From MEA 30 wt.% to demixing solvents: investigation of an aqueous-alcoholic MEA-based solution

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UMONS RESEARCH INSTITUTE FOR ENERGY

8th Post-Combustion Capture Conference
Marseille – France

16th September 2025 – Session 3A

PCCC-8

Carbon capture context

+ 1.55°C in 2024
since pre-industrial level era

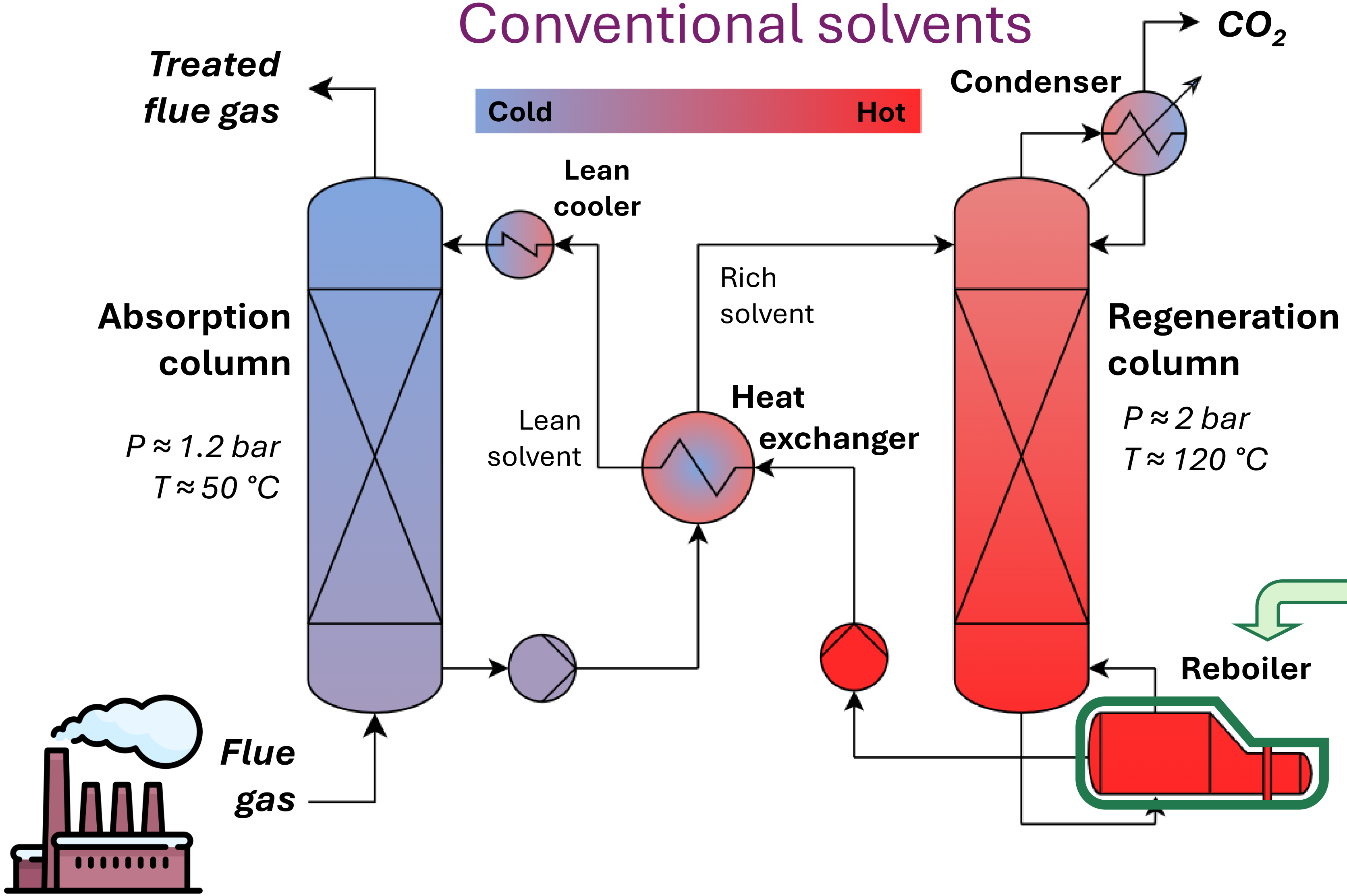
425.48 ppm in August 2025
CO_2 atmospheric concentration

