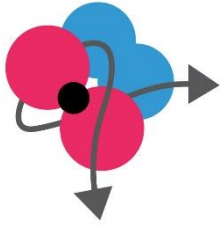


ELEGANCy

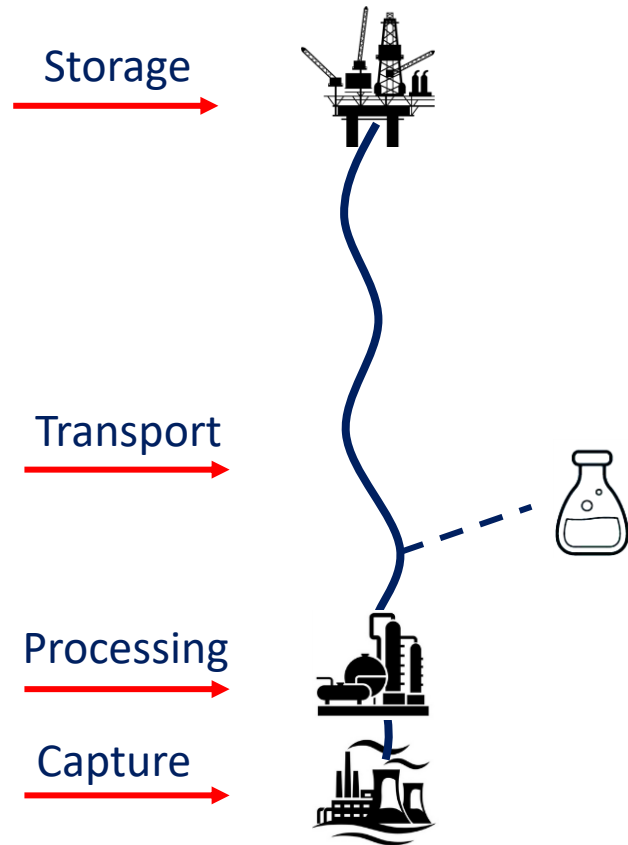
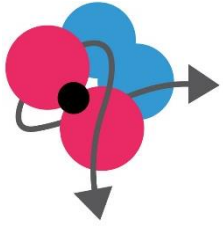


Advanced Property Models for Processing, Transport and Storage of Gas Mixtures Containing H₂

Roland Span & Robin Beckmüller

22.06.2020

Requirements on Property Models – Transport as an Example



What we discussed so far:

- Power plant close to base load as CO₂ source
- One fuel, one capture process
- Essentially a constant CO₂ stream with constant composition

- Possibly use of part of the CO₂ as feedstock



Power plant with capture



CO₂ processing and compression



CO₂ injection and storage (offshore)



Industrial site with capture



Chemical industry



Ship transport

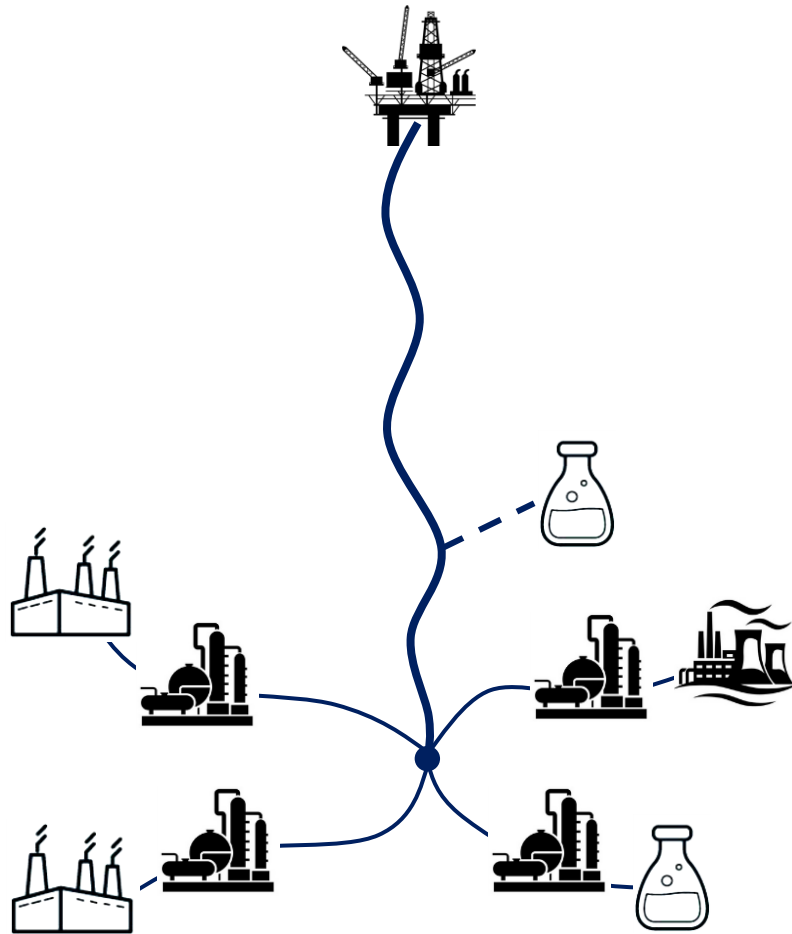
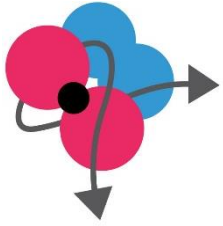


Rail transport



Truck transport

Requirements on Property Models – Transport as an Example

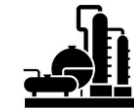


Industrial Clusters and Hubs:

- Different CO₂ sources
- Some at base load, some fluctuating
- Different origins of the CO₂
- **Different capture technologies**
- **Different impurities** – in ELEGANCY including **hydrogen**



Power plant with capture



CO₂ processing and compression



CO₂ injection and storage (offshore)



