Society of Petroleum Engineers

PACE CCS

Integrated Flow Assurance Modelling in CCS systems

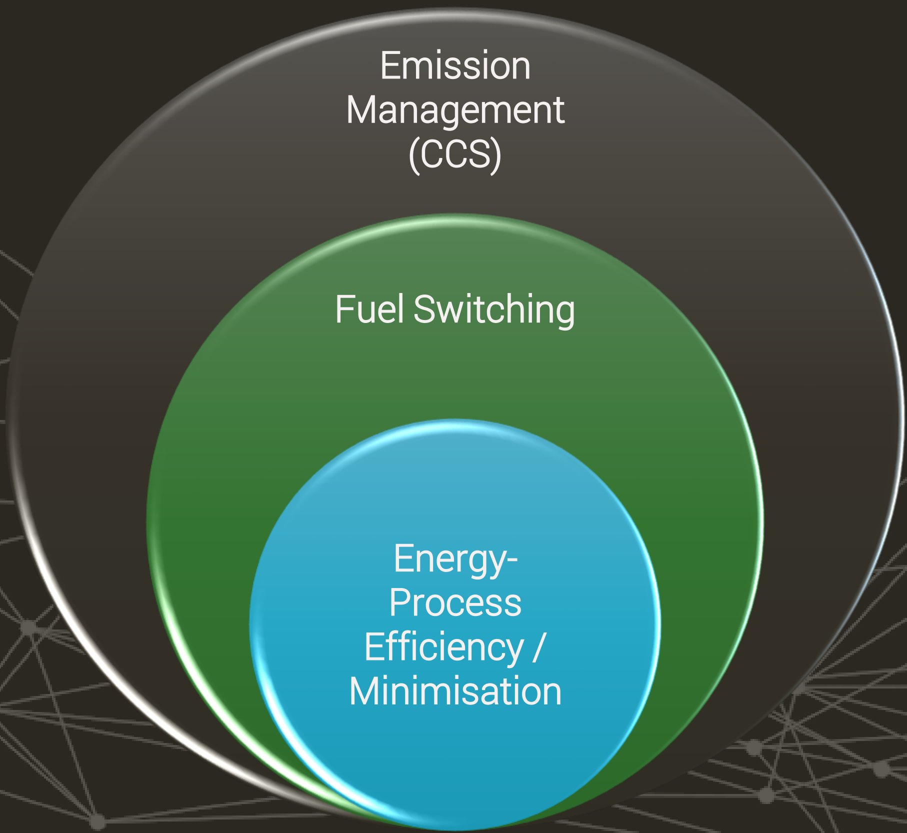
Dr Eduardo Luna-Ortiz

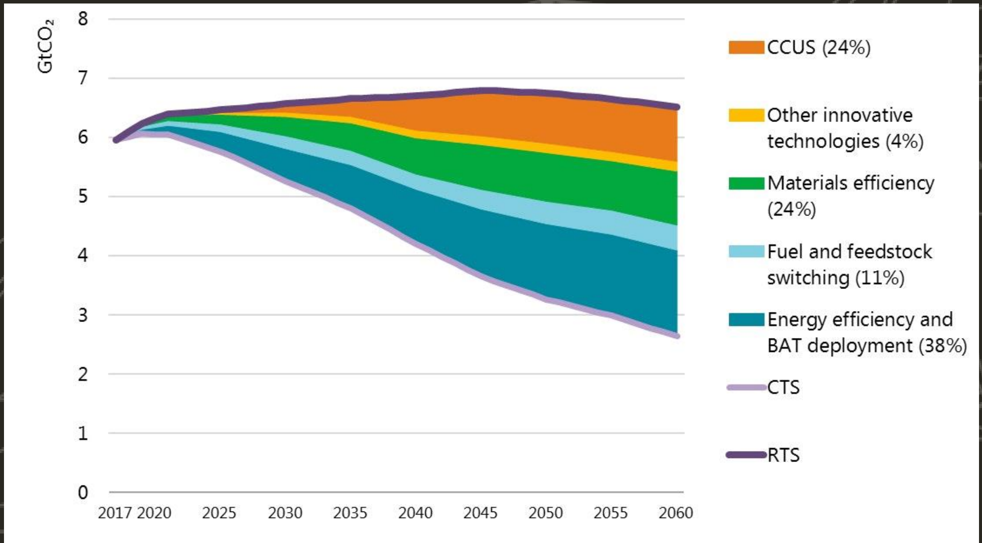
Pace CCS

London SPE Section – Net Zero Programme

June 2022

Industrial Decarbonisation





[1] Emissions reductions for key industry subsectors (cement, iron and steel, chemicals) by mitigation strategy (IEA 2019)

Decarbonisation means different things to different people

Measures

- CO_2 released versus resources used; temperature increase; …
- Effects on climate; availability of resources; uses and needs of products; …
- 17 sustainable developments UN goals

How?