Carbon capture technologies

- Absorption — TRL 9
- Adsorption
- Membrane
- Cryogenics
- Microalgae

Carbon capture Absorption-Regeneration process

Conventional solvents



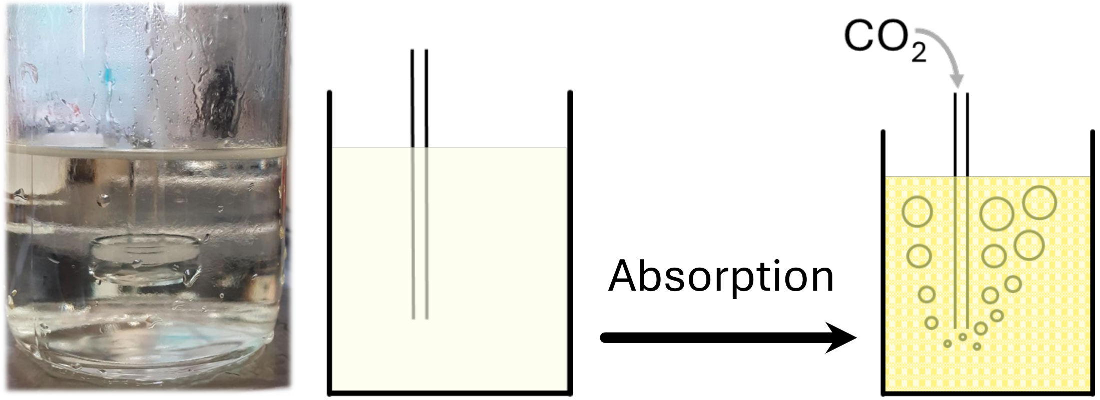
Aqueous amine-based solvents

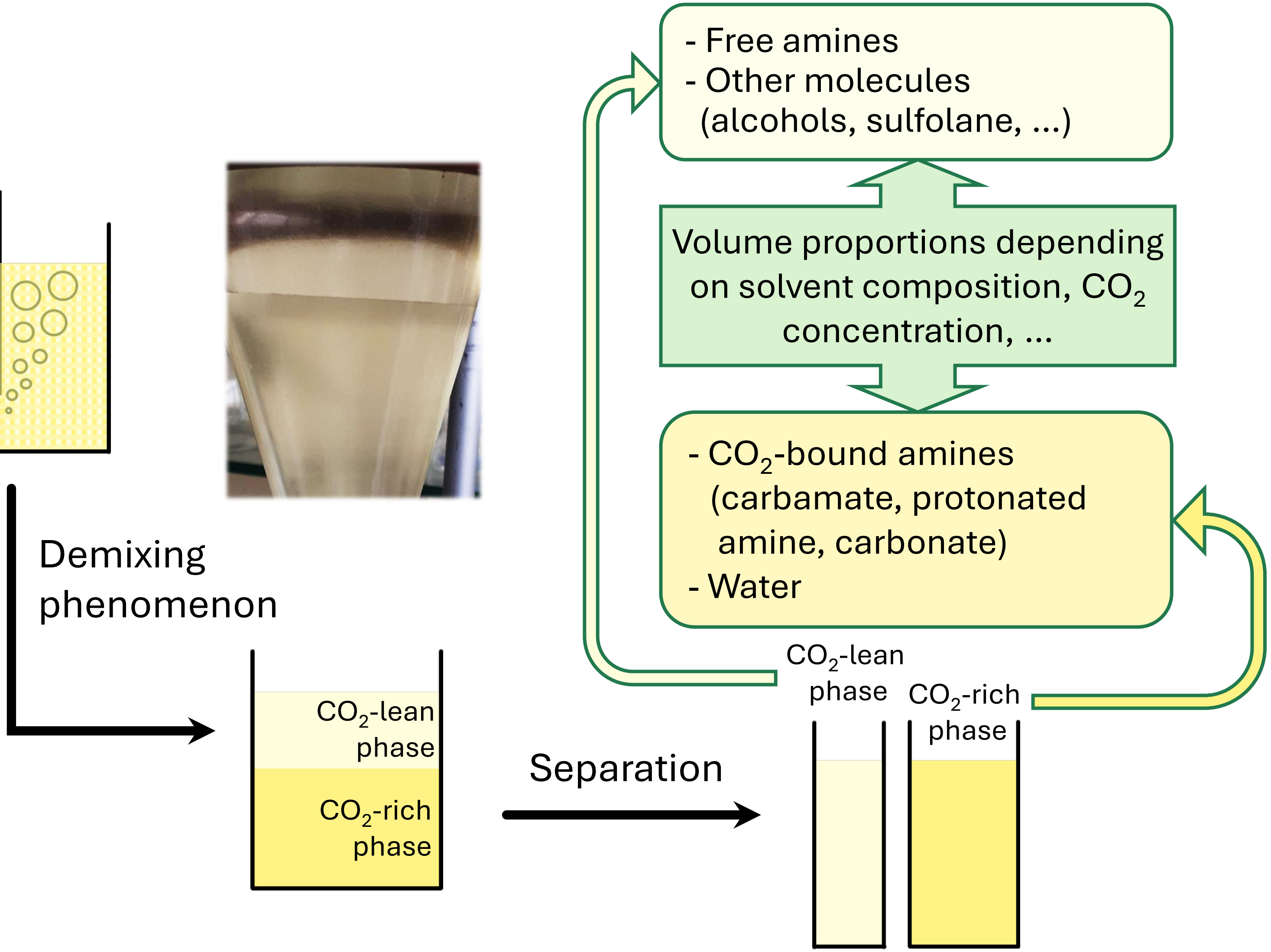
Monoethanolamine (aq. MEA 30 wt.%)

$E_{regen} \approx$ 3.4 – 4 GJ/tCO_2

Major part of the operative costs

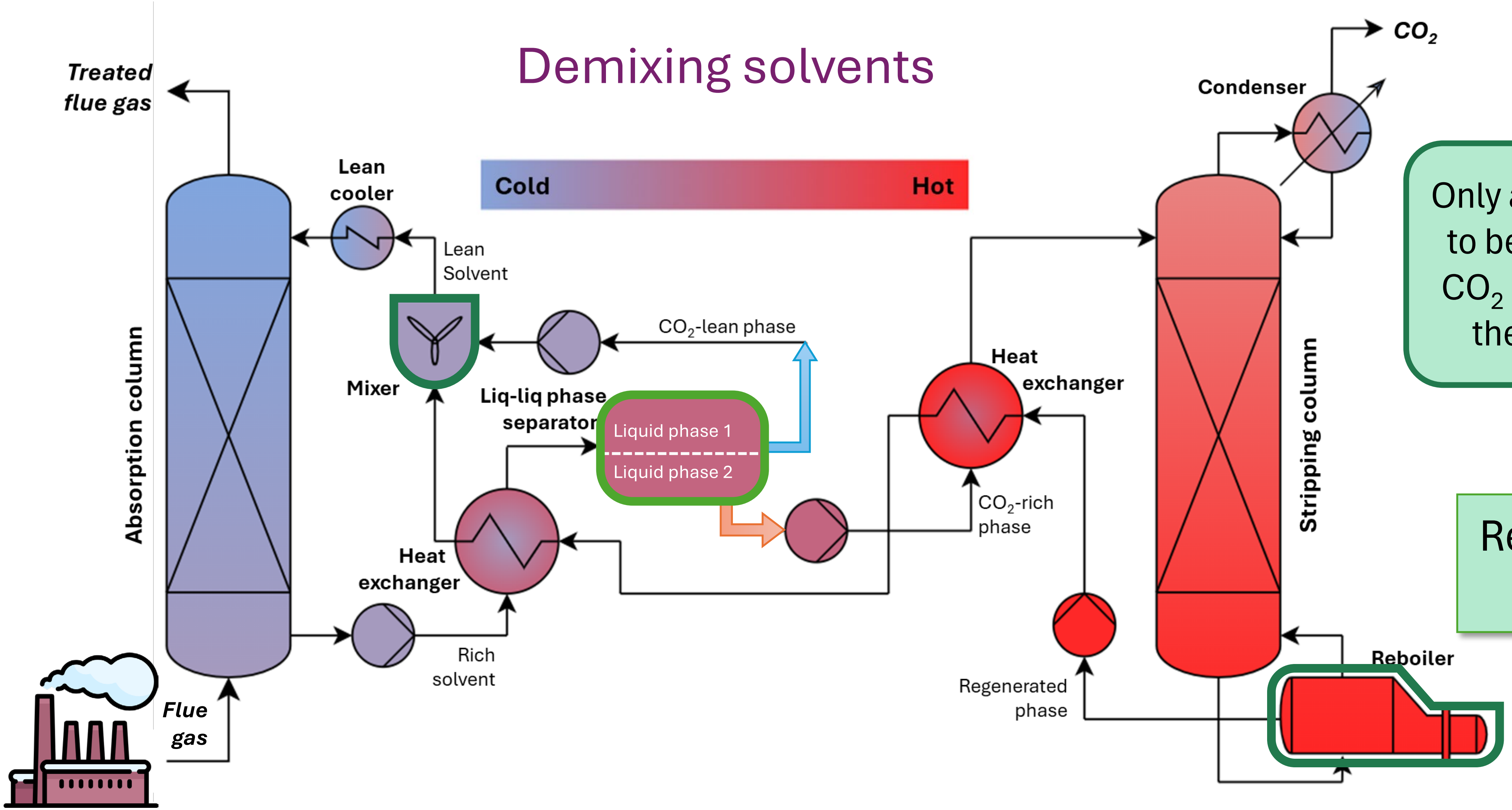
Demixing liquid-liquid amine-based solvents





- Free amines
  (primary, secondary, tertiary)
- Water
- Other molecules
  (alcohols, sulfolane, ...)