Industrial site with capture



Chemical industry



Ship transport

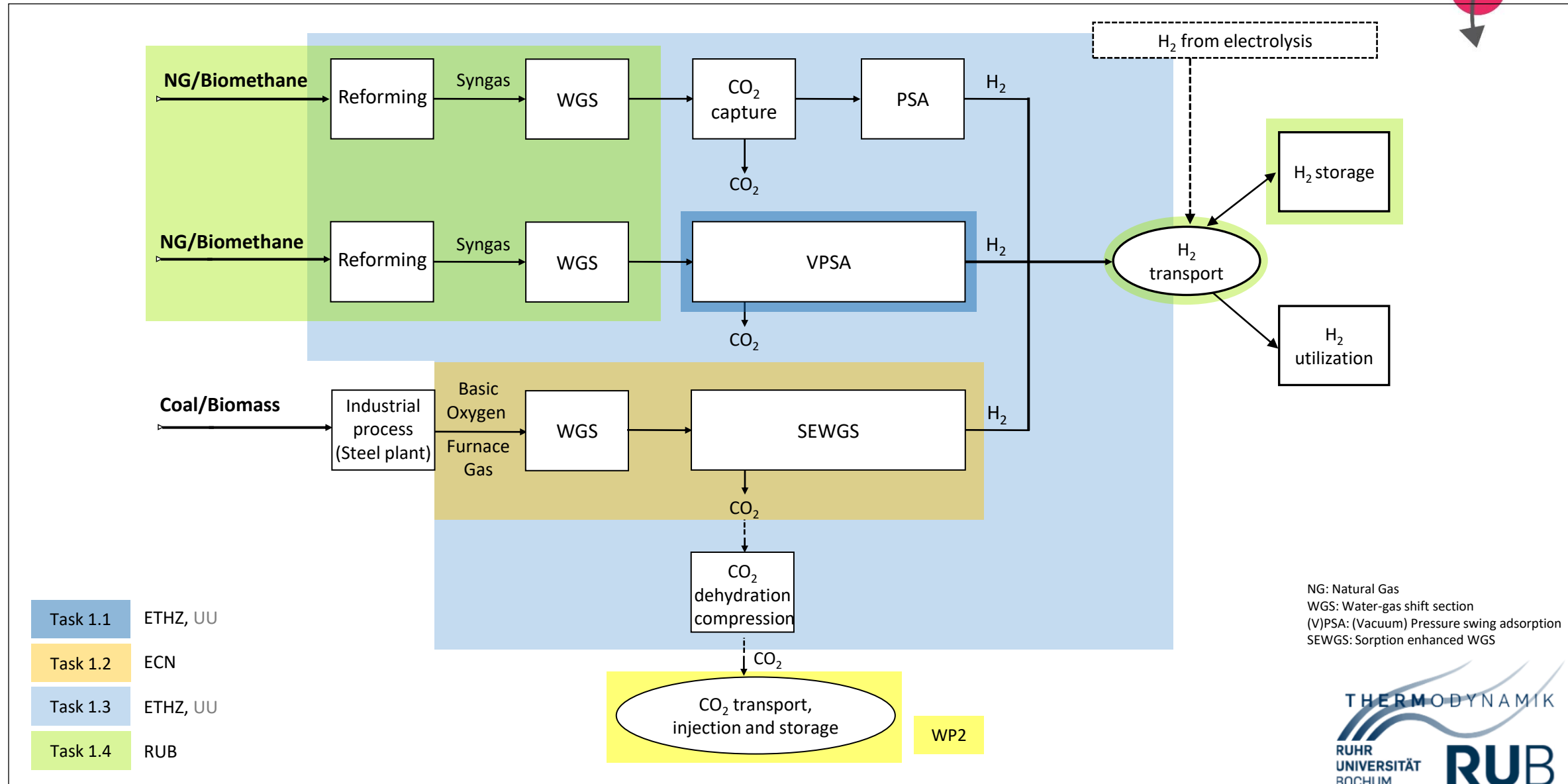
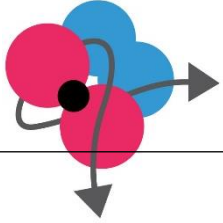


Rail transport

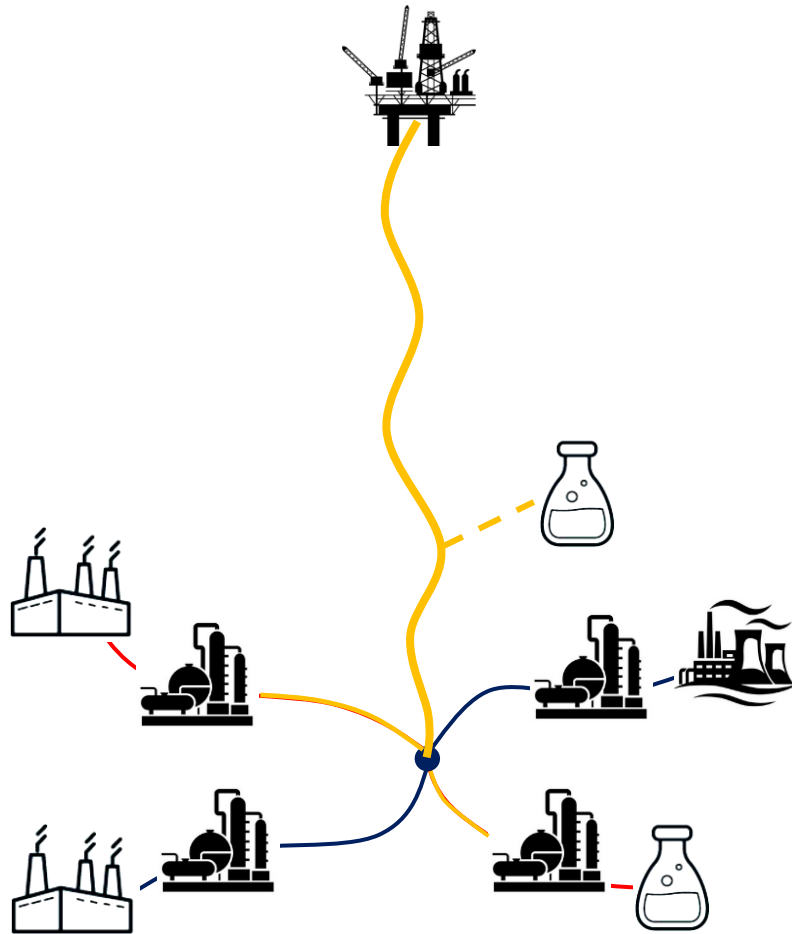
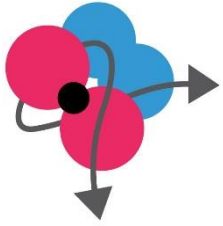