- Reduce CO_2 emission by reducing energy demand
- Utilised captured CO_2; generate only amount of CO_2 that can be captured and utilised
- Look for integrated solutions taking into account regional constraints

Means

- Integration of ideas, concepts; to develop significantly better technologies
- Use new conversion and separation technologies
- Develop and use computational methods and tools that give significantly better solutions
- Change business paradigm from maximising profits to maximizing sustainability (and including social, ethical constraints)

Energy transition: Why not only renewables?

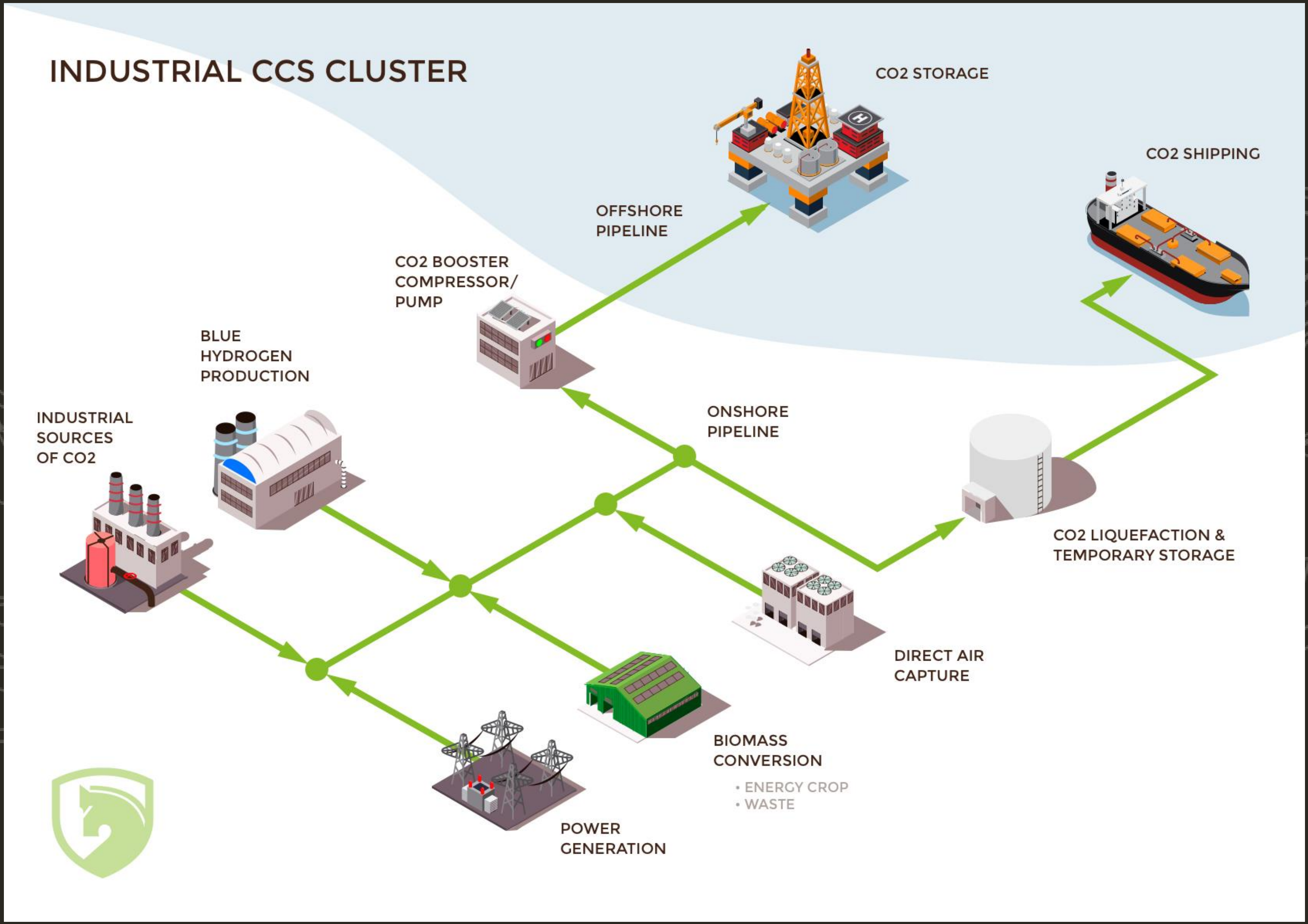
- Current deployment rates is not enough without significant de-industrialization and, a lot of investment (and perhaps political willingness)
- Realistically, we will still depend on hydrocarbons but we have to minimise emissions
- Renewables can't prevent emissions of hard-to-abate industries
- CCS as one of the pillars of the energy transition. It's not 'the' silver bullet. However, it should not prevent increasing efforts in true green energy