Carbon capture Absorption-Regeneration process



Only a solvent fraction to be regenerated ↘ CO_2 concentration in the rich phase ↗

Regeneration energy ↘

Demixing liquid-liquid amine-based solvents

- Demixing solvents review and selection methodology
- Equilibrium and kinetic data acquisition
- Micro-pilot scale solvents evaluation
- Process modelling, simulation & LCA
- Validation of the relevance of such demixing solvents

Demixing liquid-liquid amine-based solvents

Demixing solvents review

Often a primary/secondary amine with a tertiary amine

30 aqueous amine-based demixing blends

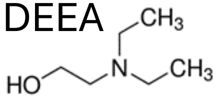
Demixing phenomenon dependent on temperature and CO_2 loading

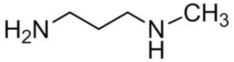
- 2-amine blends
- Presence of a phase-splitting agent
  - Sulfolane
  - Alcohols
  - Others

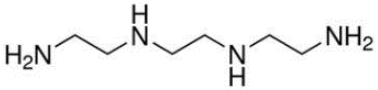
Used to induce or enhance the demixing phenomenon

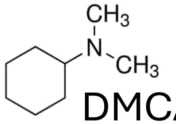
Examples of blends

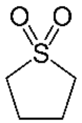
- 2-amine blends: DEEA-MAPA, TETA-DMCA
- Sulfolane: MEA-SULF, DETA-SULF
- Alcohols: TETA-PROP, MEA-PROP
- Others: DMCA-MCA-AMP, TEPA-DGME

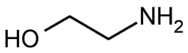
DEEA


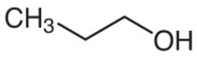
MAPA


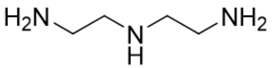
TETA


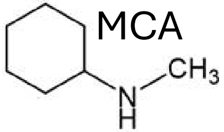
DMCA


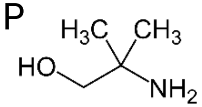
SULF


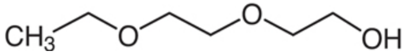
MEA


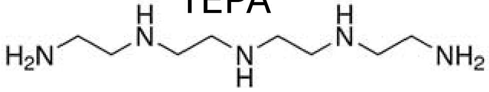
PROP


DETA


MCA


AMP


DGME


TEPA


Selection methodology of demixing solvents

Step 1 – Techno-economic evaluation

Based on 6 key indicators …	… having each a specific weight
Regeneration energy	0.42
CO_2 absorption rate	0.17
Demixing volume ratio*	0.15
CO_2 absorption capacity	0.12
Volatility of organic compounds**	0.08
Solvent cost	0.06

Scale from 1 (best case) to 5 (worst case) for each indicator

Estimated values if missing in literature

*= V_{rich}/V_{lean}

**=$y_{organic}/x_{organic}$

For each solvent $$Global\ score = \sum_{i=1}^{6} p_i * s_i$$

p_i : weight of indicator i
s_i : score of indicator i {1,2,3,4,5}

Step 2 – Health, safety and environment analysis

A solvent is **excluded** from the final ranking if at least one of its components causes:

- Death
- Serious fertility problem
- Corrosion to metals
- Very toxic to aquatic life

Rejection of 17 solvents

Database: European Chemistry Agency (CLP regulation and REACH legislation)

Selection methodology of demixing solvents

Final classification

1	TETA (30 wt.%) – PROP (50 wt.%)
2	TETA (15 wt.%) – DMCA (35 wt.%)
3	DEEA (64 wt.%) – MAPA (19 wt.%)
4	DEEA (50 wt.%) – MEA (25 wt.%)
5	DEEA (62 wt.%) – MAPA (9 wt.%)
6	DMBA (47 wt.%) – DEEA (27 wt.%)
7	TETA (31 wt.%) – 1DMA2P (22 wt.%)
8	DEEA (47 wt.%) – TETA (15 wt.%)
9	DEEA (47 wt.%) – TETA (15 wt.%) – PROP (17 wt.%)
10	MEA (30 wt.%) – PROP (40 wt.%)
11	AEP (20 wt.%) – PROP (40 wt.%)
12	MEA (30 wt.%) – BUT (40 wt.%)
13	MAE (30 wt.%) – BUT (40 wt.%)

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Methodological Selection of Demixing Liquid–Liquid Solvents Used in the Absorption–Regeneration Carbon Capture Process

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Methodological evaluation of demixing solvents used in the absorption-regeneration carbon capture process

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An aqueous-alcoholic MEA-based solution

- Monoethanolamine (30 wt.%)

- Propan-1-ol (40 wt.%)

- Water (30 wt.%)

Open access solvent

Chemical reactions

- Same as for aqueous MEA 30 wt.%
- No reaction products with propanol

$$CO_2 + 2\,MEA \rightleftarrows MEACOO^- + MEAH^+$$
$$MEACOO^- + H_2O \rightleftarrows MEA + HCO_3^-$$

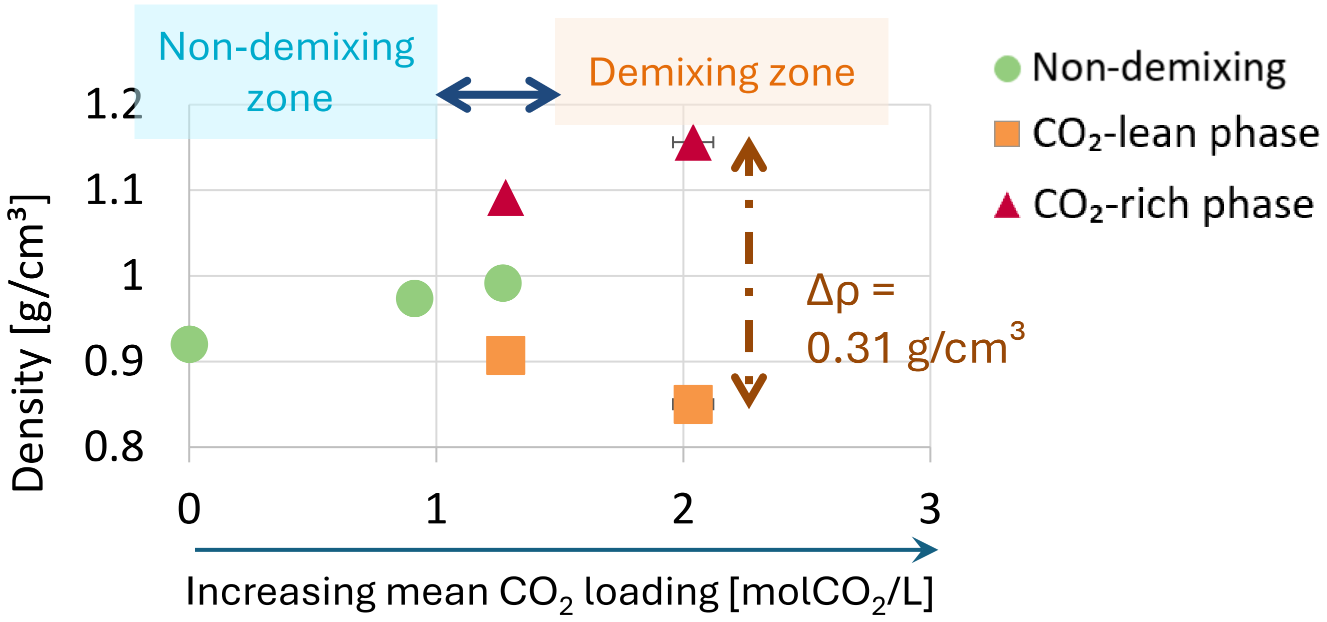
$$CO_2 + H_2O \rightleftarrows H_2CO_3$$
$$H_2CO_3 + H_2O \rightleftarrows HCO_3^- + H_3O^+$$
$$HCO_3^- + H_2O \rightleftarrows CO_3^{2-} + H_3O^+$$