Truck transport

Different CO₂ Sources and Capture Technologies



Requirements on Property Models – Transport as an Example

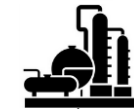


What we need to know:

- **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



Power plant with capture



CO₂ processing and compression



CO₂ injection and storage (offshore)



Industrial site with capture



Chemical industry



Ship transport

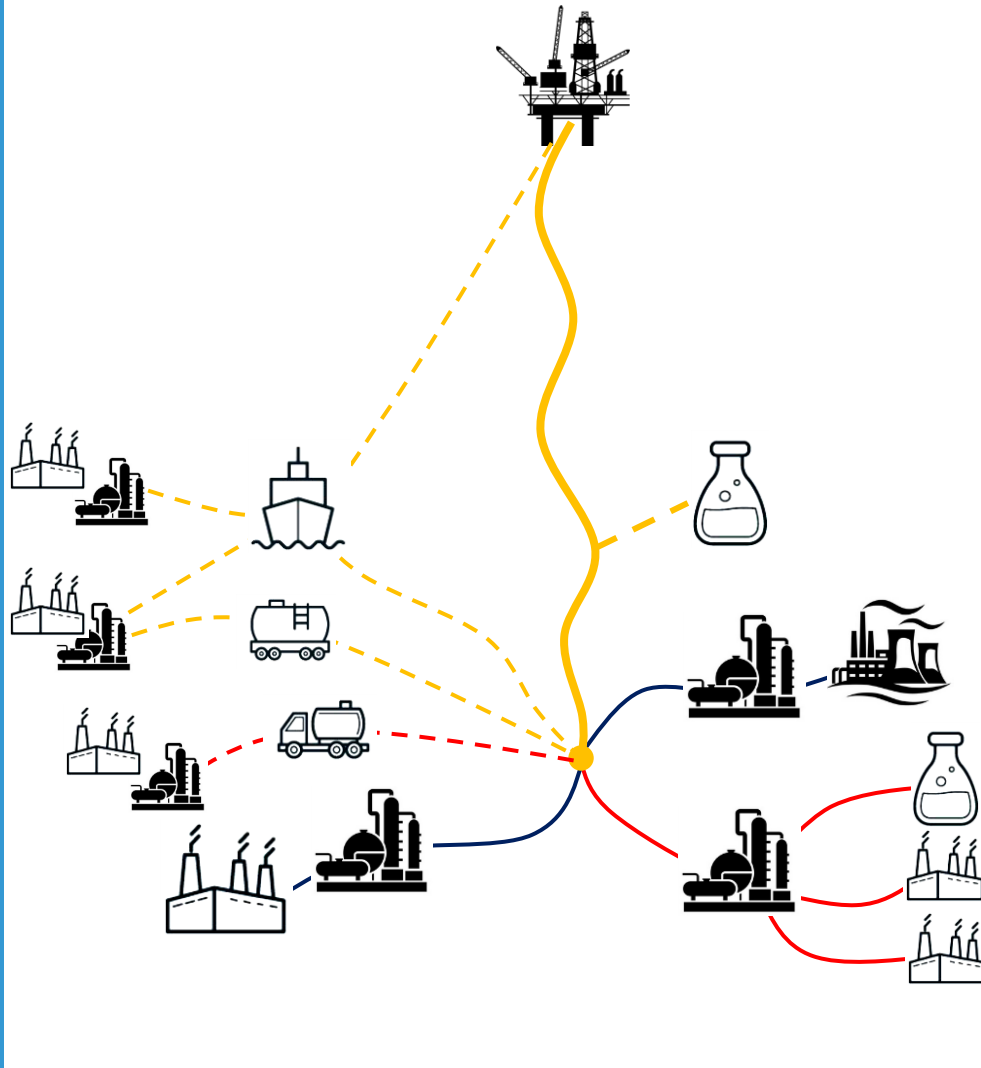
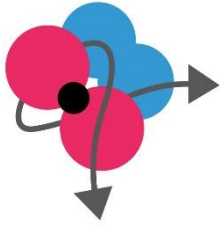


Rail transport



Truck transport

Requirements on Property Models – Transport as an Example



What we need to know:

- **Phase behaviour** needs to be known for varying composition, pressure, temperature
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Different means of capture, processing and transport require property data in a broad range of compositions, temperatures, and pressures!



CO₂ processing and compression

CO₂ injection and storage (offshore)

Industrial site with capture



Ship transport

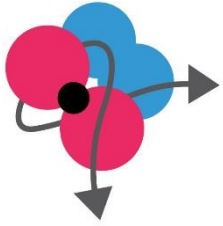


Rail transport



Truck transport

Helmholtz-Energy Based Multiparameter Mixture Models



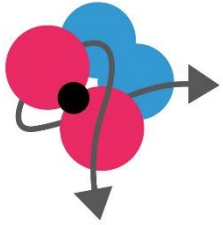
- Mixtures are described based on the 1990's approach by Lemmon & Tillner-Roth
 - Pure fluid equations of state
 - Mixing rules for δ_m und τ_m with up to 4 adjustable parameters
 - “Departure function” for an improved description of well measured mixtures

