsystems
- Hydrogen is a “difficult” component – **comprehensive sets of accurate data** required

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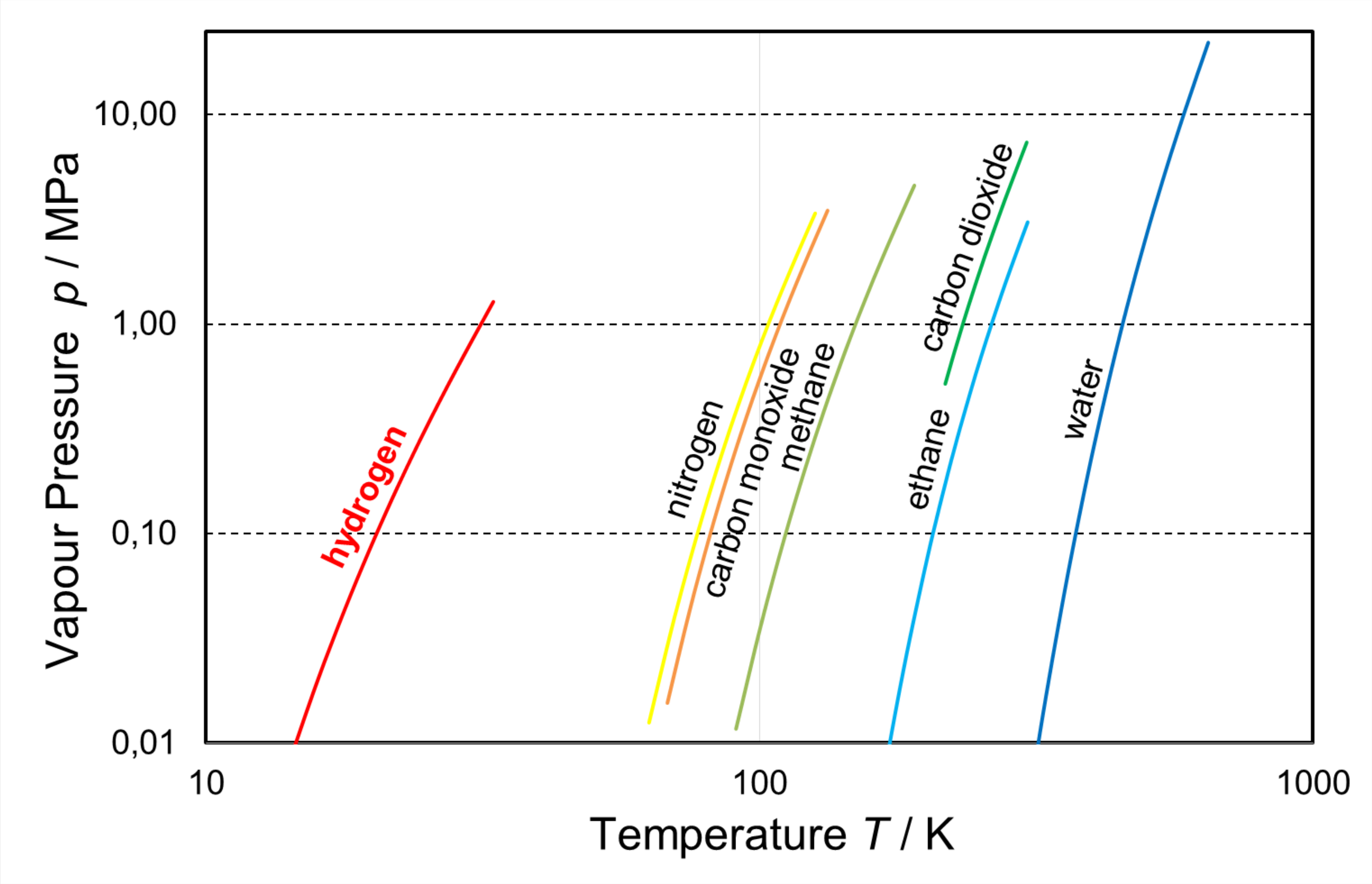