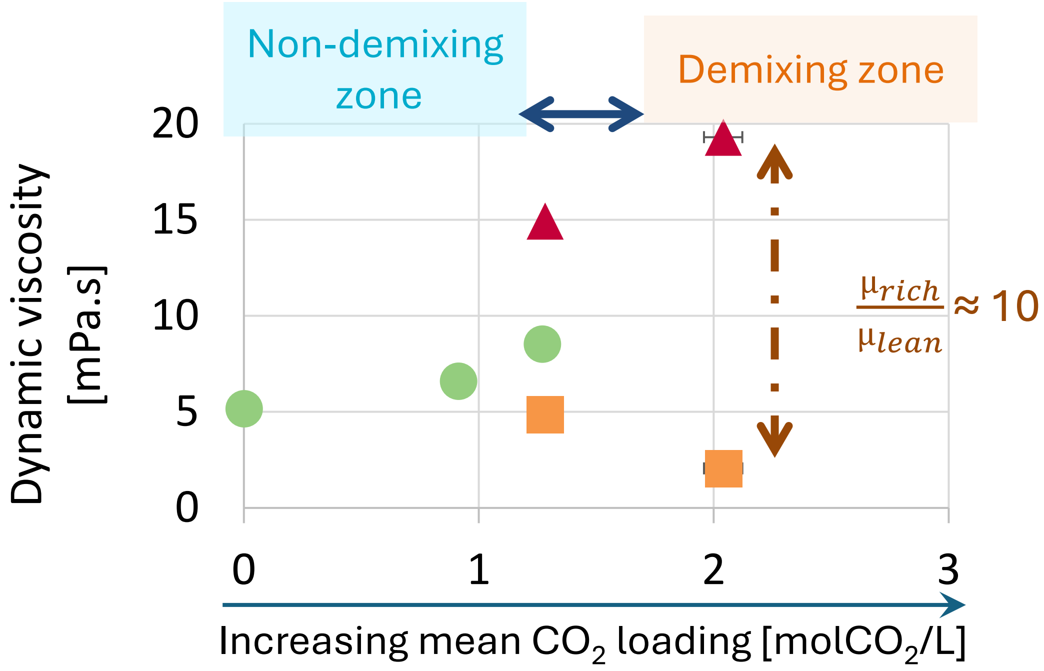
An aqueous-alcoholic MEA-based solution

MEA (30 wt.%) – PROP (40 wt.%)

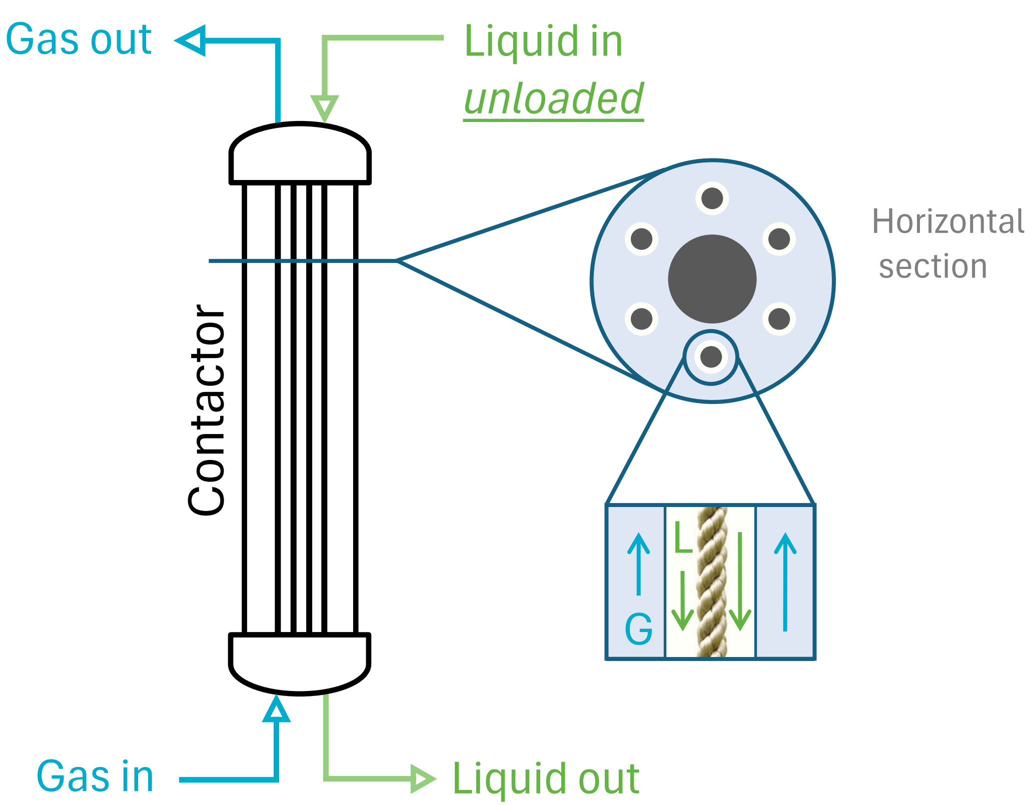
Critical CO_2 concentration at 25 °C
1.28 molCO_2/L

Volume of the CO_2-rich phase from 44 to 60%
(from 2.15 up to 3.22 molCO_2/L)





Absorption performance on cable-bundle contactor

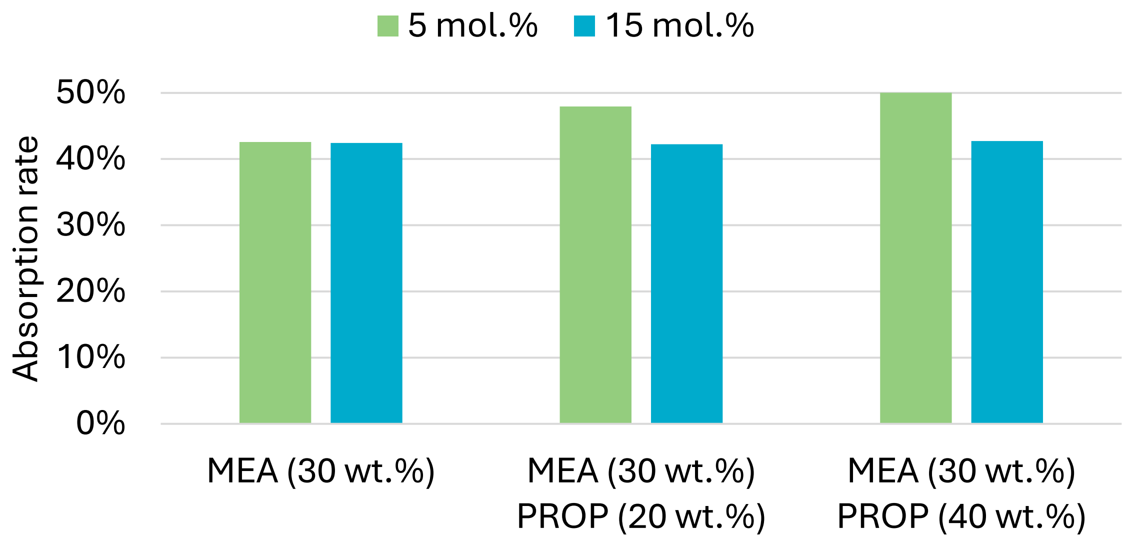


Height	54 cm
Number of cables	6
Diameter of a cable	1.6 mm

$$A = \frac{G_{CO_2,in} - G_{CO_2,out}}{G_{CO_2,in}} = 1 - \frac{y_{CO_2,out}}{y_{CO_2,in}} * \frac{1 - y_{CO_2,in}}{1 - y_{CO_2,out}}$$