Opportunities for energy efficient operations

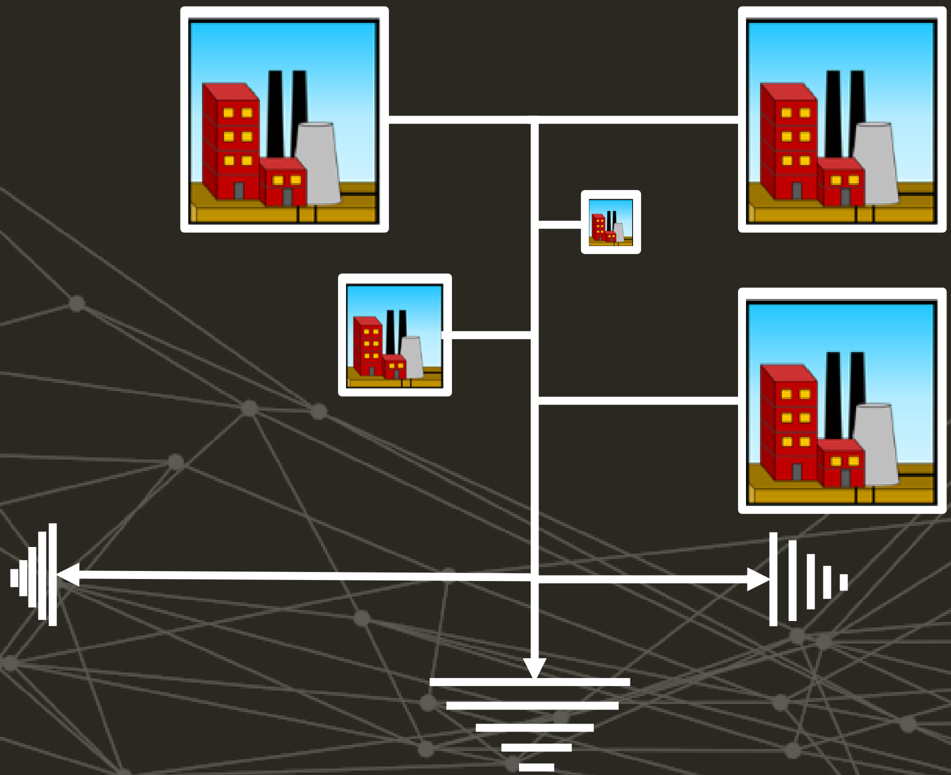
- Distillation columns are energy-intensive = emissions
  - Long-term solution: total replacement
  - Are there membranes or related materials to totally replace industrial distillation columns?
- Short-term solution: hybrid scheme
  - Integrate existing columns with small membrane operation, reduce energy consumption

- But, needs optimal design to combine both unit operations so that each operates at their highest efficiency
  - 10-50% energy savings
- There are at least 200,000 operating distillation columns worldwide

CCS-sphere


INDUSTRIAL CCS CLUSTER
CO2 STORAGE
CO2 SHIPPING
OFFSHORE PIPELINE
CO2 BOOSTER COMPRESSOR/ PUMP
BLUE HYDROGEN PRODUCTION
INDUSTRIAL SOURCES OF CO2
ONSHORE PIPELINE
CO2 LIQUEFACTION & TEMPORARY STORAGE
DIRECT AIR CAPTURE
BIOMASS CONVERSION
• ENERGY CROP
• WASTE
POWER GENERATION

Challenges



- Multiple users (present and future)
- Different sizes, industries, capture tech
- Transitions from gas, to liquid or supercritical
- **CO_2 is not pure (a lot impurities)**

PVT: know your fluid (CO_2 + …)

MAJOR

Component	Limit (% mol)	
N_2	4.0	Combined total ≤ 4
H_2	1.0	
Ar	4.0	
CO	0.2	
Methane	4.0	
Ethane	4.0	
Propane & Other Aliphatic Hydrocarbons	0.15	in total

MINOR

Component	Limit (ppm mol)
H_2O	50
O_2	10
NO_x	50
SO_x	50
H_2S	5 in total
COS	
NH_3	1500
BTEX	50
Methanol	500