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

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



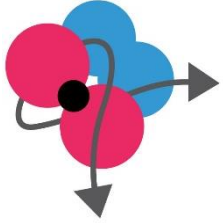
	Helium	Water	Carbon monoxide	Hydrogen	Oxygen	Argon	n-Octane	n-Heptane	n-Hexane	Isopentane	n-Pentane	Isobutane	n-Butane	Propane	Ethane	Carbon dioxide	Nitrogen
Methane	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
Nitrogen	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
Carbon dioxide	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
Ethane	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
Propane	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
n-Butane	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
Isobutane	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
n-Pentane	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
Isopentane	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
n-Hexane	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
n-Heptane	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
n-Octane	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
Argon	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
Oxygen	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
Hydrogen	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
Carbon monoxide	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
Water	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•

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

- Binary specific departure functions
- Generalised departure function for important alkanes
- Adjusted reducing functions, no departure function
- Linear combining rules, no fitting
- Lorentz-Berthelot combining rules, no fitting

Decreasing Accuracy

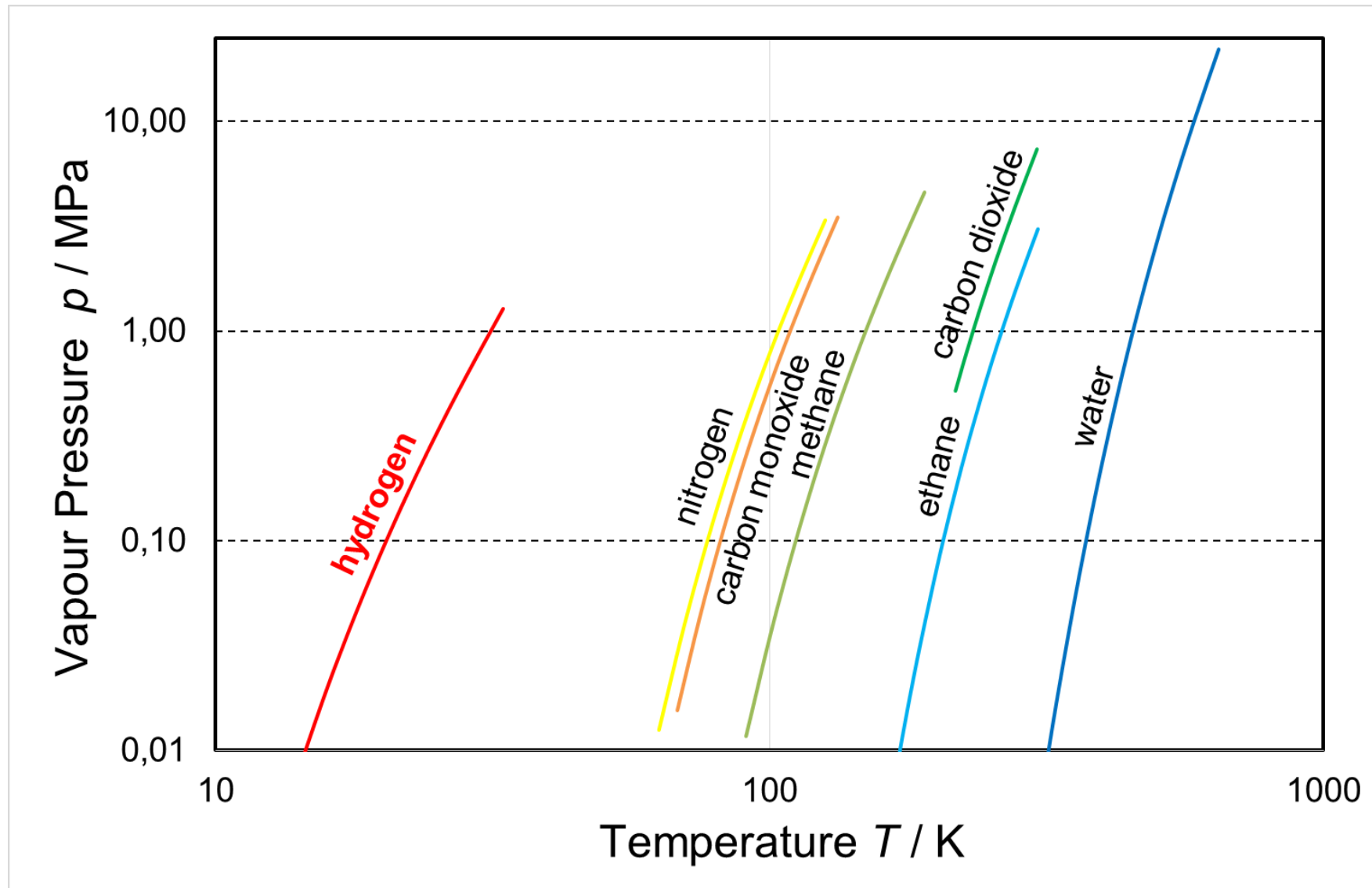
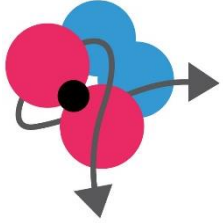
Improving GERG-2008 for Mixtures with Hydrogen