Continuous tests

a single pass of liquid



Liquid flow rate	Gas flowrate	CO_2 gas fraction
11.4 L/h	762 NL/h	5 - 15 mol.%

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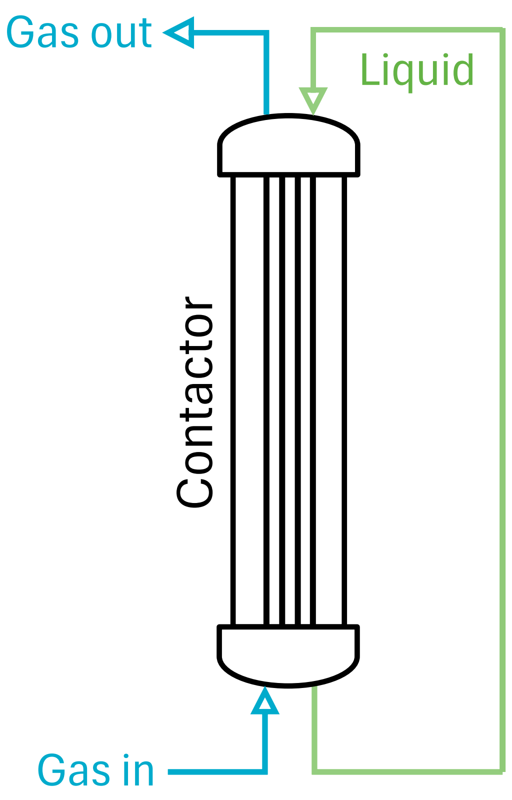


Recirculation of liquid until CO_2 saturation is achieved

Height	54 cm
Number of cables	6
Diameter of a cable	1.6 mm

$$A = \frac{G_{CO_2,in} - G_{CO_2,out}}{G_{CO_2,in}} = 1 - \frac{y_{CO_2,out}}{y_{CO_2,in}} * \frac{1 - y_{CO_2,in}}{1 - y_{CO_2,out}}$$

Semi-continuous tests

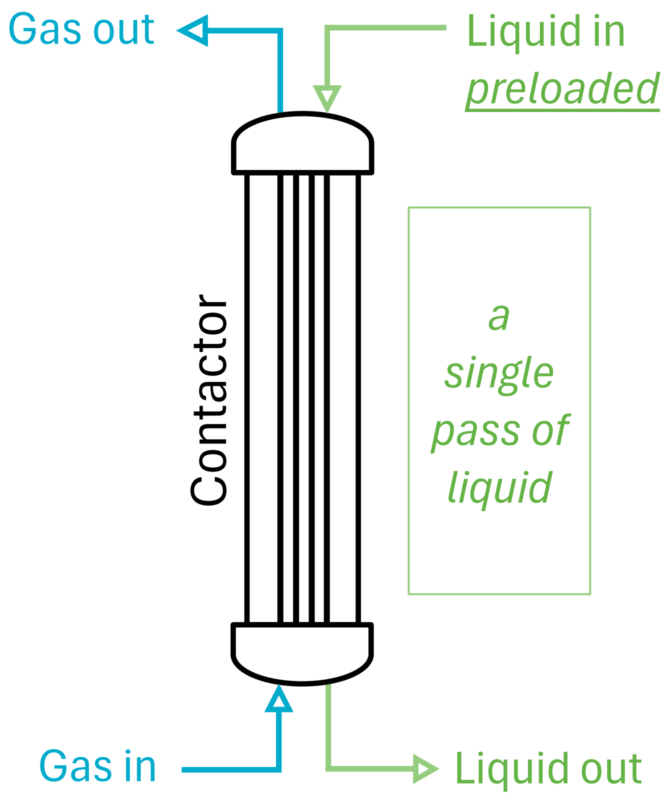
For aqueous blend
MEA (30 wt.%) – PROPAN-1-OL (40 wt.%)

Volume loss of the liquid solvent

↓

Volatility of propan-1-ol

Absorption performance on cable-bundle contactor

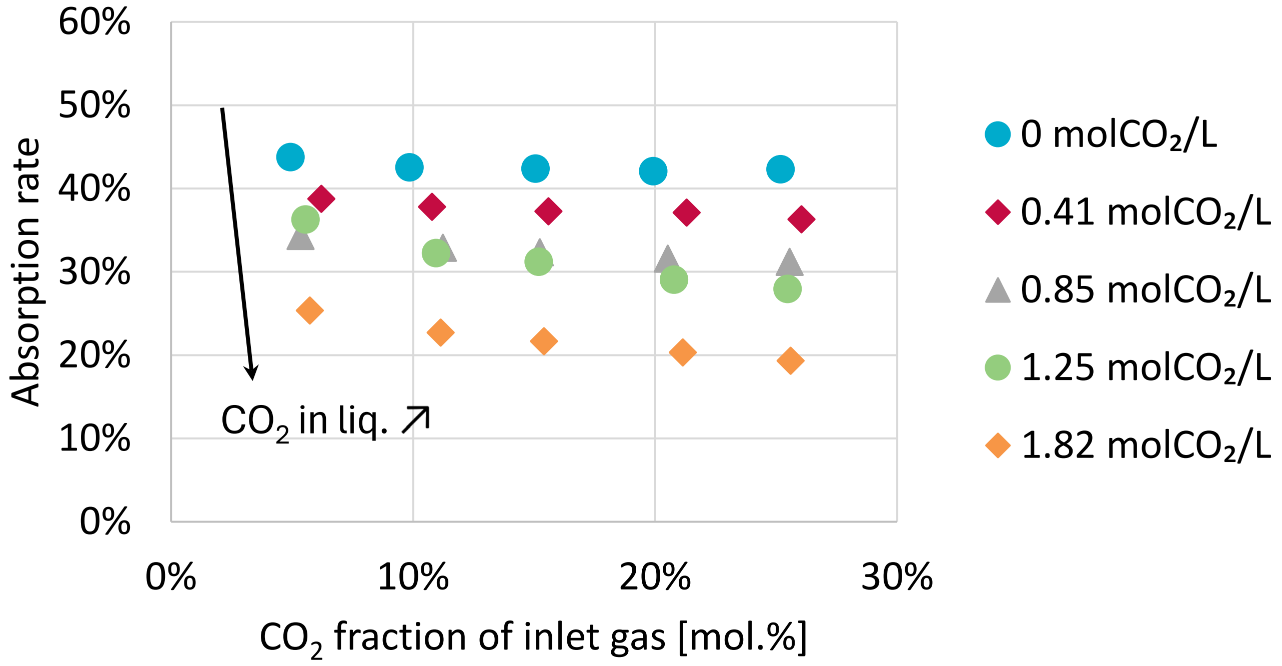


Height	54 cm
Number of cables	6
Diameter of a cable	1.6 mm

Continuous tests

$$A = \frac{G_{CO_2,in} - G_{CO_2,out}}{G_{CO_2,in}} = 1 - \frac{y_{CO_2,out}}{y_{CO_2,in}} * \frac{1 - y_{CO_2,in}}{1 - y_{CO_2,out}}$$