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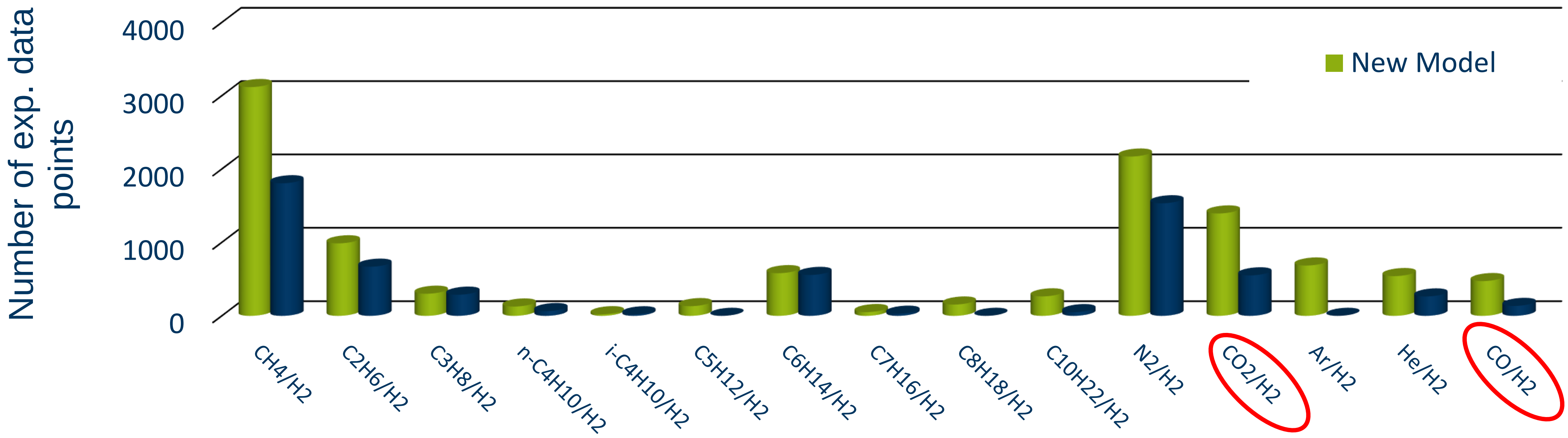
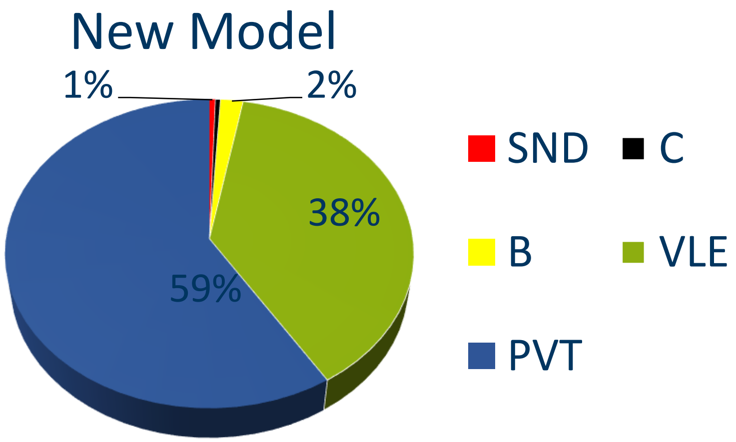
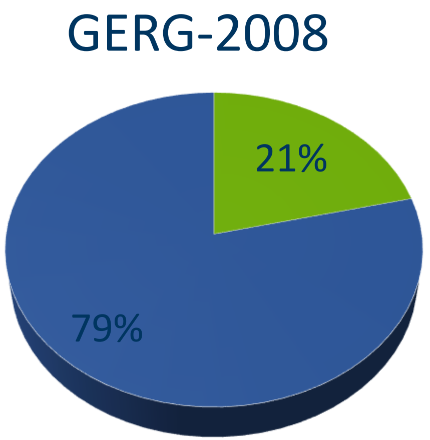