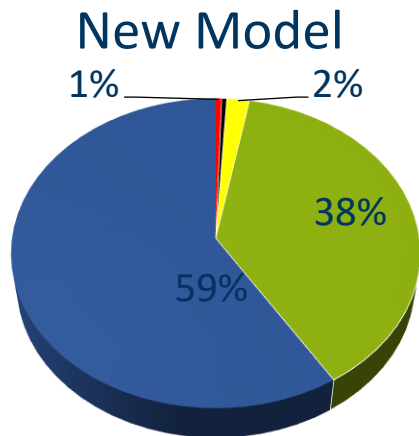
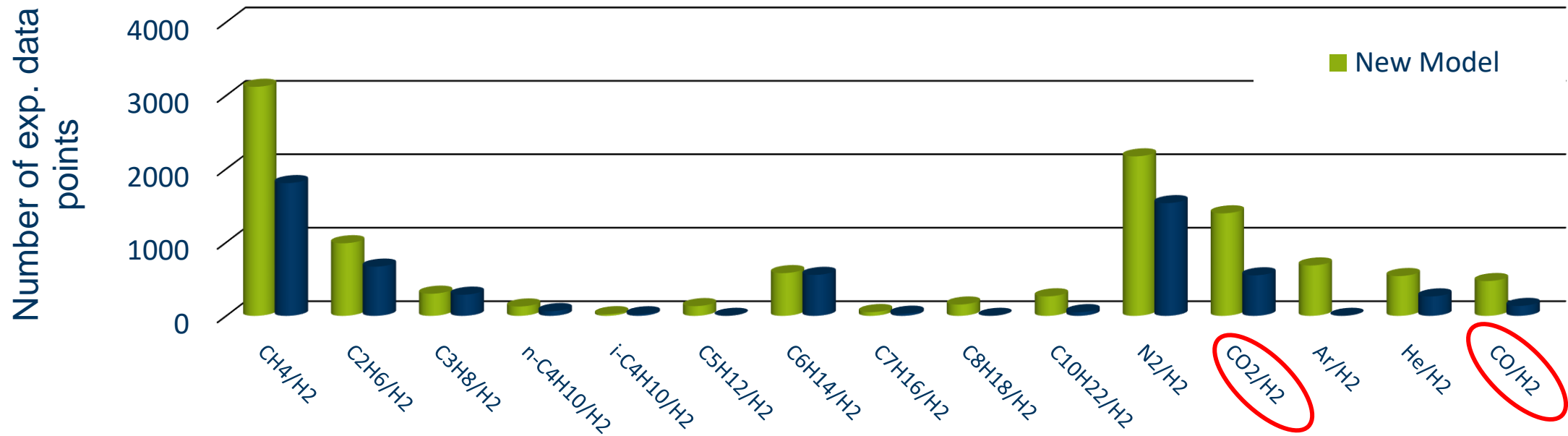
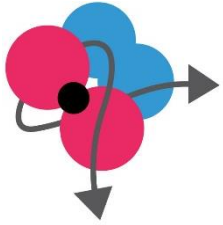
	Helium	Water	Carbon monoxide	Hydrogen
Methane	•	•	•	•
Nitrogen	•	•	•	•
Carbon dioxide	•	•	•	•
Ethane	•	•	•	•
Propane	•	•	•	•
n-Butane	•	•	•	•
Isobutane	•	•	•	•
n-Pentane	•	•	•	•
Isopentane	•	•	•	•
n-Hexane	•	•	•	•
n-Heptane	•	•	•	•
n-Octane	•	•	•	•
Argon	•	•	•	•
Oxygen	•	•	•	•
Hydrogen	•	•	•	•
Carbon monoxide	•	•	•	•
Water	•	•	•	•

- 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

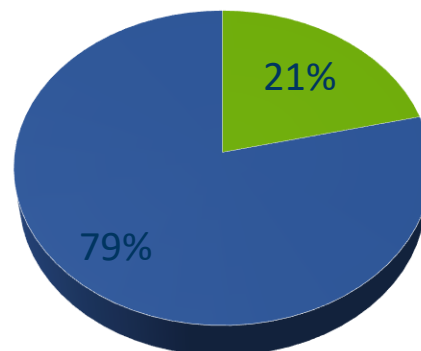
Improving GERG-2008 for Mixtures with Hydrogen



Improving GERG-2008 for Mixtures with Hydrogen



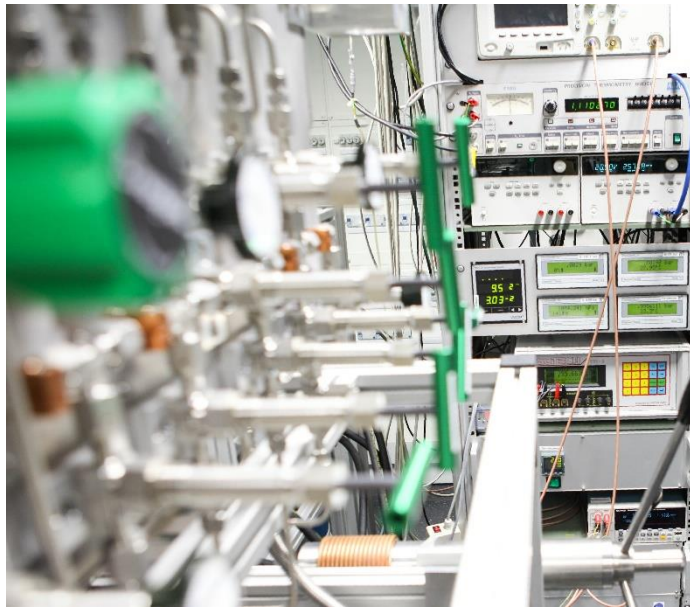
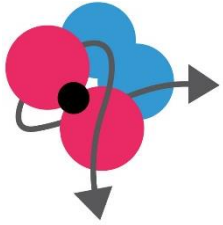
GERG-2008



New data from ...