MEA 30 wt.%

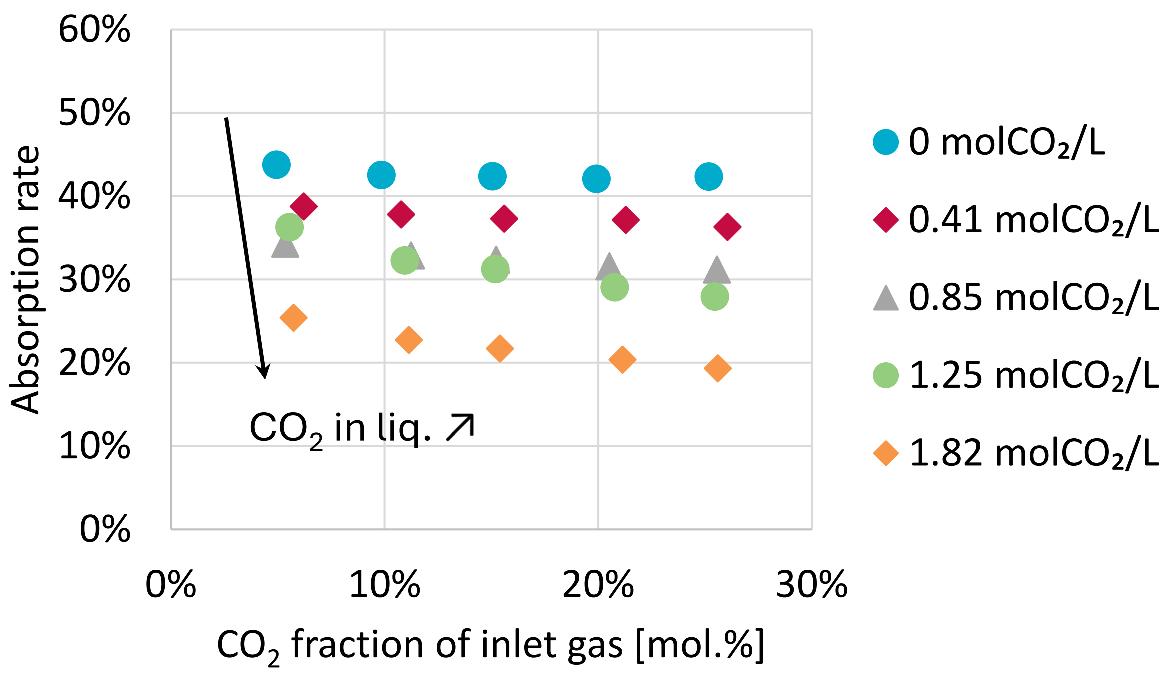


Absorption performance on cable-bundle contactor

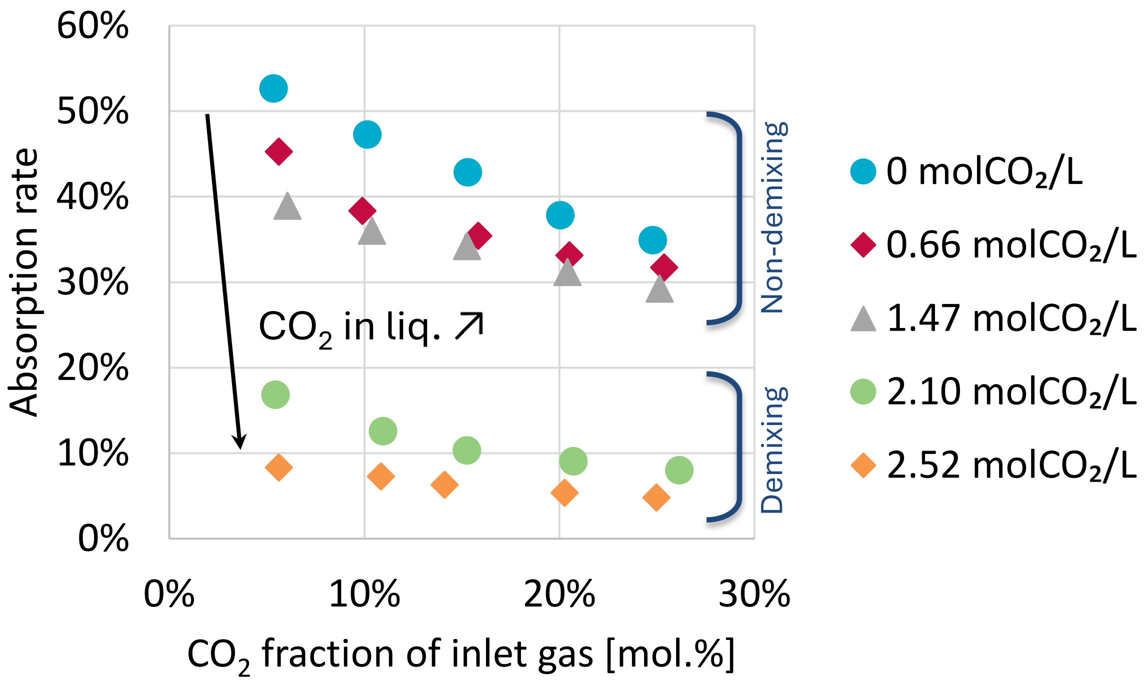
Continuous tests

$$A = \frac{G_{CO_2,in} - G_{CO_2,out}}{G_{CO_2,in}} = 1 - \frac{y_{CO_2,out}}{y_{CO_2,in}} * \frac{1 - y_{CO_2,in}}{1 - y_{CO_2,out}}$$

MEA 30 wt.%



MEA 30 wt.% - PROP 40 wt.%



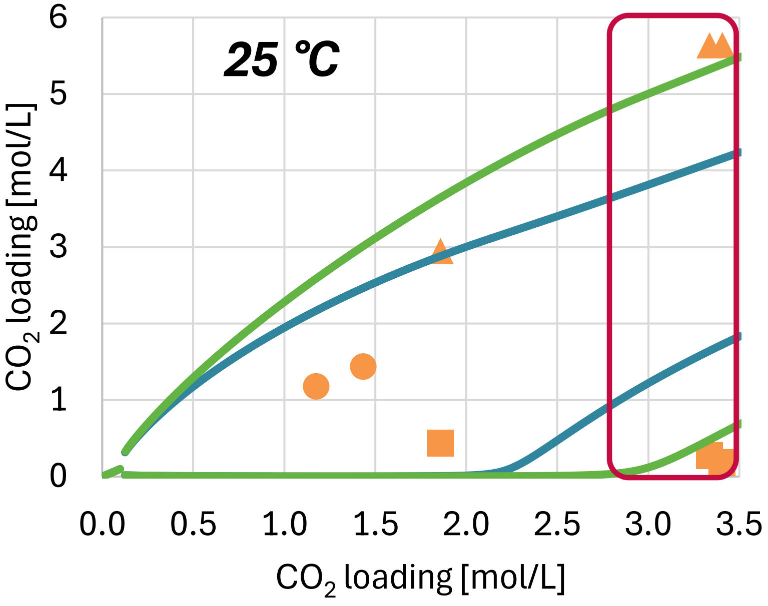
Liquid-liquid equilibrium modelling

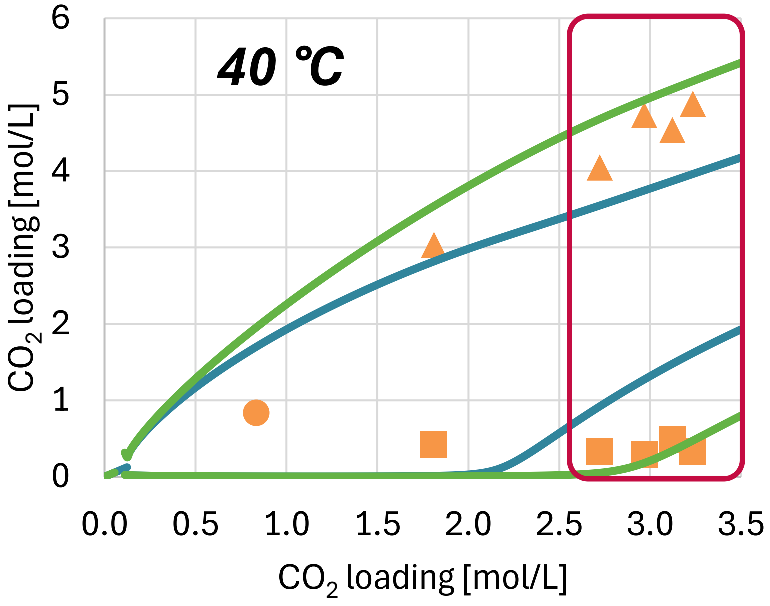
MEA (30 wt.%) – PROP (40 wt.%)

Modelling using two different thermodynamic models for liquid phases:

- Electrolyte Non-Random Two-Liquid (eNRTL) Wang et al., 2019
- Electrolyte Non-Random Two-Liquid with the Helgeson model (eNRTL-HG)

