Investigating the impact of impurities in the CO_2 streams for the Carbon Capture and Transportation value chain using MATLAB and CAPE-OPEN

Outline

- 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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PhD Chem. Eng.
CAPE-OPEN Conference
Nancy, France
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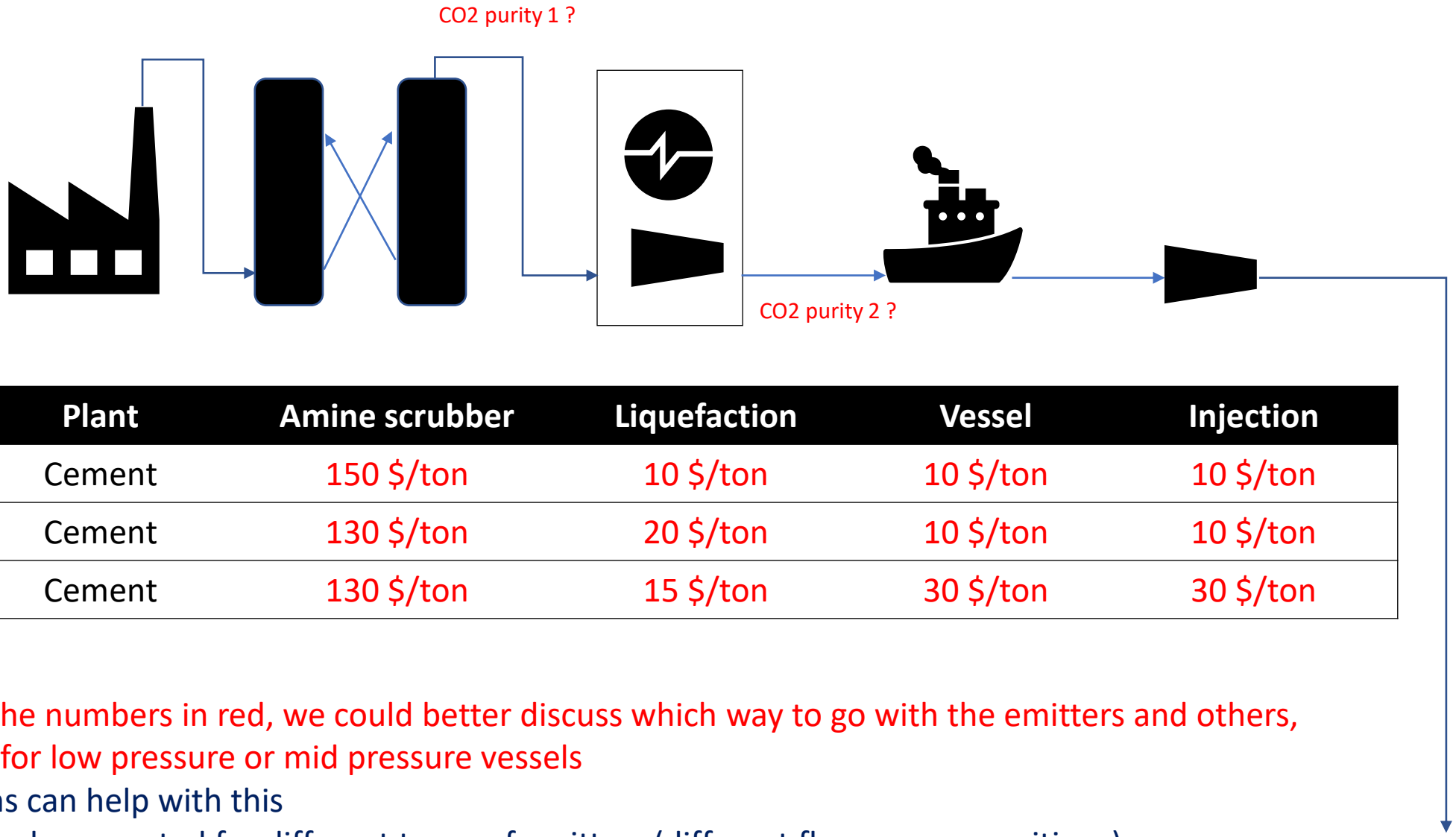
CO2 Value chain