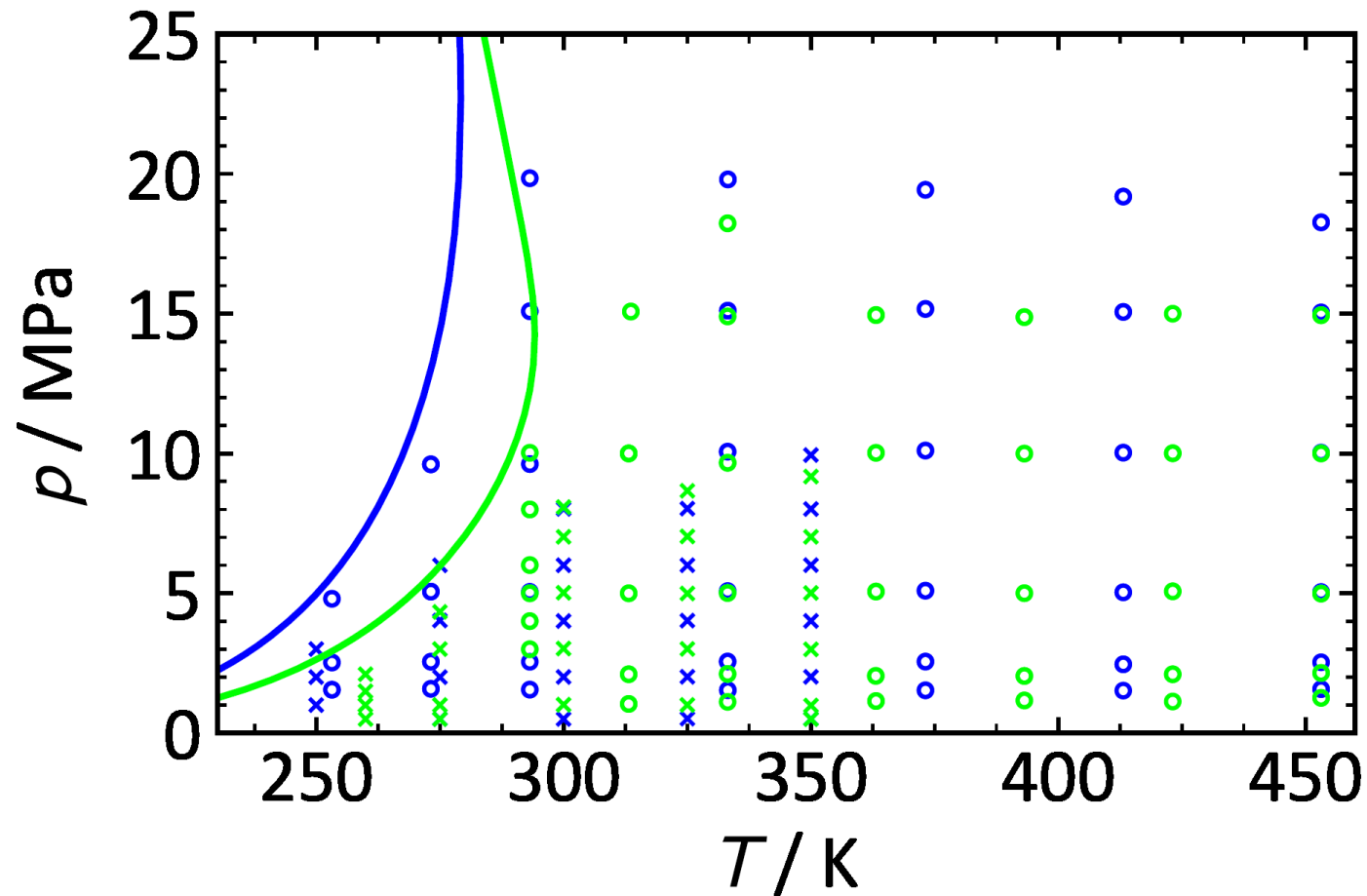
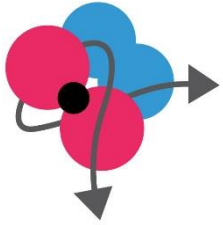
- extensive literature search
- synergies to other projects
- own measurements in **ELEGANCY**