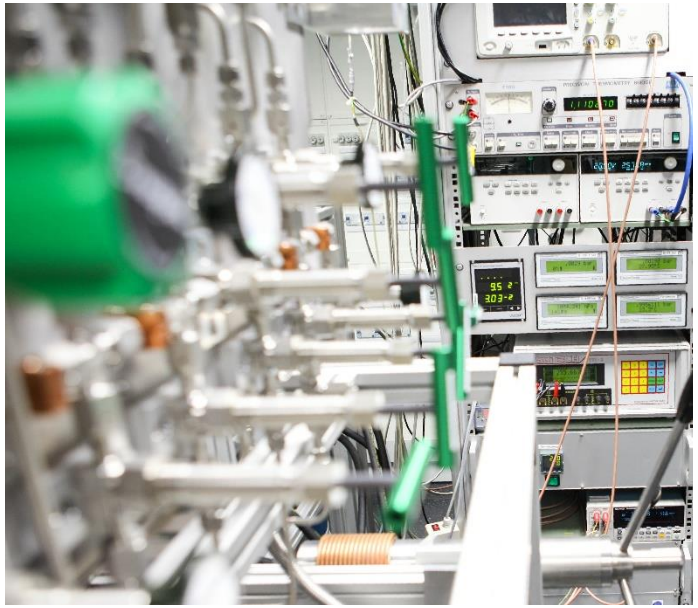


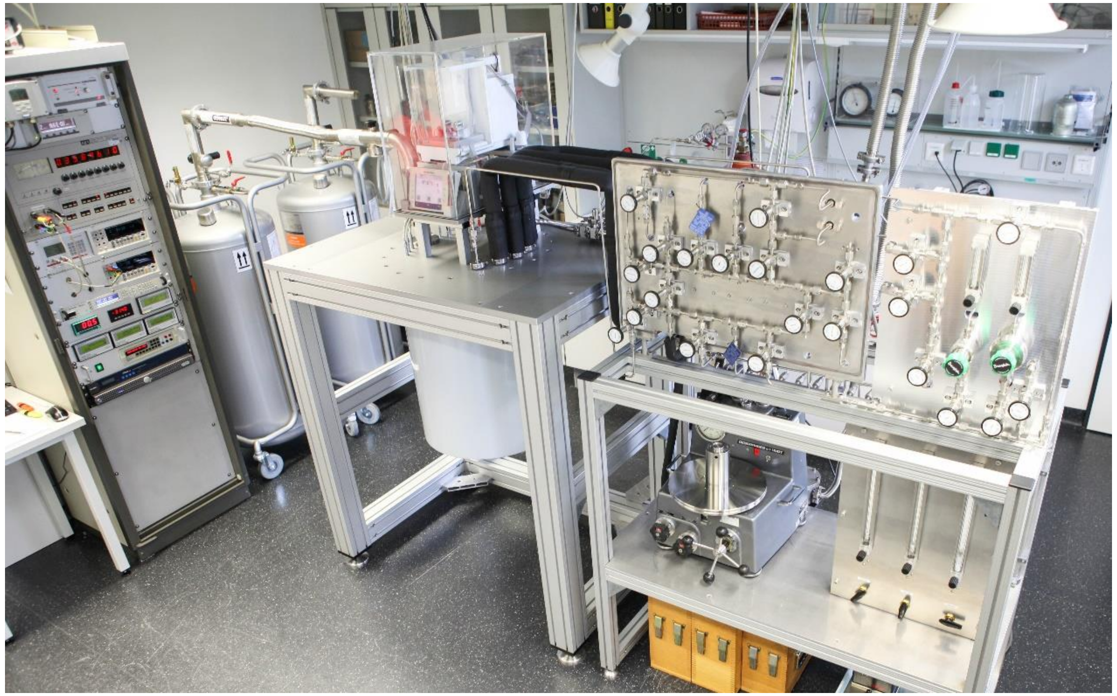


New data from …

- extensive literature search
- synergies to other projects
- ***own measurements in ELEGANCY***