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

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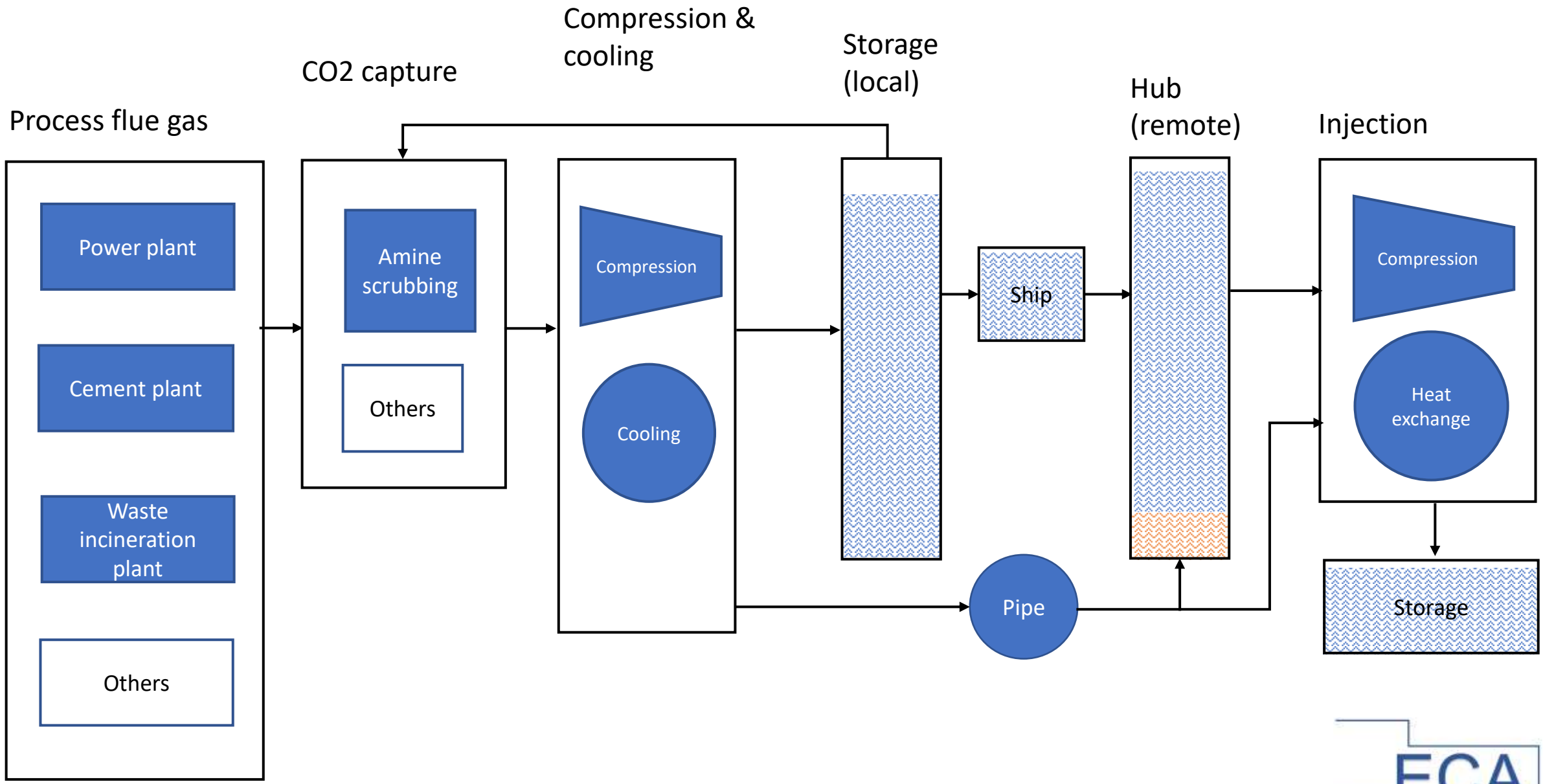
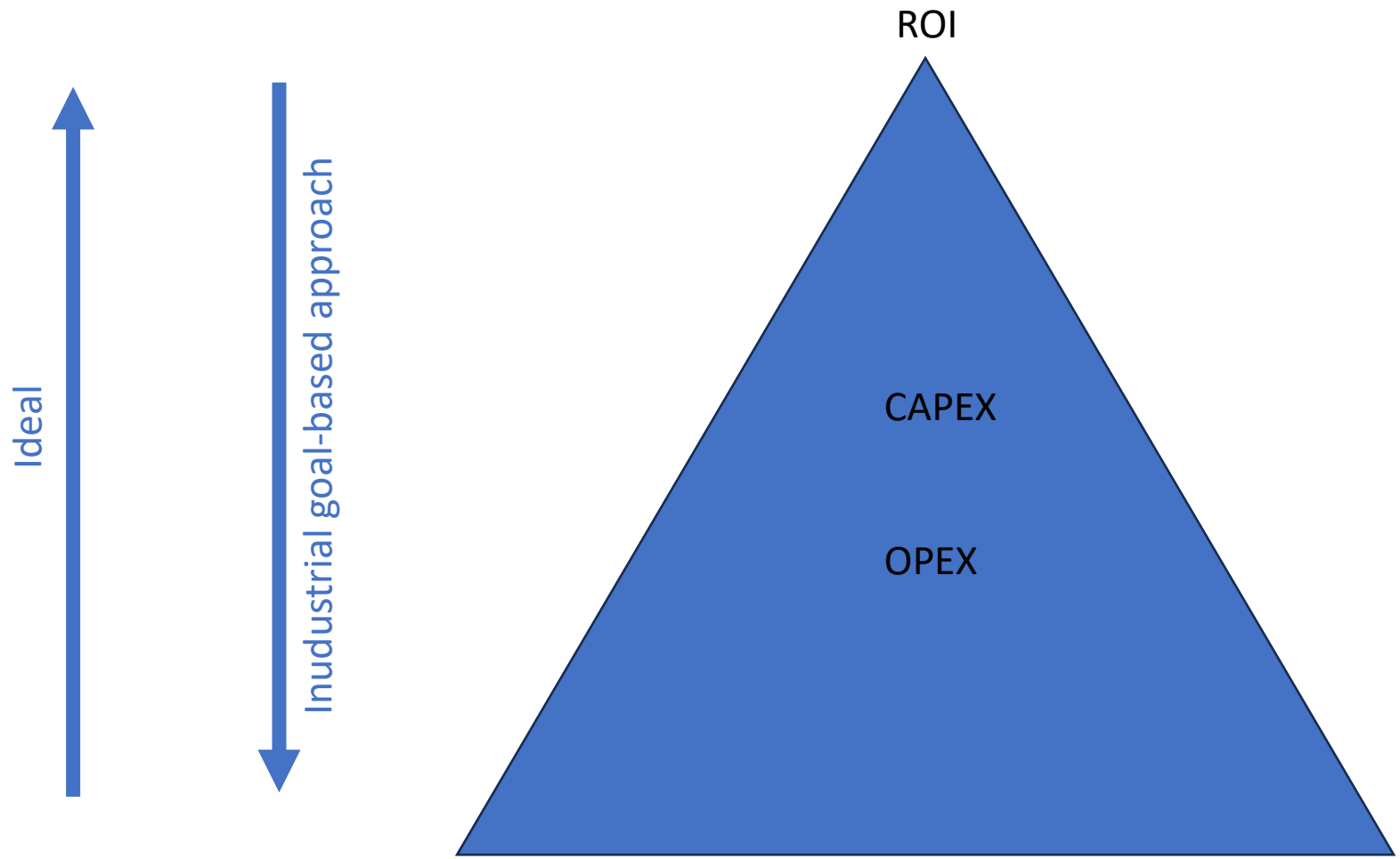
Process simulations