TRACES

Component	Unit	Limit
Solid Particulates (Max size of particulate: 1 µm) (Ash, dust, Na, K, Mg, Cr, Ni, Cd, Hg, Tl, Pb, As and Se)	mg/Nm³	1 in total
Cd (Max size of particulate: 1 µm)	mg/Nm³	0.15
VOCs (formaldehyde, acetaldehyde, dimethyl sulfide, ethanol)	mg/Nm³	150
Acid Forming Compounds (Cl_2, HF, HCl, HCN)	mg/Nm³	150
Amines (Max size of liquid droplet: 2 µm) (MEA, MDEA, DEA, AMP, piperazine)	ppb mol	100
Glycols (Max size of liquid droplet: 2 µm) (TEG, MEG, DEG)	ppm mol	1
Nitrosamines and Nitramines (NDMA, NMEA, NDEA, NDELA, NPIP, NMor)	µg/Nm³	3
Naphthalene	ppb mol	100
Dioxins and Furans (PCDD, PCDF)	ng/Nm³	0.02
Selexol (polyethylene glycol dimethyl ether)	mg/Nm³	100

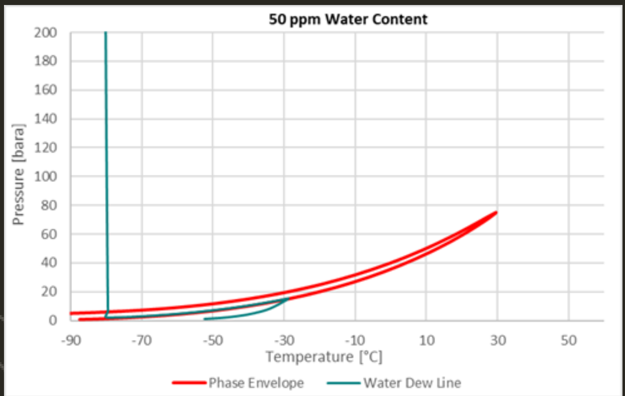
OTC-32103-MS

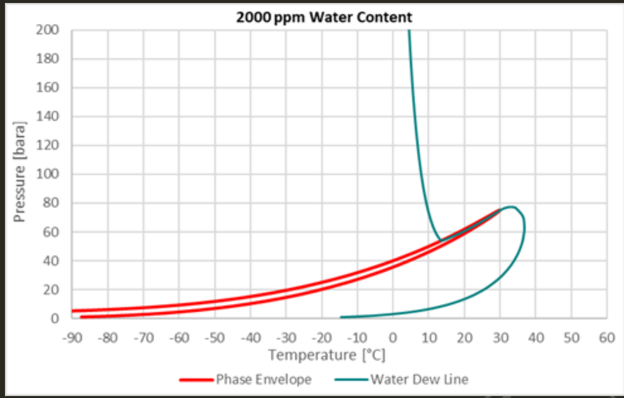
Development of A CO_2 Specification for Industrial CCS Transport Networks: Methodology, Limitations and Opportunities

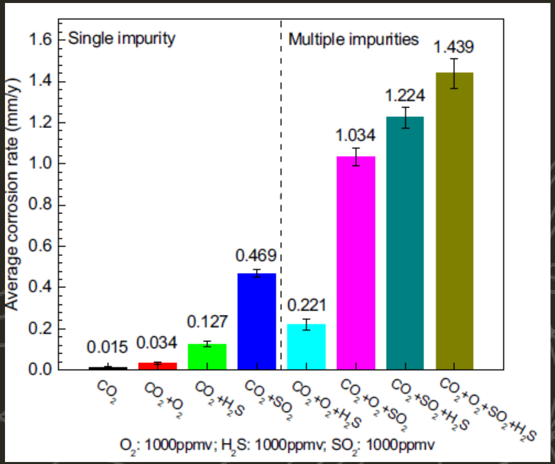
Eduardo Luna-Ortiz, Cathy Yao, Jon Barnes, Matthew Winter, and Matthew Healey, Pace CCS Ltd

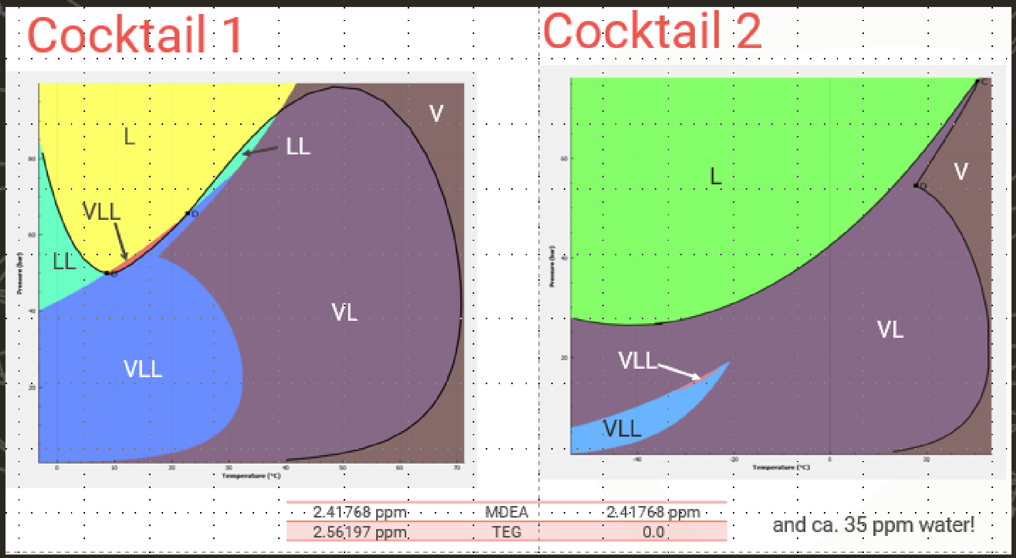
This paper was prepared for presentation at the Offshore Technology Conference held in Houston, TX, USA, 2 – 5 May, 2022.