Experimental Work in ELEGANCY



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

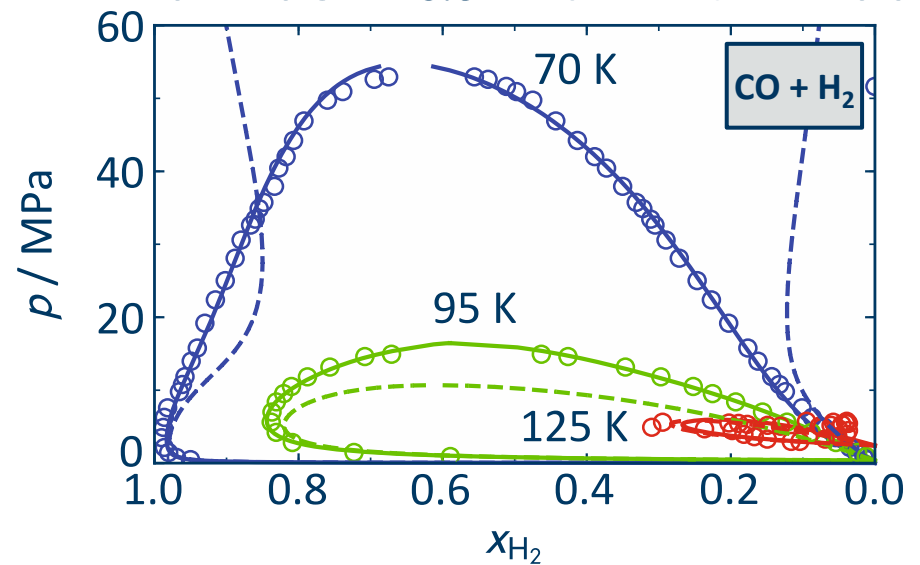
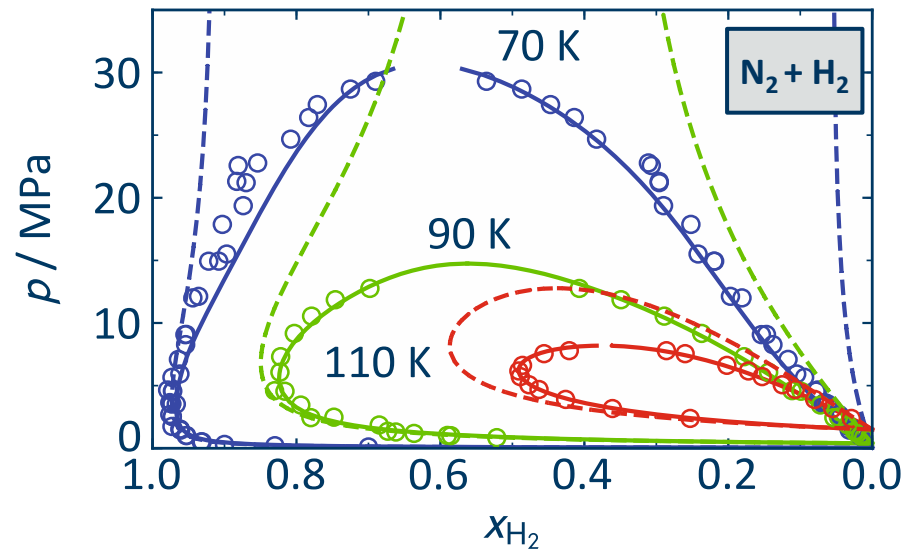
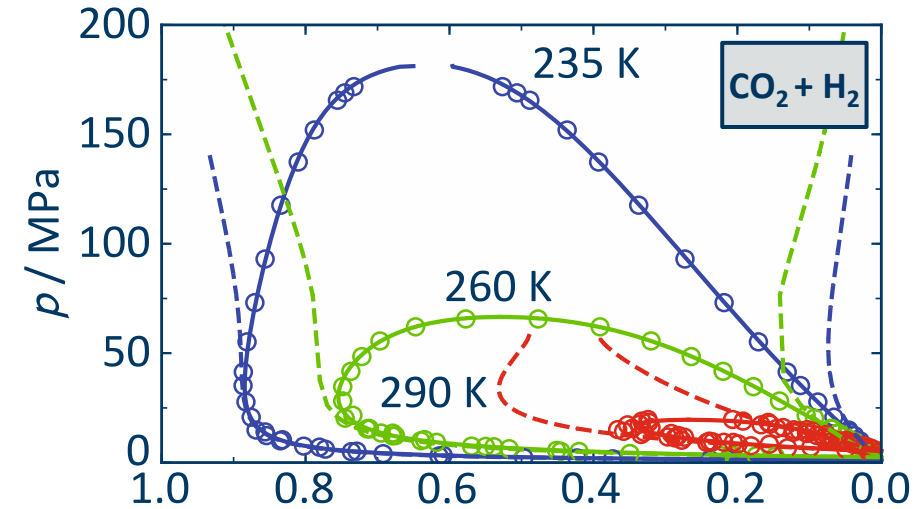
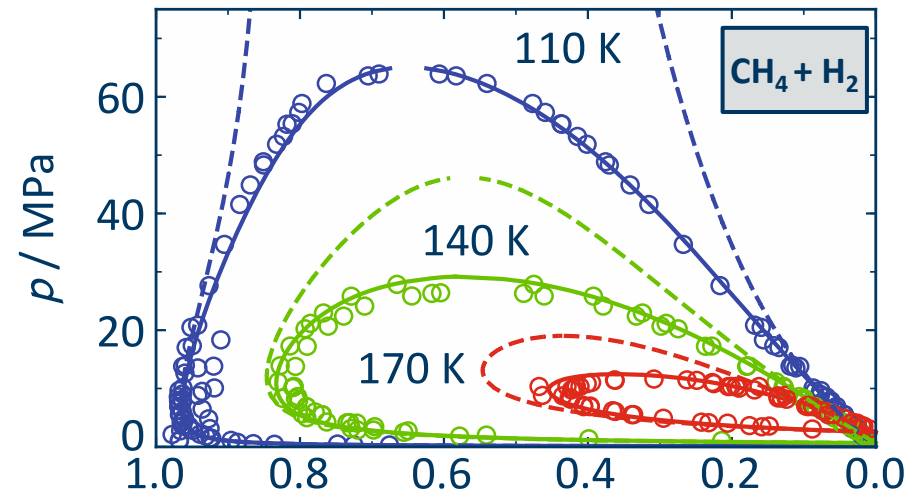
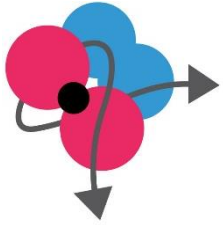
Experimental Work in ELEGANCY



- \circ ρ Scholz *et al.* 0.28 H_2 + 0.72 CO_2
- \circ ρ Scholz *et al.* 0.45 H_2 + 0.55 CO_2
- \times w Maurer *et al.* 0.25 H_2 + 0.75 CO_2
- \times w Maurer *et al.* 0.45 H_2 + 0.55 CO_2
- 0.25 H_2 + 0.75 CO_2
- 0.45 H_2 + 0.55 CO_2