Considerations regarding choice of simulation software



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 ☺
- 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)

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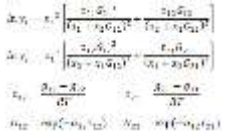
Life of a process simulation engineer

I don’t have time enough!
That is not my education!
Will they help me to solve all the chemistry?



Boss

IT details

Wife

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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

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Examples and status of work

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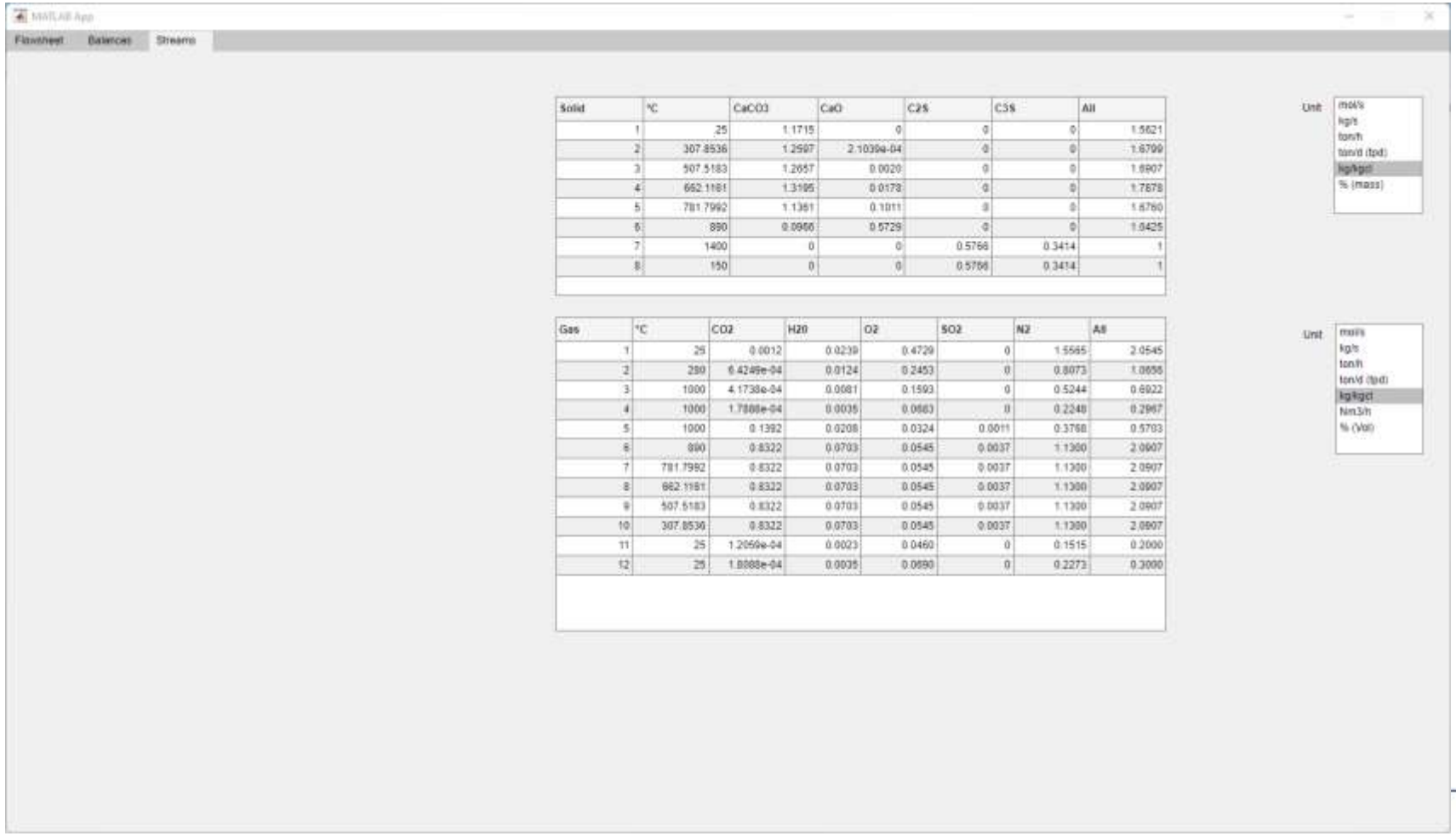
Process flue gas model