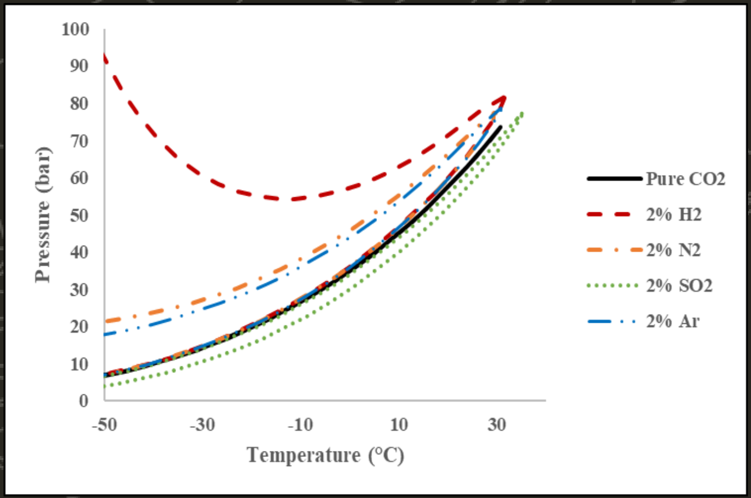
Effect of impurities







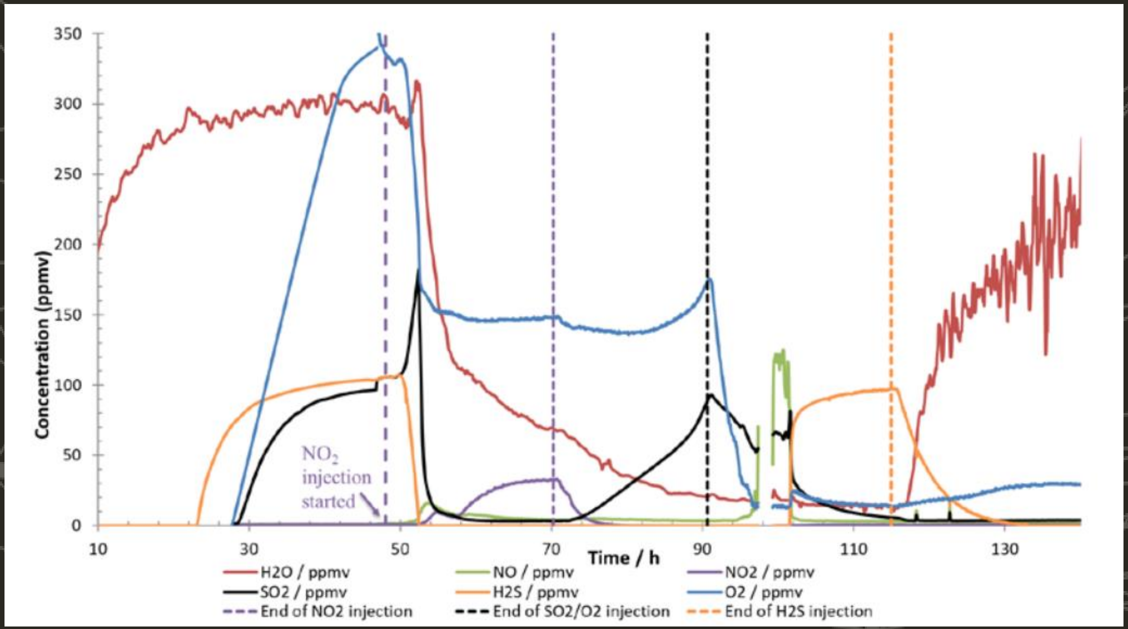




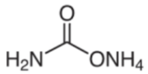
- Impurities (even at ppm level) have an impact (assume pure CO_2 at your own peril!)