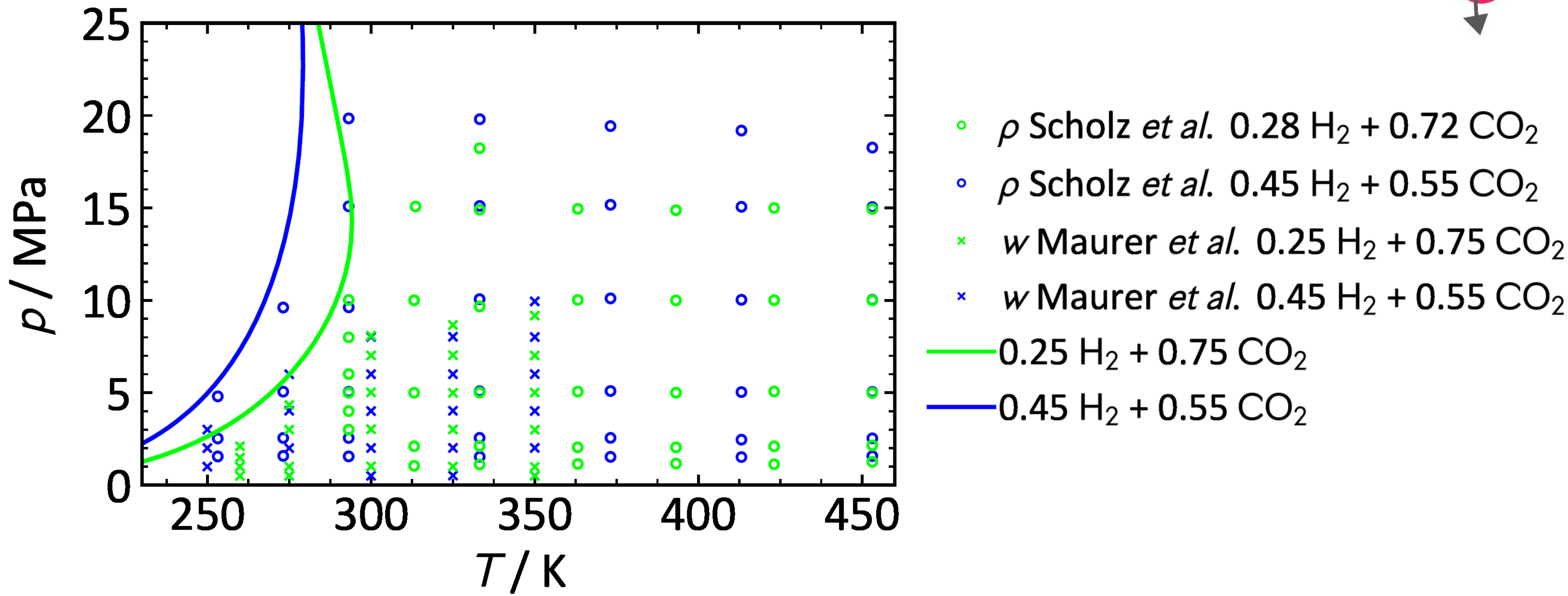
Experimental Work in ELEGANCY





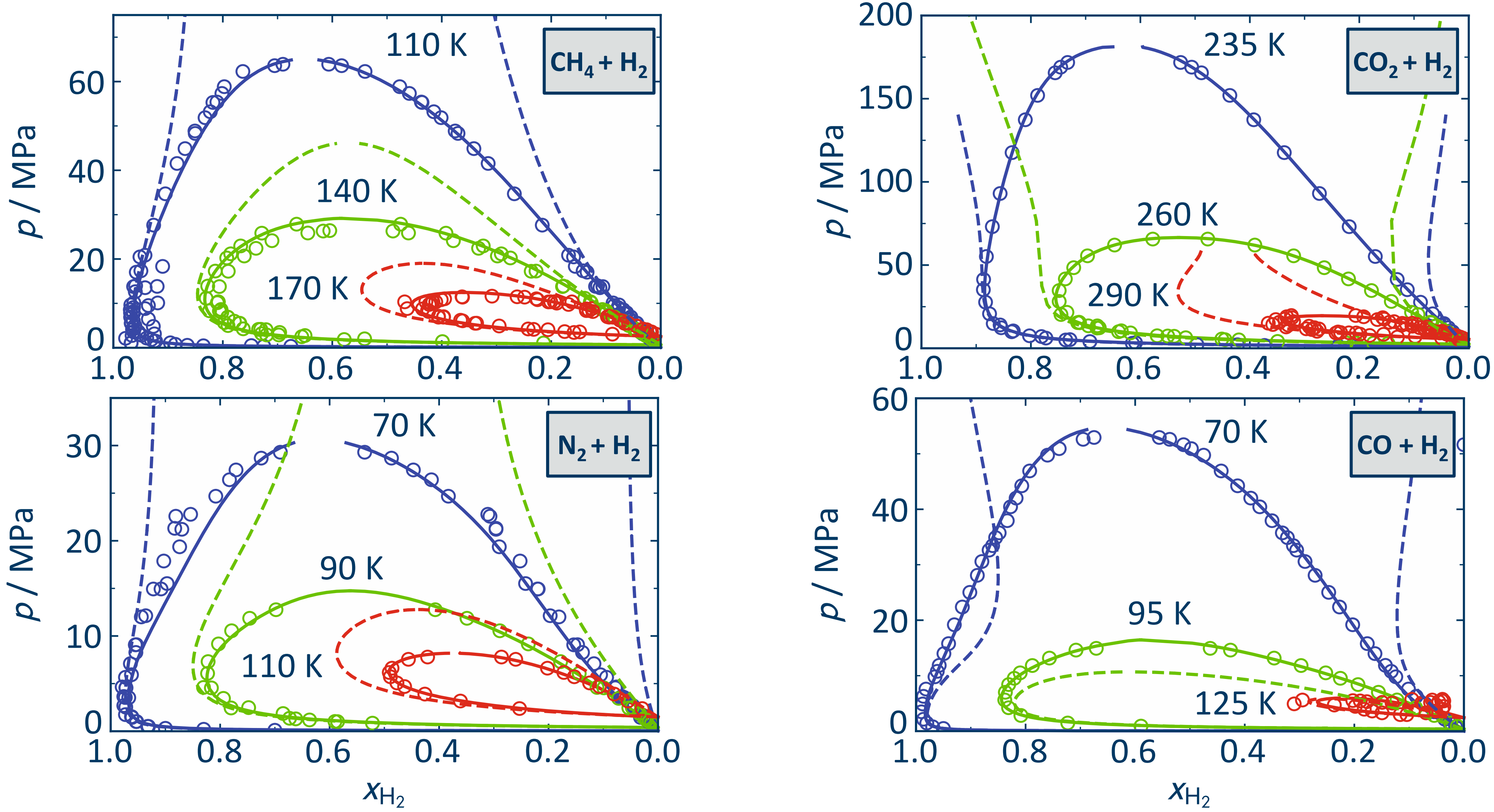
Thermodynamics laboratories at RUB are highly specialised in accurate density (and speed of sound) measurements