- 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

Detailed information about each stream



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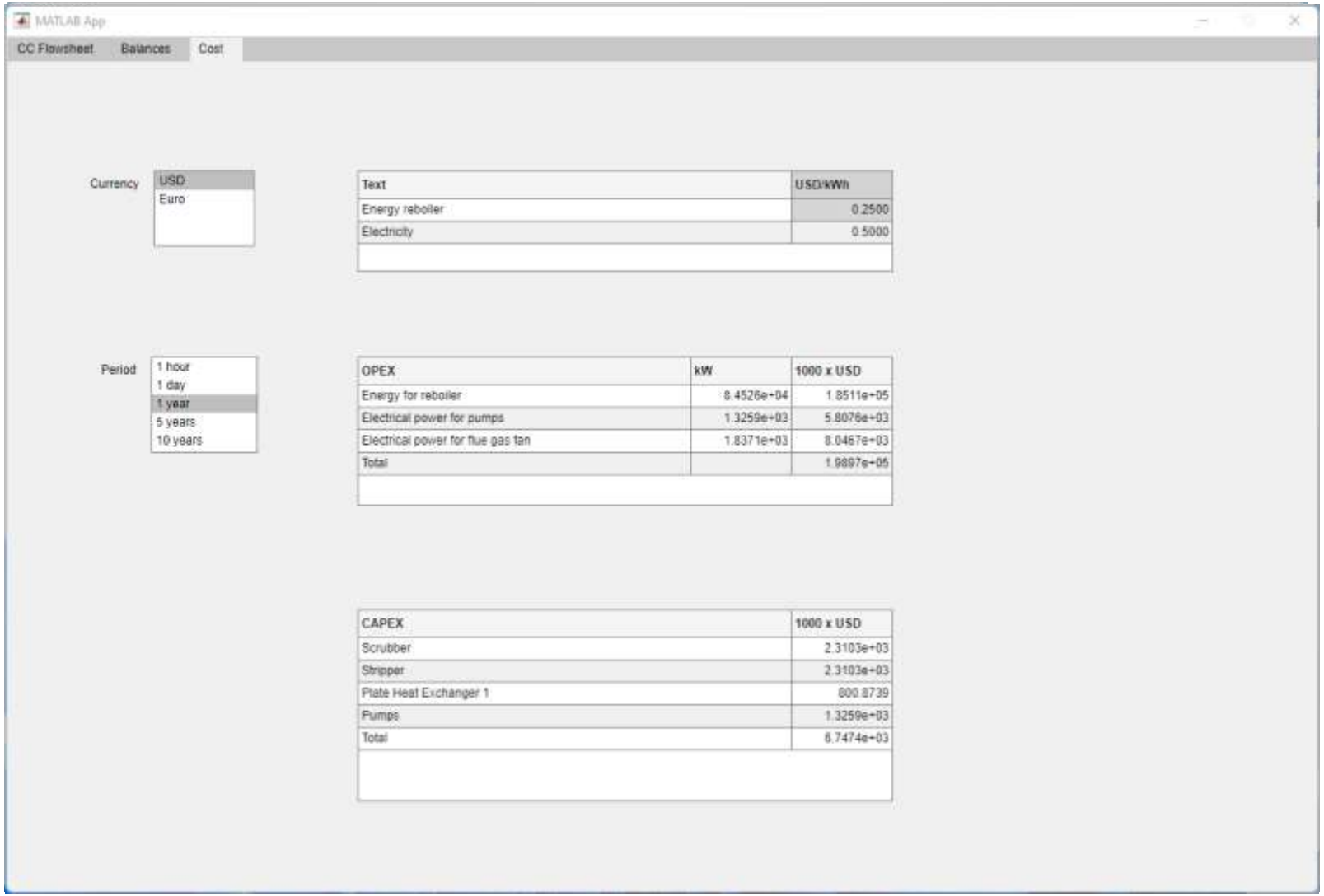
CO2 scrubbing model

- 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

Detailed cost overview (OPEX and CAPEX)



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Liquefaction model

MATLAB App

Plant | Capture | Liquefaction | Storage | Transportation | Storage | Injection | Entire Value Chain

Process: Internal

Purge [%]: 19.31

Number of compression stages: 4

Comp. efficiency [%]: 70

Flowsheet | Diagram | Balances | Streams | Purge | Settings | All simulations

Package Manager: TEA (CAPE-OPEN 1.1)

Package: CO2_N2 (PR)