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

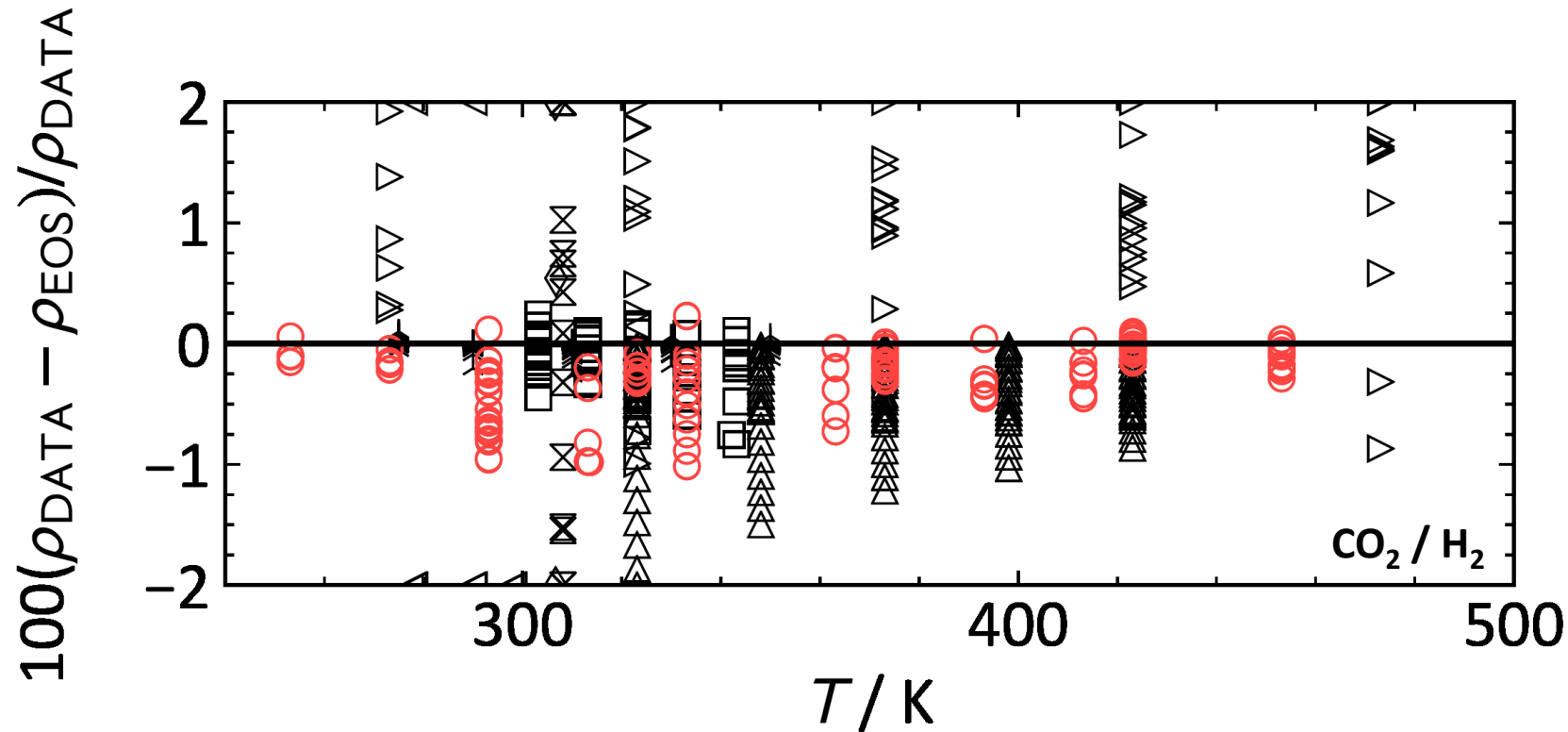
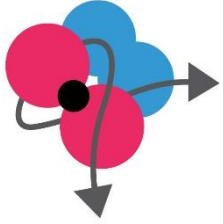
Improved Description of Phase Equilibria



solid lines = new model

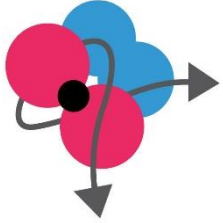
dashed lines = GERG-2008

Improved Description of Homogeneous States



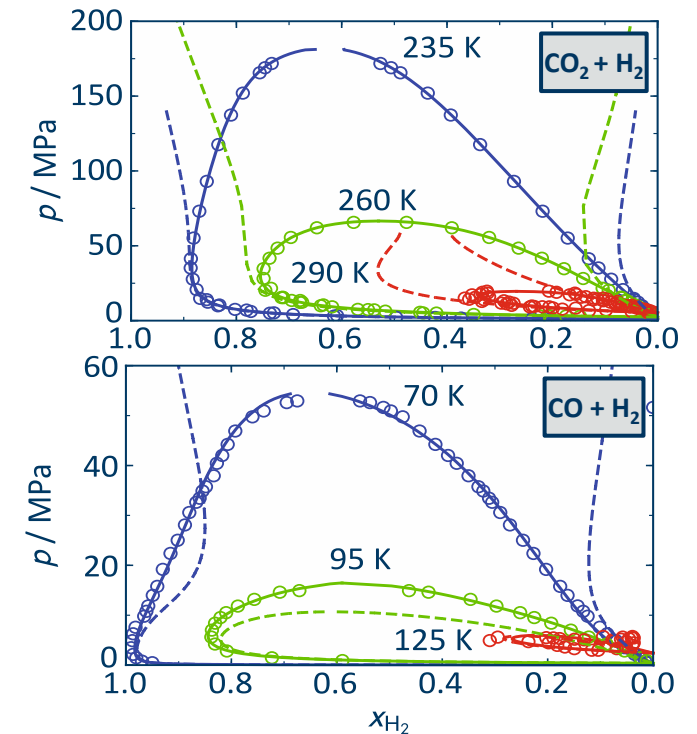
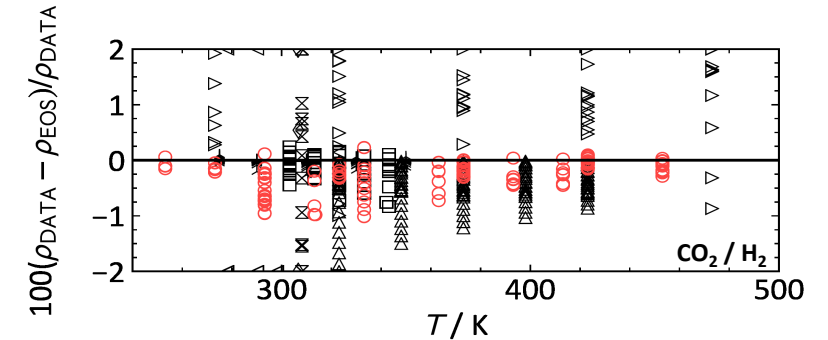
- Ababio & McElroy (1993)
- ◁ Bezanhtak *et al.* (2002)
- ⋈ Jaeschke & Humphreys (1990)
- ▷ Kritschewsky & Markov (1940)
- △ Mallu & Viswanath (1990)
- ◇ Pinho *et al.* (2015)
- Scholz *et al.* (2018)
- ⊗ Zhang *et al.* (2002)

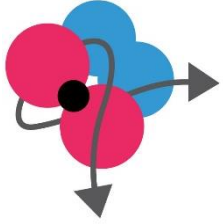
Take Away Messages



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

ACT ELEGANCY, Project No 271498, has received funding from DETEC (CH), BMWi (DE), RVO (NL), Gassnova (NO), BEIS (UK), Gassco, Equinor and Total, and is cofunded by the European Commission under the Horizon 2020 programme, ACT Grant Agreement No 691712. This project is supported by the pilot and demonstration programme of the Swiss Federal Office of Energy (SFOE).