Experimental Work in ELEGANCY



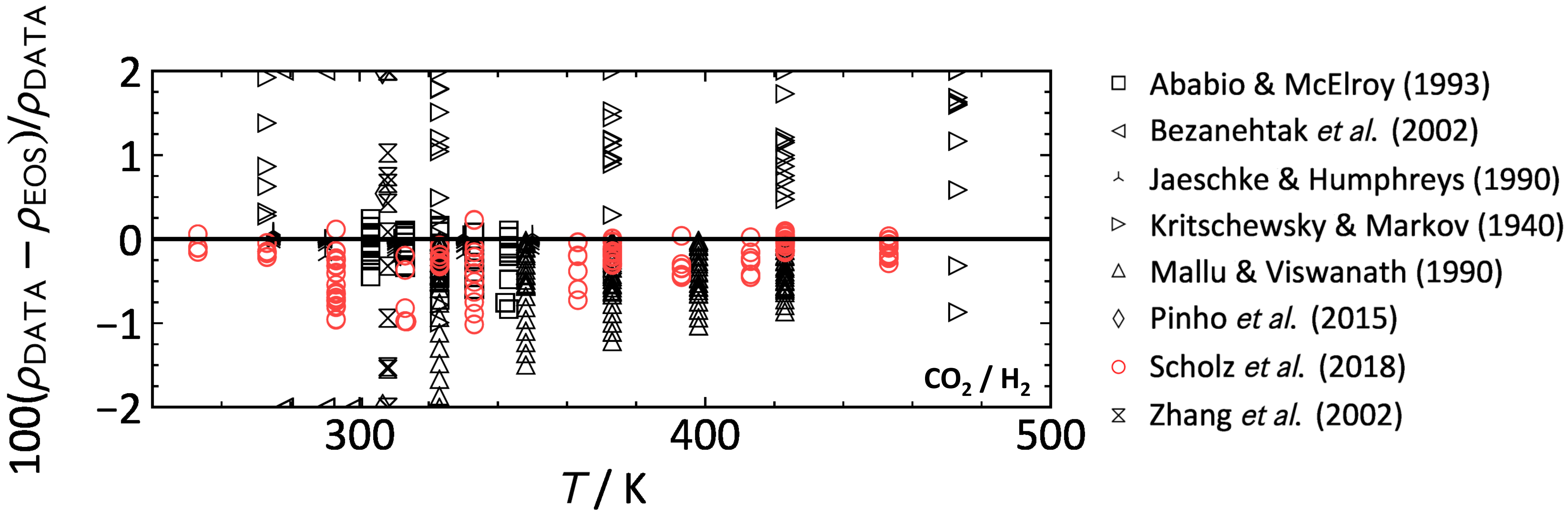
For the most relevant binary subsystems, the data situation at homogeneous states could be largely improved as a result of our work in ELEGANCY.