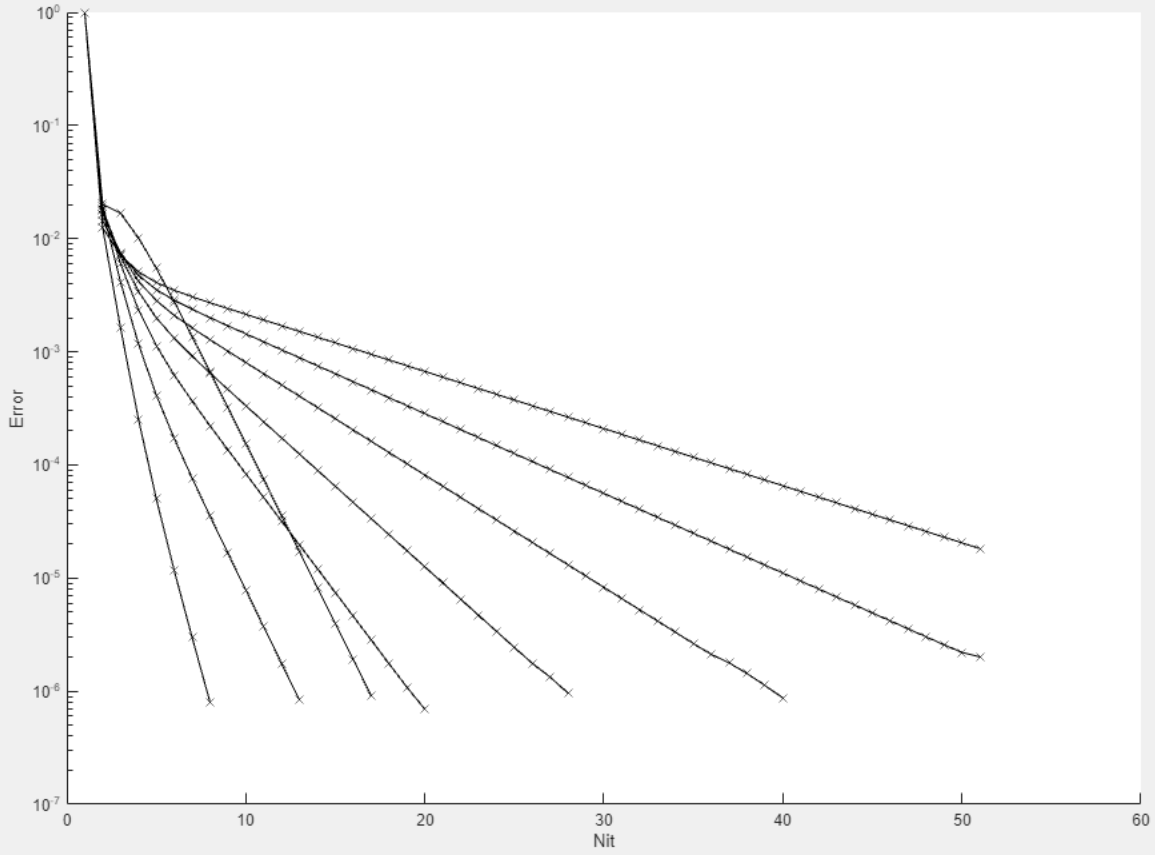
- CO2_N2 (PR)
- CO2 (PR)
- Methanol
- Ammonia
- Methane
- test
- CO2_N2_O2 (PR)
- CO2_N2_O2 (SRK)
- CO2_H2O (PR)
- CO2_N2_H2O (PR)

Log (max error)

