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# Industry Guidelines for Setting the CO<sub>2</sub> Specification in CCUS Chains

Joint Industry Project

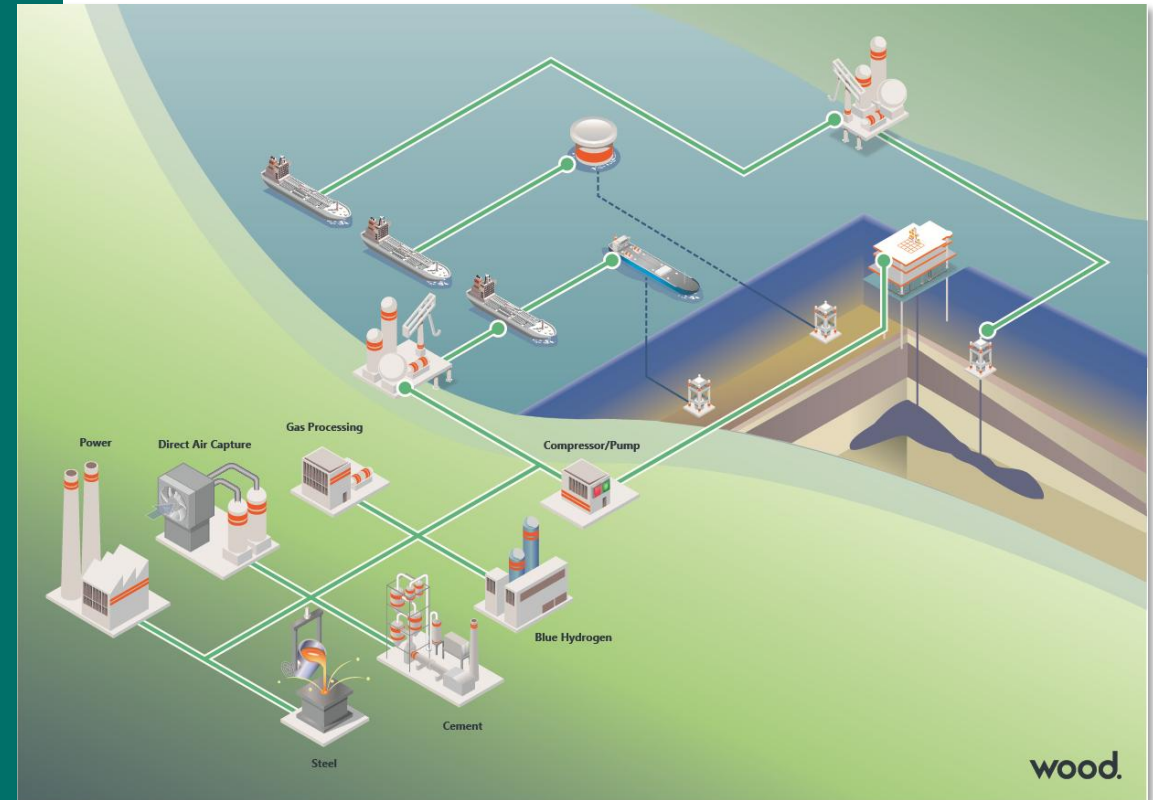
Craig McKay



# CO<sub>2</sub> Specification in CCUS Chains

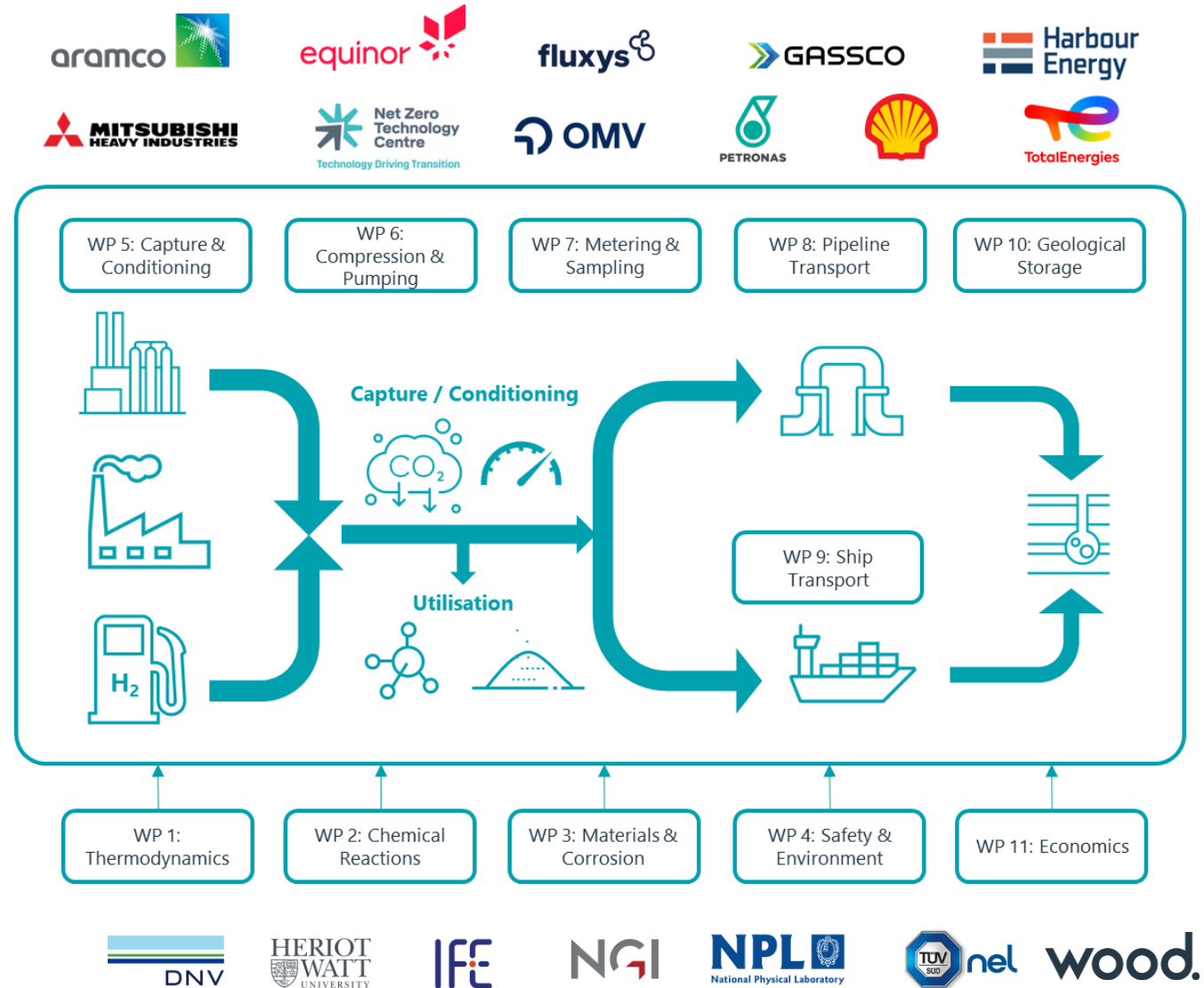


- Impurities in captured CO<sub>2</sub> can adversely affect factors such as material integrity and operation in CCUS chains. Can significantly impact the cost of processing and storage.
- There is limited guidance that considers the whole CCUS chain when setting the level of impurities in CO<sub>2</sub>.
- A Joint Industry Project (JIP) was therefore formed to collate current knowledge surrounding impurities and to create guidelines to support industry when setting CO<sub>2</sub> specifications for safe and economic CCUS chains.



# Industry Guidelines for Setting the CO<sub>2</sub> Specification for CCUS Chains

- The guidelines cover the full CCUS chain from CO<sub>2</sub> capture from various industries through to storage.
- Targets the cost optimisation of CCUS by recognising the interdependence between each part of the chain.
- Reviews the required CO<sub>2</sub> conditioning to meet safety, environmental, technical and operational requirements.
- The JIP collaborated with research and industry experts to provide a comprehensive and holistic understanding of the impact of impurities across the entire chain.