Tanger et al., 1988





Experiment :
- Non-demixing
- CO_2-rich phase
- CO_2-lean phase

Relative deviations between experiments and modelling

		25 °C	40°C
CO_2-rich phase	eNRTL	27%	17%
	eNRTL-HG	**5%**	**9%**

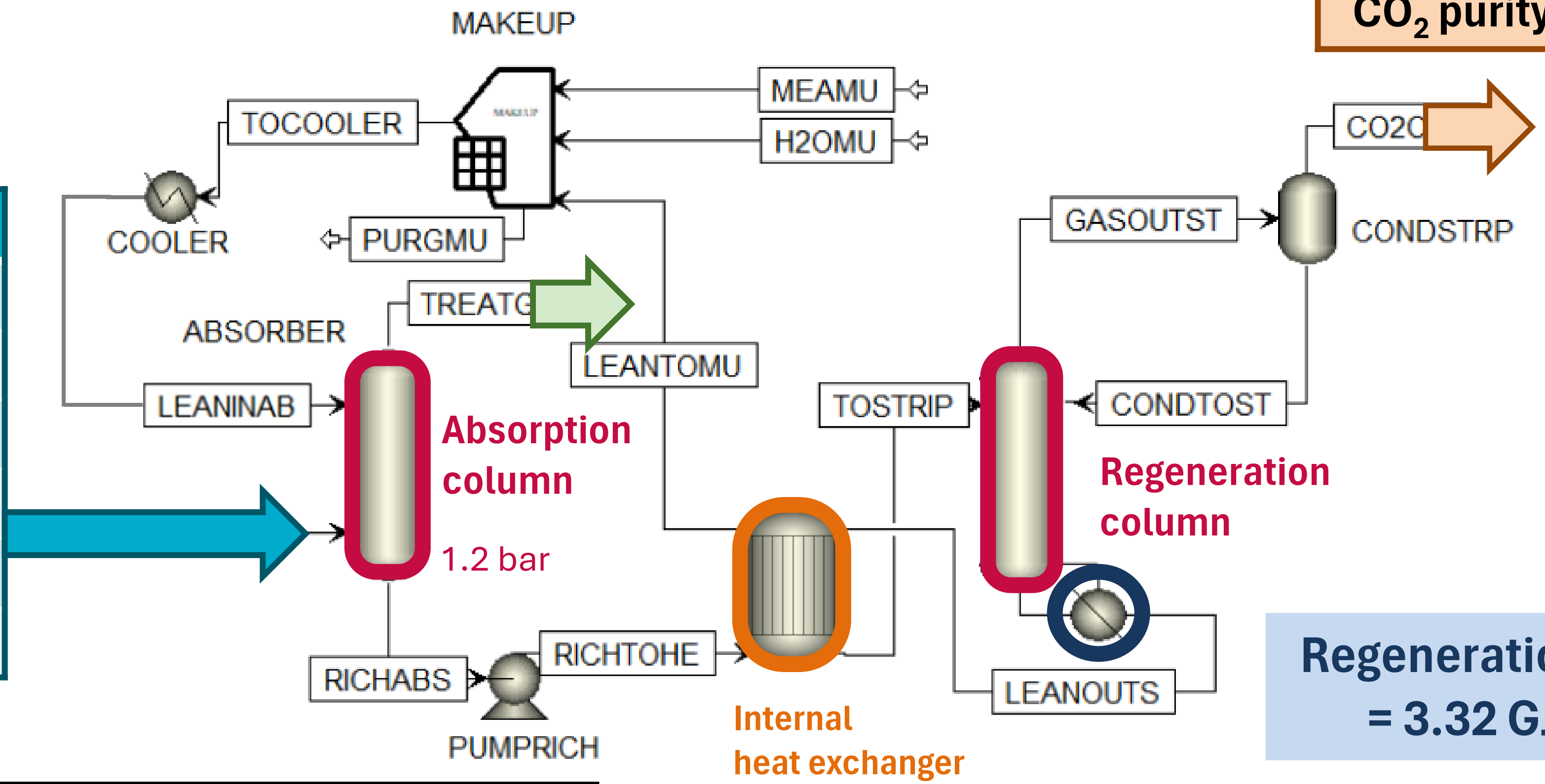
Absorption-Regeneration process modelling

MEA (30 wt.%)

Absorption rate	90%

CO_2 purity	98 mol.%

Flue gas from lime plant		
Flow		32 000 m^3/h
Temperature		50 °C
Molar fractions	CO_2	24%
	N_2	63%
	O_2	8%
	H_2O	5%



Regeneration energy = 3.32 GJ/tCO_2

Optimal L/G vol.: $6.8*10^{-3}$

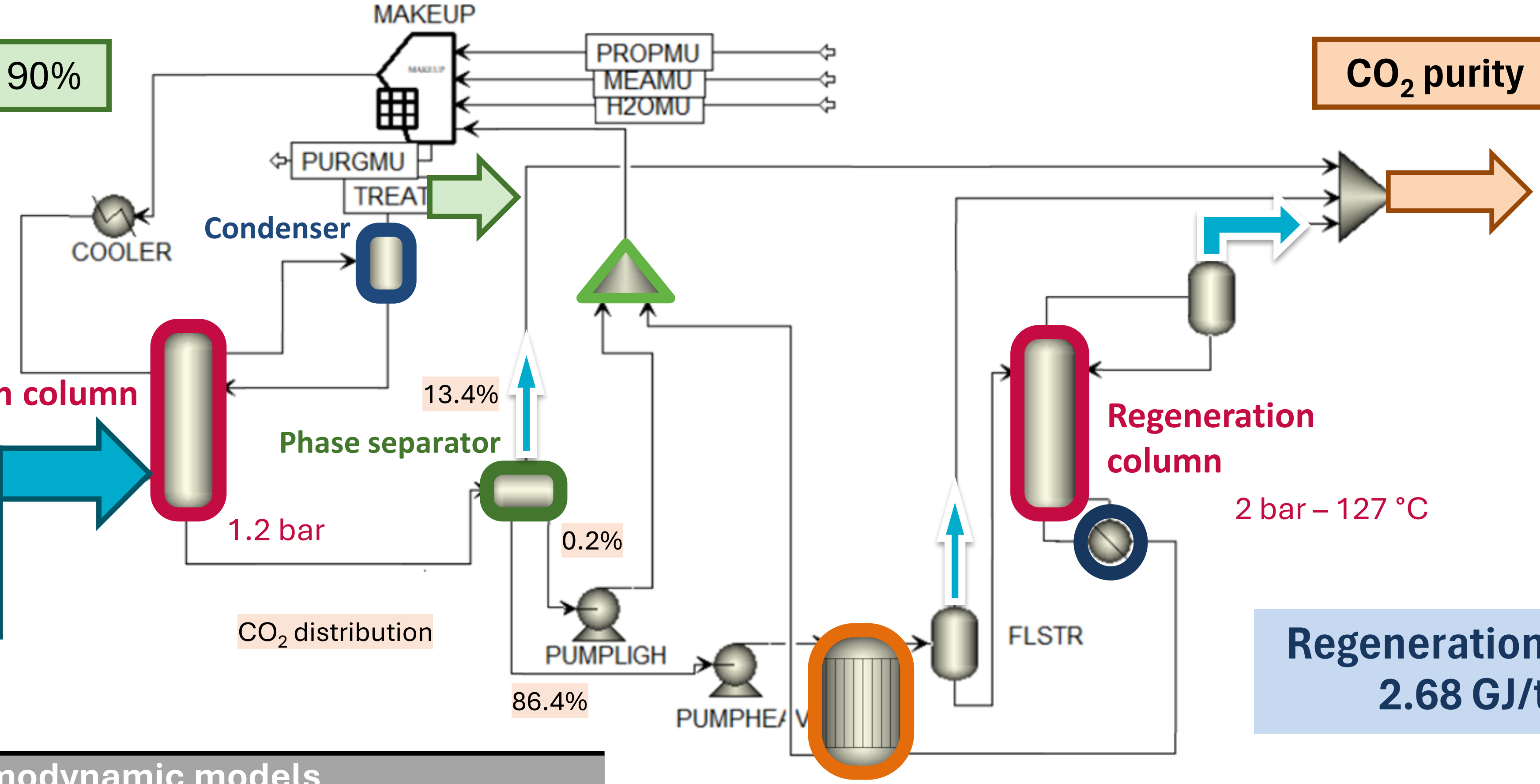
Thermodynamic models	
Gaseous phase	Redlich Kwong (RK)
Liquid phase	Electrlolyte Non-Random Two Liquid (eNRTL)