Max number of iteratio

Plot iteration

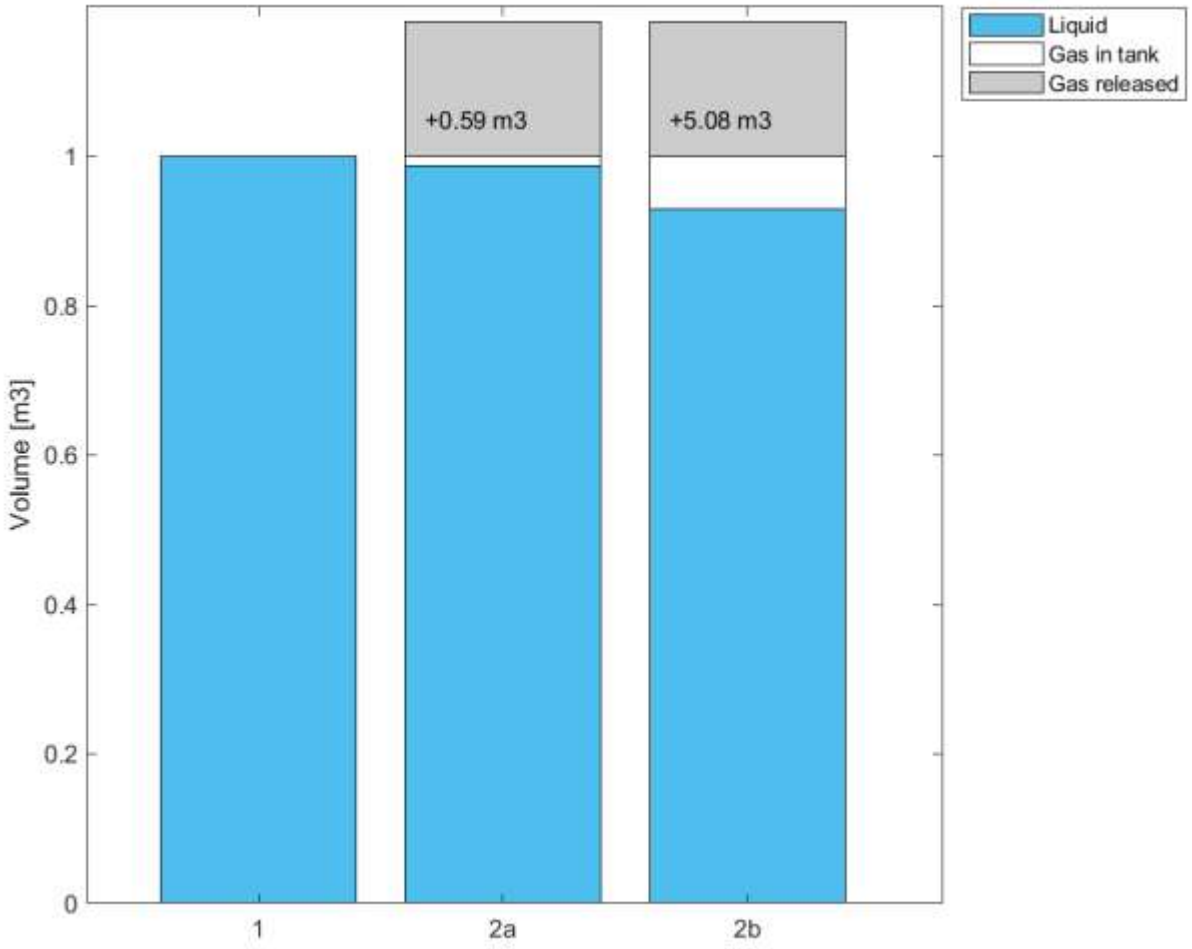
Show phase bound

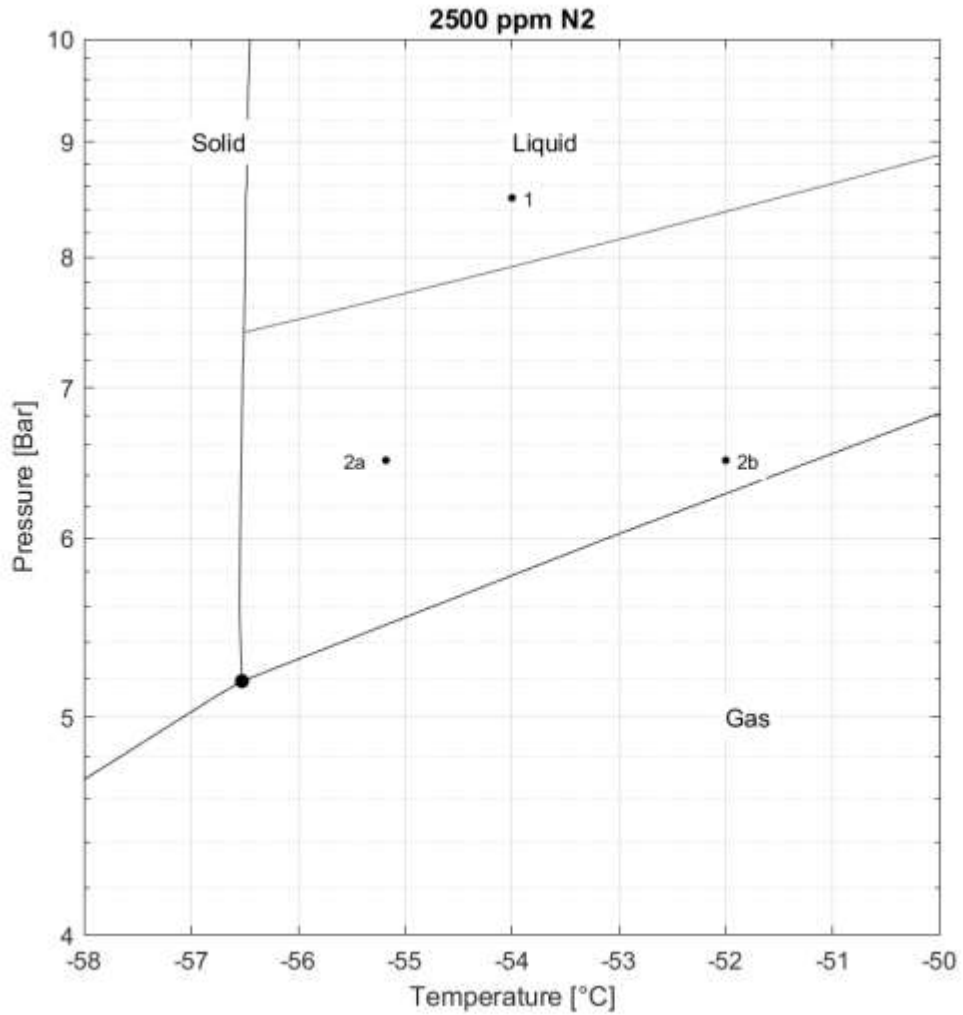


Calculate | Clear | Reset | Save | Optimize Purge

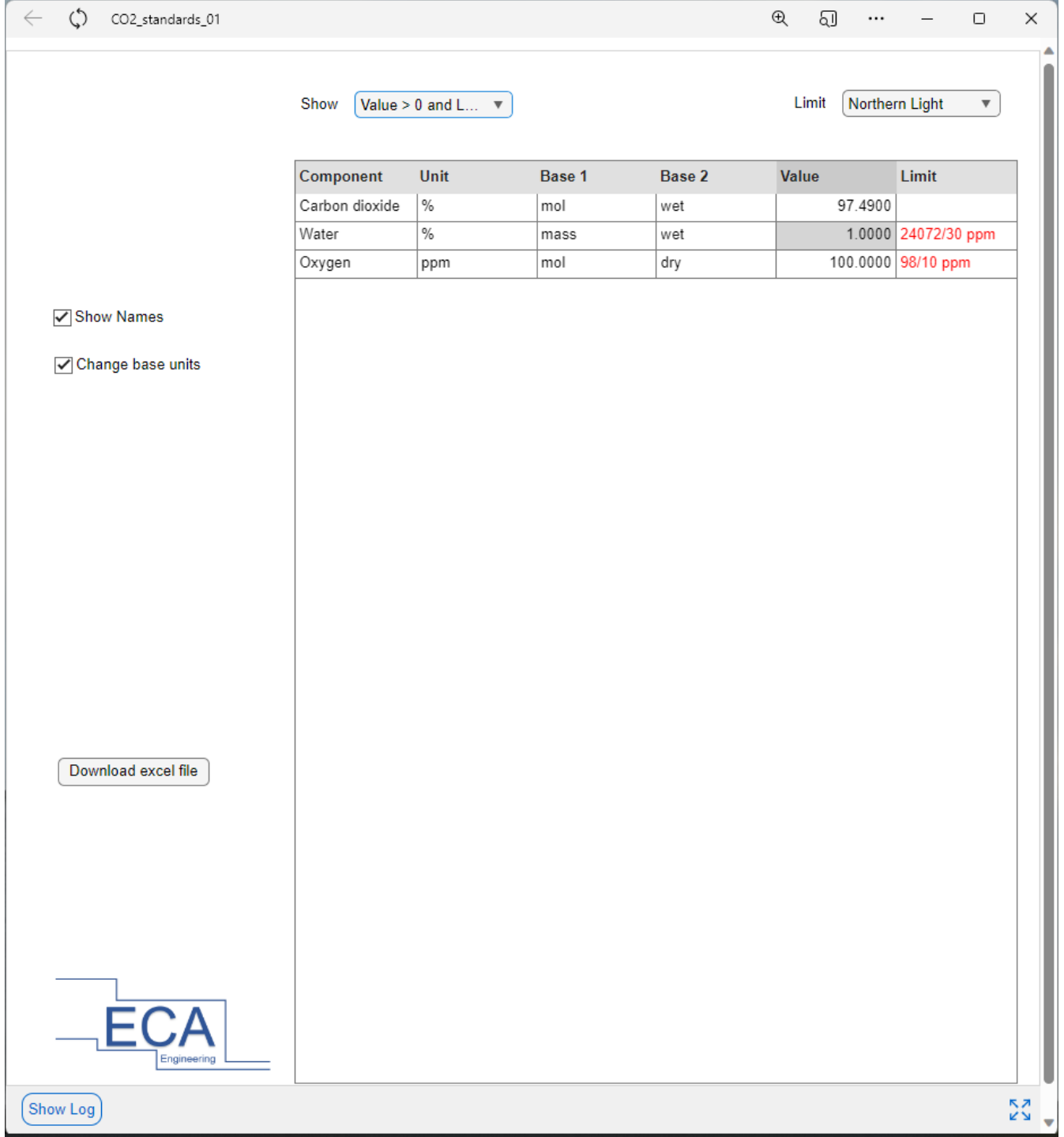