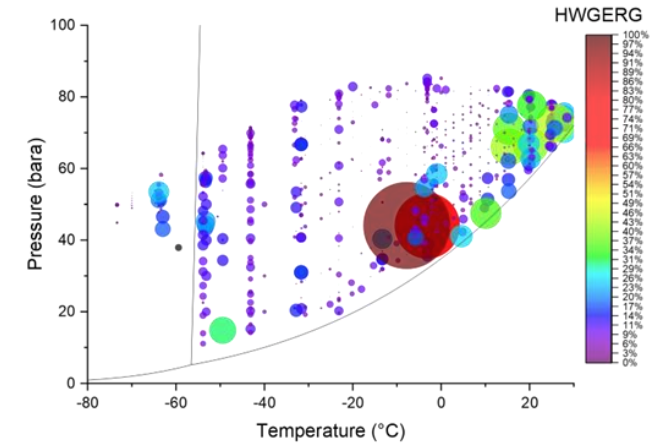


# WP1 – Thermodynamics

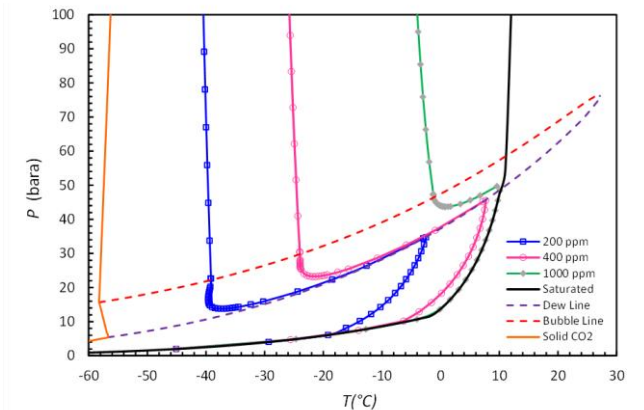
## Key Findings

- Heriot Watt University gathered > 1.5 M experimental data points from the literature for >30 impurities within CO<sub>2</sub> streams for gap analysis and validation of existing modelling methodologies.
- Reported modelling error margins for predicting the properties of interest using most advanced modelling methodologies.
- There is no single solution that provides a comprehensive solution for modeling CO<sub>2</sub> fluids. Depending on the composition, pressure, and temperature range of interest and the nature of the properties required for certain assessments, different modelling methodologies may need to be applied.
- Provided a guideline on the selection of the most appropriate modelling approach.
- **Provided example thermodynamic properties for binary and mixtures to allow the end user to confirm the validity of their modelling tools.**

## Availability of data and accuracy of modelling



## Example cases for validation of industrial tools



Hydrate Curves using CPA (95% CO<sub>2</sub> + 5% CH<sub>4</sub>)

# WP1 – Thermodynamics – Worked Examples

Here we present an example of a comparison made to the pseudo-experimental provided. The data was provided for **4 multicomponent mixtures** at a **range of conditions across the full CCS value chain**

Comparison performed using commonly available models and software packages:

- Package 1 is commonly used by **process engineers** for design work;
- Package 2 is used by **flow assurance engineers** and follows the modelling recommendations given by WP1 prior to tuning.

## IMPACT OF FLUID PROPERTIES



### DENSITY

**Pressure drop calculations (WP8):**  
over/underprediction of pressure drop, incorrect equipment sizing and/or risk of phase split



### HEAT CAPACITY

**Compression (WP6):**  
Key variable in the prediction of compression requirements and aftercooling duties



### JT COEFFICIENT

**Decompression (WP4/8):**  
Minimum temperatures during steady-state (gas transport systems) and depressurisation



### SPEED OF SOUND

**Flow assurance (WP8/9):**  
predicted surge pressures and the rate of depressurisation

# WP1 – Thermodynamics – Worked Examples

NB: -

- The AADs reported are between models, and not the deviation from experimental data.
- These AADs are weighted towards CCS fluid within gas phase conditions. At critical/supercritical conditions we see a greater error (especially for cubic models).

Composition	Package 1 (PR-Sour)				Package 2 (GERG-2008)			
	Density	Cp	JT	SoS	Density	Cp	JT <sup>Note 2</sup>	SoS
A	1.07%	2.88%	-	-	0.26%	1.51%	0.69%	0.29%
B	0.99%	3.31%	-	-	0.57%	1.05%	1.89%	0.21%
C	1.15%	3.11%	-	-	0.08%	0.28%	0.17%	0.18%
D	2.12%	3.95%	-	-	0.01%	0.58%	0.13%	0.12%

Notes:

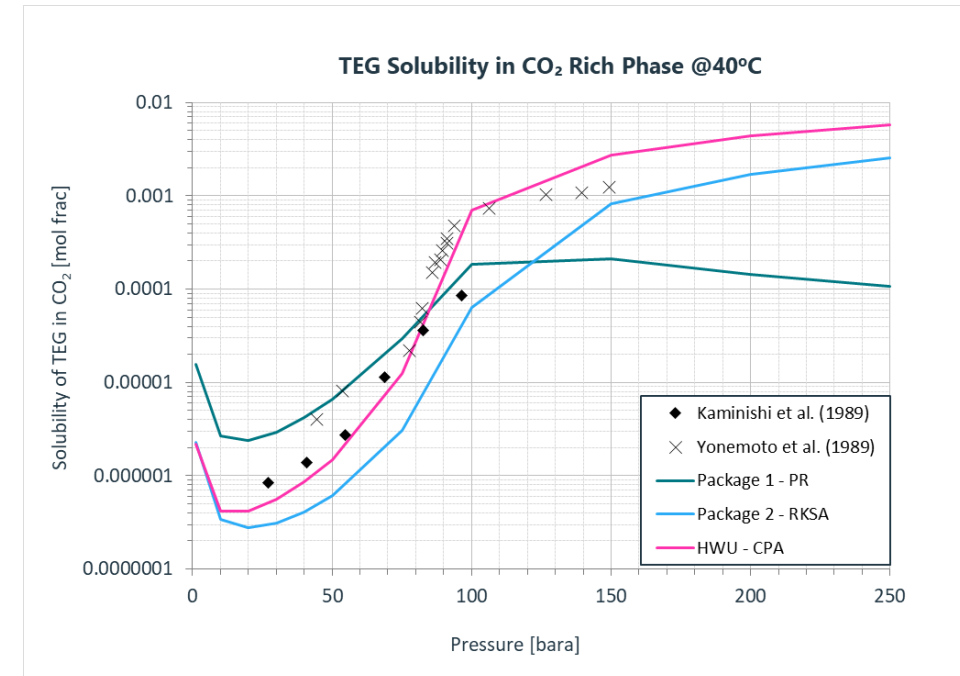
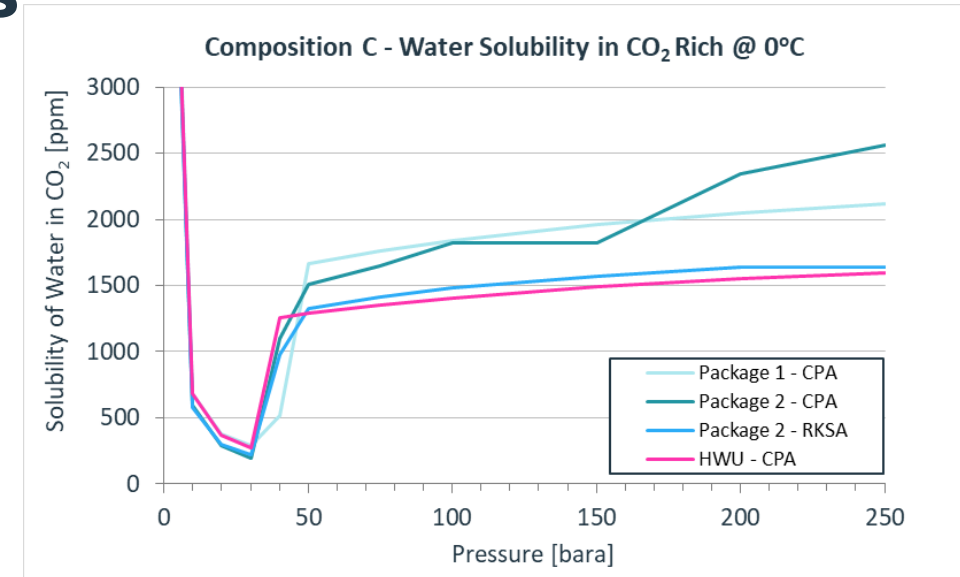
1. Vapour phase only

# WP1 – Thermodynamics – Worked Examples

Recommended EOS: CPA

- “Composition C” (from typical pipeline transport project) was used for a high-level comparison of EoS performance in prediction the water & TEG solubility within CO<sub>2</sub>;
- The results indicate that the performance of EoS is closely related to the thermodynamic property package used;
- Not only is performance related to the property package, but also the **version** of that package.

*Note: Composition C includes both methanol and ethanol – hydrate inhibitors*



# Conclusions

## Whole chain alignment

- Specifications must consider all stakeholders

## Impurities drive design

- Impacts must be understood end to end

## WP1: Models need validation

- Benchmark and perform sensitivities in absence of data

## Gaps remain

- Further research required across thermodynamics, reaction chemistry and corrosion



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# Acknowledgments

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Lastly, we are grateful to the many licensors and suppliers who provided advice on the impact of impurities on processes and equipment.

## Disclaimer

- The guidelines have been approved by the JIP Steering Committee and are intended to provide general information on the topic. The Steering Committee makes no representations or warranties of any kind, express or implied, regarding the accuracy, completeness, or suitability of the information contained herein. Users of these guidelines assume all risks associated with their application. The Steering Committee accepts no liability for any reliance placed on these guidelines or for any consequences arising from their use.

## Guidelines