Improved Description of Phase Equilibria



solid lines = new model   dashed lines = GERG-2008

Improved Description of Homogeneous States



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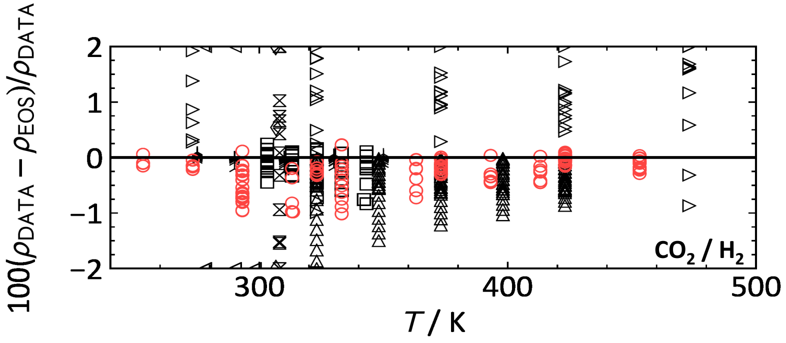
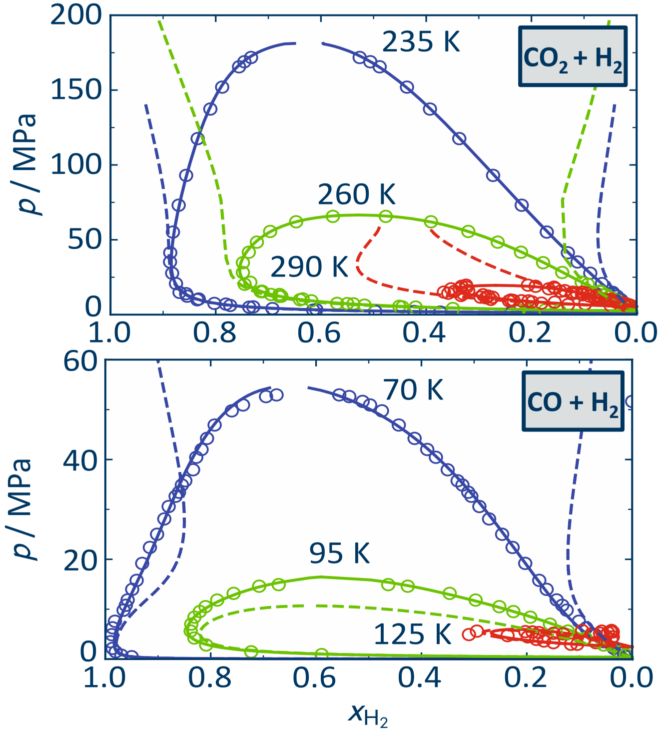
Take Away Messages

Thermophysical properties work in WP1 of ELEGANCY …

- utilizes synergies with experimental and theoretical work in other projects (DYNAFLEX, NCCS) at RUB
- utilizes synergies with experimental and theoretical work at other laboratories (SINTEF Energy, Imperial College, and others)
- leads to a new generation of accurate property models that allow for a consistent description of mixtures typical for CCS processes involving hydrogen
- enables a consistent and accurate description of properties and phase equilibria from capture to well head based on openly available models and software (WP4)





Acknowledgement

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