LCO2 transport model

- 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)



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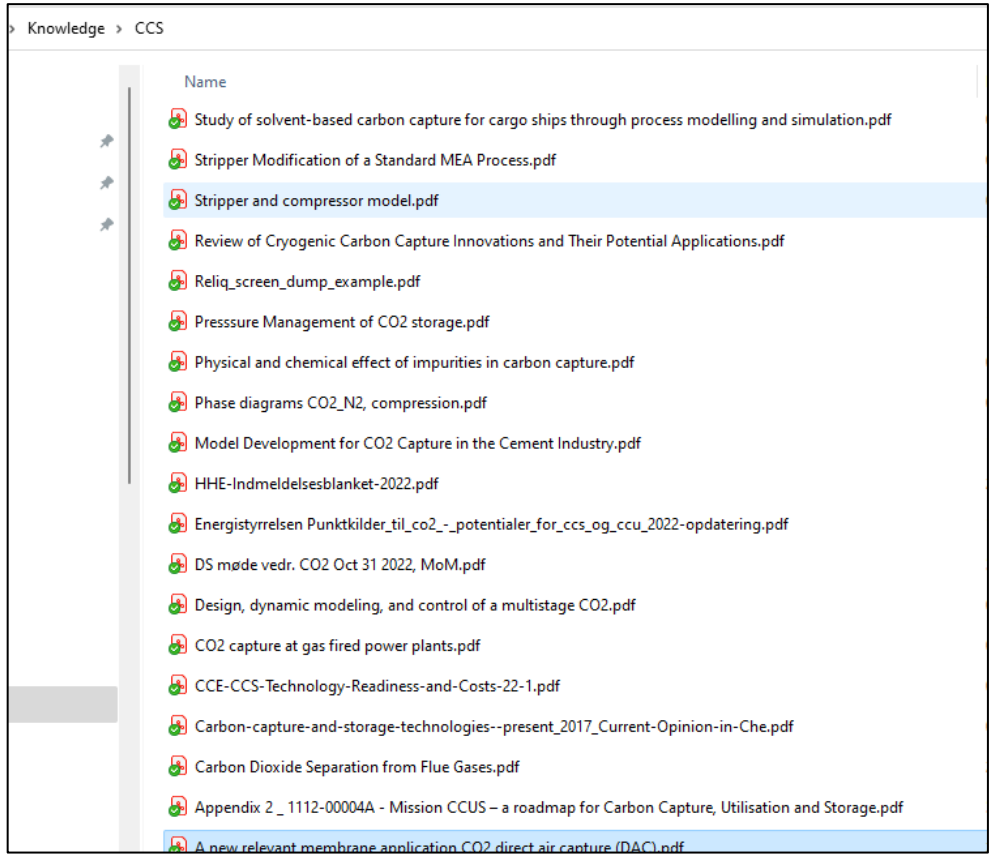
REFERENCES

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.



