Investigating the impact of impurities in the CO<sub>2</sub> streams for the Carbon Capture and Transportation value chain using MATLAB and CAPE-OPEN

<u>Outline</u>

- The CCS value chain and contribution of process simulations
- Considerations and choice of software
- Business model for process simulations (general)
- Examples and status of work

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### CO2 Value chain



Purity 1	Purity 2	Plant	Amine scrubber	Liquefaction	Vessel	Injection
High	High	Cement	150 \$/ton	10 \$/ton	10 \$/ton	10 \$/ton
Low	High	Cement	130 \$/ton	20 \$/ton	10 \$/ton	10 \$/ton
Low	Low	Cement	130 \$/ton	15 \$/ton	30 \$/ton	30 \$/ton

- If we really knew the numbers in red, we could better discuss which way to go with the emitters and others, and better decide for low pressure or mid pressure vessels
- Process simulations can help with this
- The simulations can be repeated for different types of emitters (different flue gas compositions)

### **Process simulations**

An obvious tool to use for investigating CO2 transportation by ships and in pipes because:

- We need to find and select the most optimal processes to help the emitters to overcome the current "hen and egg" situation as well as to ensure the lowest price per tons CO2 at storage and at the lowest CO2 footprint.
- The emitters don't know their compositions because they don't have any carbon capture plant up running yet.
- The optimal CO2 transportation is coupled to the upstream and down-stream processes and therefore cannot be considered alone.
- The basic unit operations are well-known whereby we can also simulate any combined processes
- Value Chain too big, expensive and slow just to build and try all the different options



#### **Process simulations**



Engineering

## Considerations regarding choice of simulation software



All detailed models and parameters in place



#### Choice of simulation software

- Experiences: Excel, Pascal, Fortran, Matlab, C++, ASPEN Plus, CFD, HSC chemistry, EES, gPROMS
- Many sub-functions build up during the last ~25 years in matlab
- No inbuild thermodynamics or any chemical unit operations in matlab 🛞
- MATLAB CAPE-OPEN thermo-sockets from AmsterCHEM ③
- Direct link to sale and customers: GUI, Process diagrams, BOM
- Co-operation internally and externally
- Not solely focus on the chemical process engineering details (structure and process all available information especially also guestimates of capex/opex)
- My background is chemical process engineer (not programmer)



#### Life of a process simulation engineer



ECA

## **Business model**

- How do we unleash the potential?

Huge, huge potential in process simulations but....

- More public / political focus on demonstration projects and "visible action"
- Investors more focused on overall feasibility studies
- CEO's, CFO's, sales managers are usually more focused on commercial sales tool
- Mechanical engineers more focused on testing
- Disturbed a bit by buzzwords like IoT, AI, BigData, etc
- Underlying process simulation models rarely acknowledged when millions are saved

A healthy business model is required to ensure the resources for success:

- We need to explain about the possibilities in public
- We need to pay the developers for their huge effort especially in case of commercial success
- We need to co-operate



# Examples and status of work



# Process flue gas model

- Calculates the heat and mass balances for all unit operations involved
- Example shown for a cement production process, but
- Easy to adapt to other combustion processes by combining the unit operations in different ways





# CO2 scrubbing model

- Calculates the heat and mass balances for all unit operations involved
- Easy to adapt to other processes by combining the unit operations in different ways

Currency	USD	Text		USD/kWh	
	Euro	Energy reboller		0.2500	
		Electricity		0.5000	
	10 C				
Period	1 hour	OPEX	kW	1000 x USD	
	1 day	Energy for rebailer	8.4526e+04	1.8511e+05	
	5 years	Electrical power for pumps	1.3259e+03	5.8076e+03	
	10 years	Electrical power for flue gas tan	1.8371e+03	8.0467e=03	
		Total		1.9897e+05	
				P	
		P		1	
		CAPEX		1000 x USD	
		Scrubber		2.3103e+03	
		Stripper		2.3103e+03	
		Ptate Heat Exchanger 1		800.8739	
		Pumps		1.3259e+03	
		the second se			

### Liquefaction model



Calculate

Clear

Reset

Save

Optimize Purge

# LCO2 transport model

• What happens when we transfer the liquid from a terminal to a ship and when heat penetrates the tanks during sailing?





# CO2 purity specification (web app)

$\varphi \  \   \varphi$	CO2_standards_01					⊕ ၃] …	– 🗆 X
		Show Value >	0 and L ▼			Limit Northe	ern Light
		Component	Unit	Base 1	Base 2	Value	Limit
		Carbon dioxide	%	mol	wet	97.4900	
		Water	%	mass	wet	1.0000	24072/30 ppm
		Oxygen	ppm	mol	dry	100.0000	98/10 ppm
✔ Sho	ow Names ange base units						
Dow	rnload excel file						
Show Log	ECA						52



# REFERENCES



# Literature review

- A lot of knowledge about CCS is already published and are carefully reviewed
- Interview with relevant emitters and stakeholders
- Co-operation with AAU and DTU (examiner in CCS projects)
- Co-operation with Force Technology regarding their detailed CFD simulation model of an amine scrubber.

Knowledge > CC	-5
1	Name
	🛃 Study of solvent-based carbon capture for cargo ships through process modelling and simulation.pdf
*	🛃 Stripper Modification of a Standard MEA Process.pdf
*	🔗 Stripper and compressor model.pdf
*	🔗 Review of Cryogenic Carbon Capture Innovations and Their Potential Applications.pdf
	🔗 Reliq_screen_dump_example.pdf
	Presssure Management of CO2 storage.pdf
	Physical and chemical effect of impurities in carbon capture.pdf
	Phase diagrams CO2_N2, compression.pdf
	Model Development for CO2 Capture in the Cement Industry.pdf
1	🔗 HHE-Indmeldelsesblanket-2022.pdf
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	B Carbon-capture-and-storage-technologiespresent_2017_Current-Opinion-in-Che.pdf
	🛃 Carbon Dioxide Separation from Flue Gases.pdf
	🛃 Appendix 2 _ 1112-00004A - Mission CCUS – a roadmap for Carbon Capture, Utilisation and Storage.pdf
	A new relevant manhance analization CO2 direct direct two (DAC) and

# Run simulations from any web-browser:

- No need to install any software
- Always latest updates

# Model details:

- Solving mass and heat balances of all unit operations involved
- Data and costs from major equipment suppliers
- Thermodynamic data from NIST Standard Reference Database 23
- Thermodynamic models: Peng Robinson, SRK, UNIFAC ao.
- The core simulation model is programmed in Matlab<sup>®</sup>
- CAPE-OPEN standard
- +20 years experience in the field





# Member of CAPE-OPEN standard organisation

https://www.colan.org/





# Member of ISO Technical Committee

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#### CARBON CAPTURE PROCESSES

Let's calculate the cost for your different options



PROCESS DESIGN

Let's solve the energy and mass balances for your process based on our extensive libary of pre-defined functions



DATA ANALYSIS

Tired of spreadsheets? Let's help to visualize and analyze your data based on the power of Matlab





# DESM