Absorption-Regeneration process modelling

MEA (30 wt.%) – PROP (40 wt.%)

Absorption rate	90%

CO_2 purity	98 mol.%



Flue gas	
Flow	32 000 m^3/h
CO_2	24%

Regeneration energy = 2.68 GJ/tCO_2

Optimal L/G vol.: $1.0*10^{-2}$

Thermodynamic models	
Gaseous phase	Redlich Kwong (RK)
Liquid phases	eNRTL (Phase separator: eNRTL-HG)

Conclusion

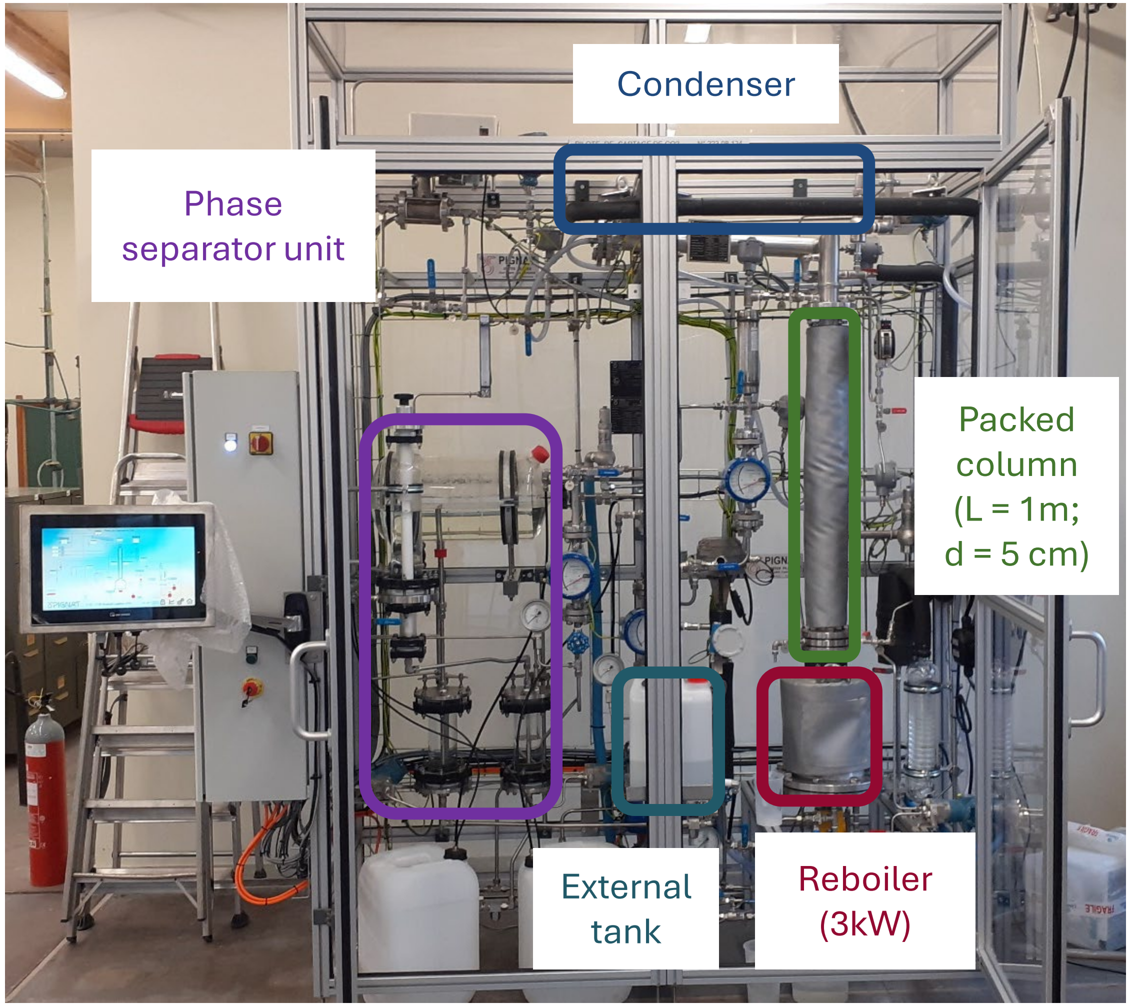
Aqueous-alcoholic MEA-based solution

- Same fast chemical reactions as for the MEA benchmark
- Propan-1-ol used as a demixing inducer
- Up to **97.9% of the CO_2 in the rich phase** (60% of the total volume)
- Challenge about the alcohol volatility (condenser / intercooling)
- <u>20%-reduction for regeneration energy</u> >< aqueous MEA (30 wt.%) solvent (despite higher liquid flow rate)

Perspectives

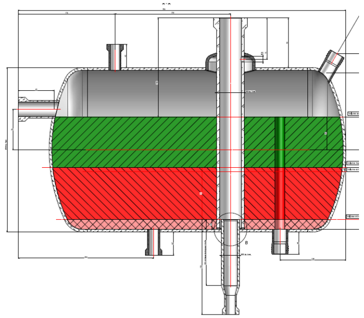
- Micro pilot Absorption-Regeneration unit tests + simulations

Micro pilot Absorption-Regeneration unit



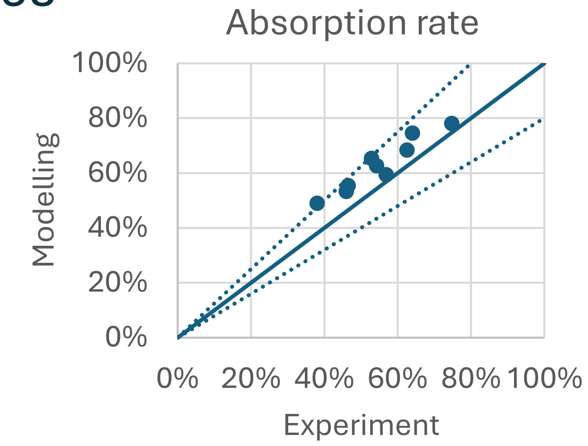
Multiple possibilities of use

- <u>Two modes</u>
  - ✓ Absorption
    - Continuous tests
    - Semi-continuous tests
  - ✓ Regeneration
- Regeneration under **pressure** (up tu 3 barg)
- Use of **demixing** solvents (with phase separator unit)



Objectives

- **AspenPlus model validation**
  - ✓ experimental vs modelling on AspenPlus at this scale
    - First promising results with aq. MEA (30 wt.%)



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Perspectives

- Micro pilot Absorption-Regeneration unit tests + simulations
- Other aqueous-alcoholic solvents

Thank you very much for your attention

Any QUESTIONS?

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