And maybe even chemical reactions

$$H_2S + 3\,NO_2 \rightarrow SO_2 + H_2O + 3\,NO$$
$$2\,NO + O_2 \rightarrow 2\,NO_2$$
$$SO_2 + H_2O + NO_2 \rightarrow NO + H_2SO_4$$



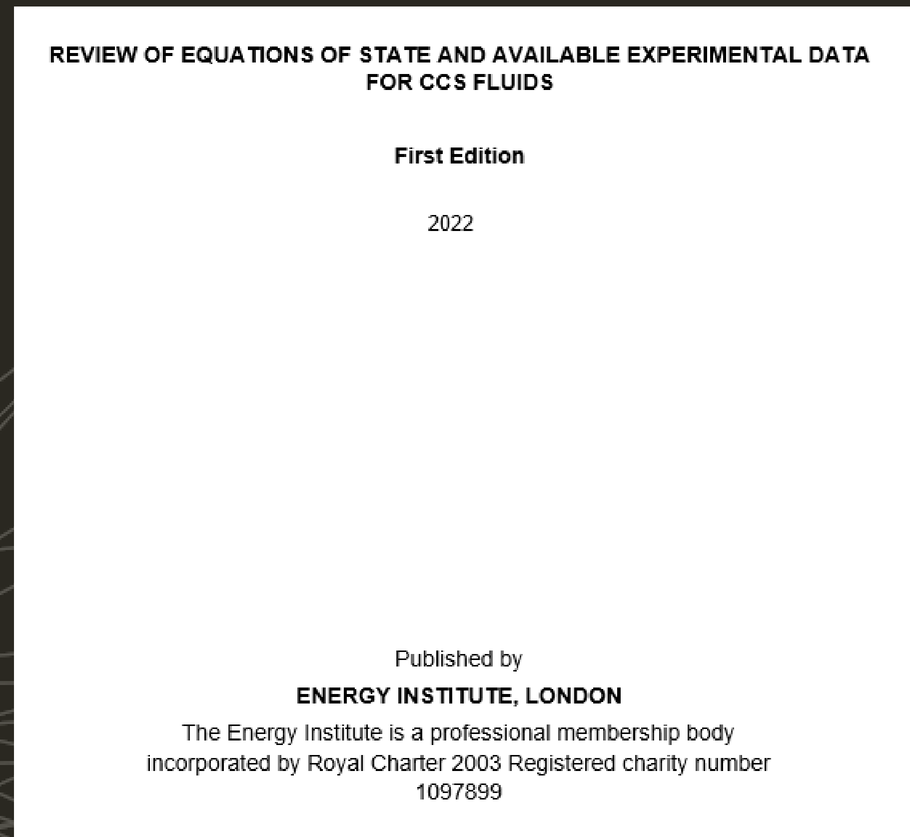
$$CO_2 + NH_3 \rightleftharpoons CO_2 \cdots NH_3 \rightleftharpoons NH_2CO_2H$$
$$NH_2CO_2H + NH_3 \rightleftharpoons NH_2CO_2NH_4$$



$$CO_{2(g)} + 2NH_{3(g)} \rightleftharpoons NH_2CO_2NH_{4(s)};\ K_{eq(273\,K)} = 2.35 \times 10^4$$

The ubiquitous presence of thermodynamics (a.k.a. fluid modelling)

- What's the 'best' model?
- It depends on the chemical nature of the compounds
- How the model and theirs results are going to be used?
- Implementation


REVIEW OF EQUATIONS OF STATE AND AVAILABLE EXPERIMENTAL DATA FOR CCS FLUIDS

First Edition

2022

Published by

ENERGY INSTITUTE, LONDON

The Energy Institute is a professional membership body incorporated by Royal Charter 2003 Registered charity number 1097899

Chemical Engineering Science: X 7 (2020) 100060

Contents lists available at ScienceDirect

Chemical Engineering Science: X

journal homepage: www.elsevier.com/locate/cesx

Equations of state in three centuries. Are we closer to arriving to a single model for all applications?

Georgios M. Kontogeorgis [a,*], Xiaodong Liang [a], Alay Arya [a], Ioannis Tsivintzelis [b]

Especially, based on the current status, it is difficult to conclude that we are, as yet, close to a single thermodynamic model for all or even for many applications (which Prausnitz et al. hoped in 1983 that it might be the case in the future). We also believe that the advanced association models have enhanced somewhat our capabilities from an engineering point of view, while it is not entirely clear how much they have enhanced our understanding of complex intermolecular interactions.