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®
- CAPE-OPEN standard
- +20 years experience in the field

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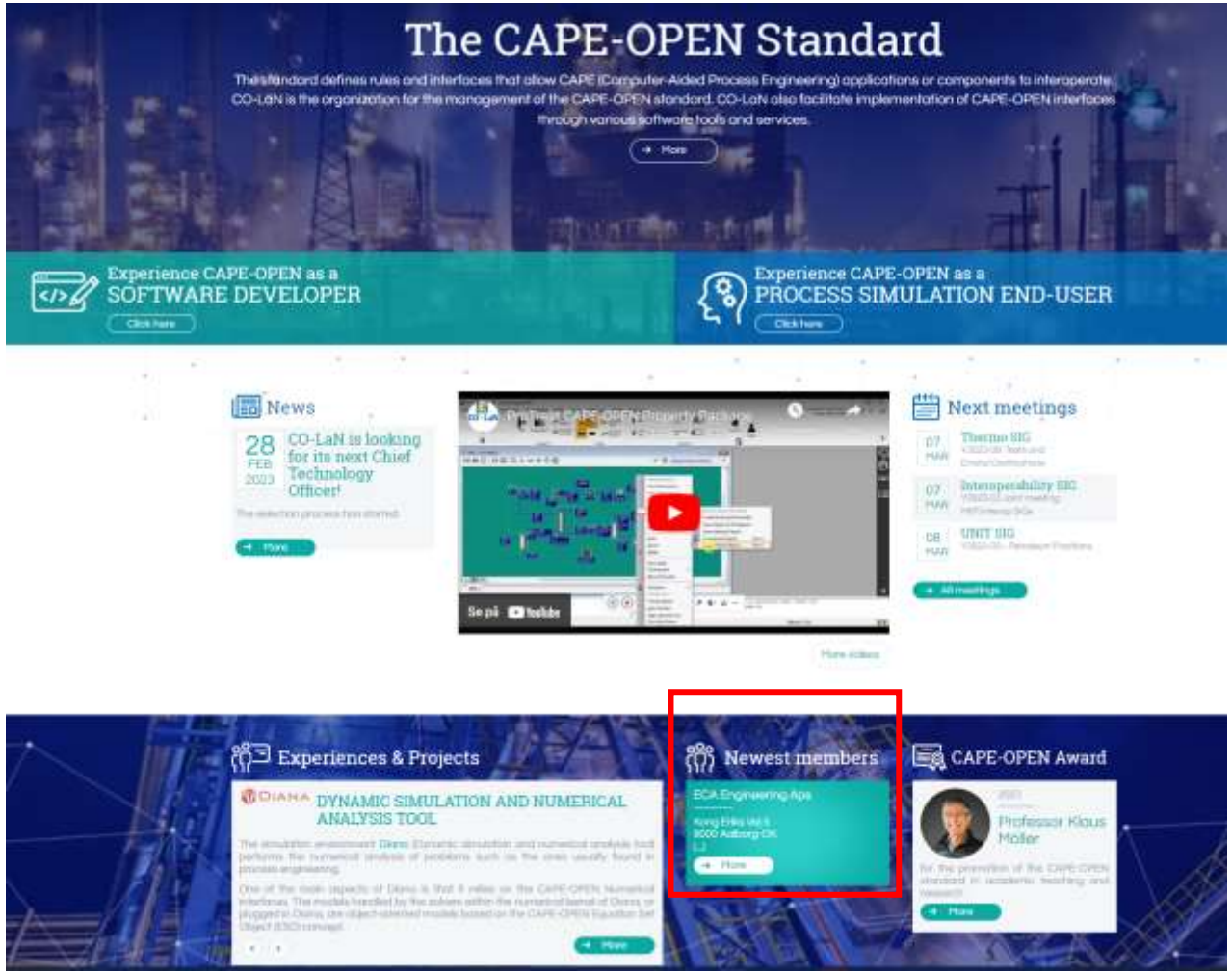
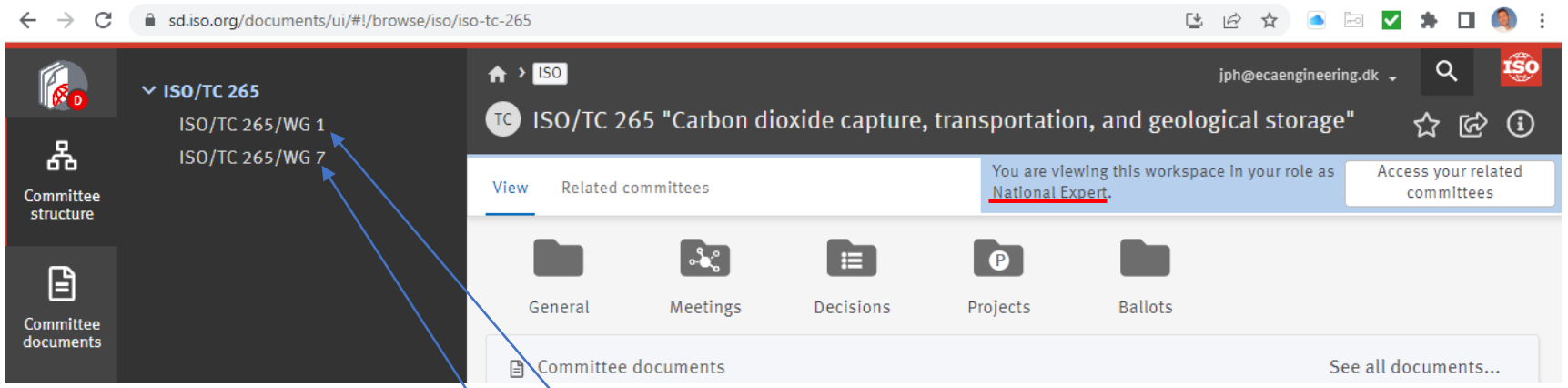
Member of CAPE-OPEN standard organisation

https://www.colan.org/



Member of ISO Technical Committee



WG1: new standards to describe the performance of carbon capture plants and different absorbents (national expert)

WG7: new standards for transportation of CO2 onboard ships (contributing with thermodynamic simulations and the practical impacts of impurities)

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