The ubiquitous presence of thermodynamics (a.k.a. fluid modelling)

- All models have limitations (failure near critical region, poor liquid density predictions, computationally expensive, compatibility, etc.)
- All models should be tuned with experimental data (but data for multicomponent and even binary mixtures is scarce)

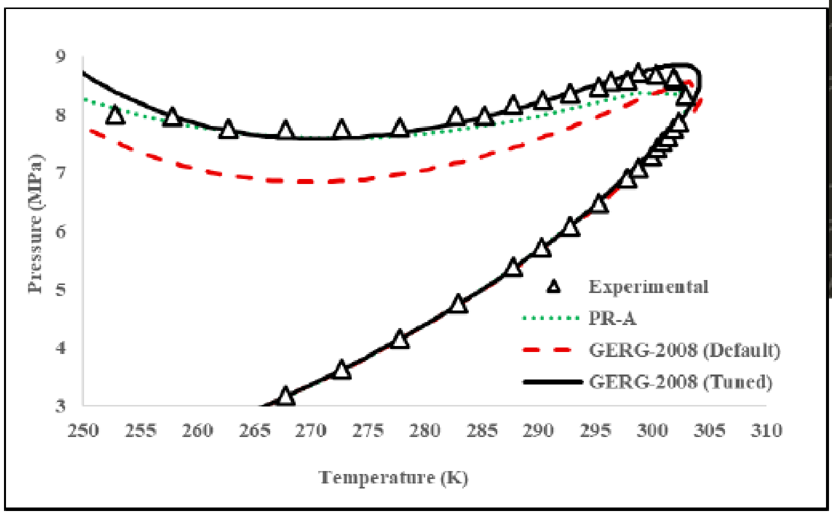


Fig. 12. Comparison of experimental data and EoS models for a binary mixture of CO_2 with 3% mol H_2.

ghgt-15

15th International Conference on Greenhouse Gas Control Technologies, GHGT-15

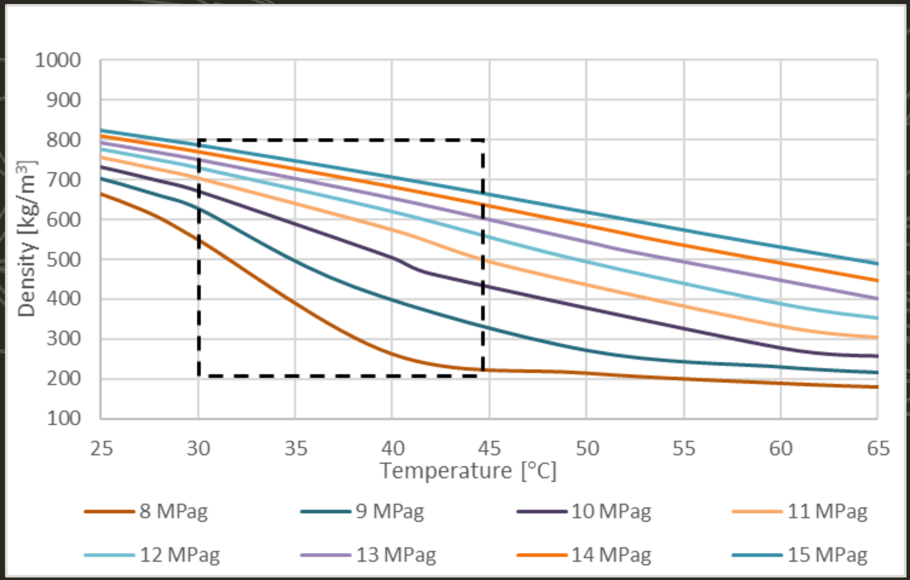
15th 18th March 2021 Abu Dhabi, UAE

Impact of Hydrogen as Impurity in the Physical and Transport Properties of CO_2 Streams in CCS/CCUS Transport Systems: A Technical Discussion

Eduardo Luna-Ortiz[a,*], Kamila Szklarczyk-Marshall[a], Matthew Winter[a], Emilio McAllister-Fognini[a]

Consistent EoS

- Ensure consistency through the nodes of the CCS system
  - Plant captures and compresses X MTPA
  - Pipeline transport Y MTPA
  - Reservoir stores Z MTPA
- Subsurface/surface segregation leads to discrepancies




OTC-31536-MS

Case Study: The Importance of Integrated Flow Assurance Modelling for Carbon Capture and Storage CCS Project

Mohd Uzair Zakaria, Wan Mahsuri Wan Hashim, Nik Fauziah Nik Omar, Rohaizad M. Norpiah, M Azuan Abu Bakar, and Wan Amni Wan Mohamad, PETRONAS

Copyright 2022, Offshore Technology Conference DOI 10.4043/31536-MS

This paper was prepared for presentation at the Offshore Technology Conference Asia held in Kuala Lumpur, Malaysia, 22 - 25 March 2022.

Options for integrated modelling to ensure thermodynamic consistency


1052 Review Chemie Ingenieur Technik

CAPE-OPEN: Interoperability in Industrial Flowsheet Simulation Software

Jasper van Baten[1,*] and Michel Pons[2]

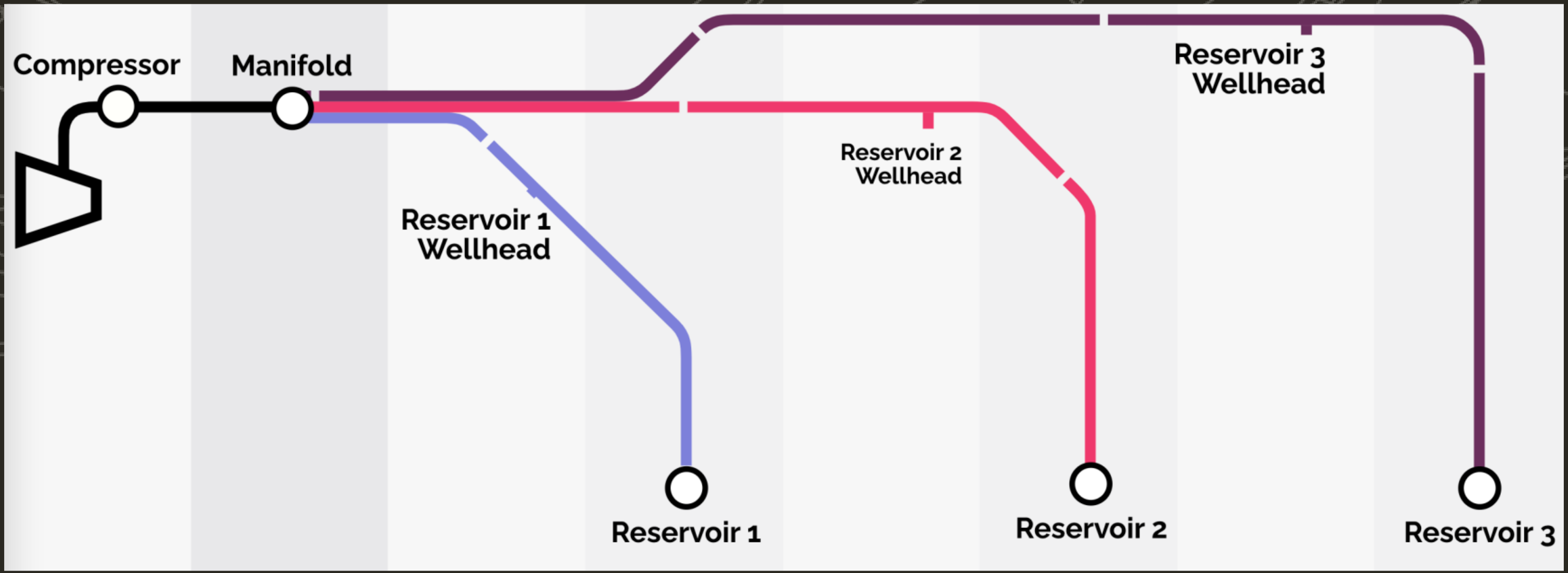
- CAPE-OPEN
  - Allows using a thermodynamic model in a plug-and-play in various simulators
    - Thermo model in Multiflash
    - Process in HYSYS using the Multiflash model
    - Allows using a thermodynamic model in a plug-and-play in various simulators
  - But not all simulation tools are CAPE-OPEN compliant
- Maximus - IPM
  - Third-party simulator with Multiflash
    - Connects to PETRO-SIM
    - Rigorous pipeline/well thermal-hydraulics
    - Tank model
    - Life-of-field simulation

Options for integrated modelling to ensure thermodynamic consistency

- Digital CCS Simulator
  - How do we quickly understand how a CCS network will operate across project cycle
    - Multiple emitters connecting to a transport network, to multiple wells/reservoirs
    - Changing conditions over field life, reservoir pressure increases, flowrates changes, composition changes, phased development
    - Limited operational experience
  - We develop a custom-made web-based software
    - Uses thermodynamic model of choice via either look-up tables or maybe a ML model
    - Transient thermo-hydraulic model for single phase elements
    - Surrogate model or tank model for storage

CCS Digital Twin: Parallel filling of multiple injection reservoirs

- How does flow split at an uncontrolled offshore manifold?
- How do reservoir pressures increases over field life
- Integrated flow assurance, well and reservoir models without any third-party software
- Well and reservoir model uses surrogate to match OLGA and ECLIPSE



Concluding Remarks

- Integrated surface/subsurface approach is more crucial in CCS projects
- Thermodynamic modelling remains a challenge. Keeping consistency across the whole-chain is key.
- Various options to integrate subsurface/surface with consistent thermodynamics

PACE