PCCC-8

Development of a new CESAR1 carbon capture model across various scales and CO_2 contents

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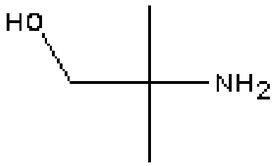
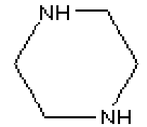
NKL Project

Wallonie Relance

CESAR1 is the new benchmark amine solvent

Aq. 27 wt.% 2-amino-2-methyl-1-propanol (AMP) + 13 wt.% piperazine (PZ)





Developed in the CESAR European funded-project

20-25% less energy consumption than MEA

Potential higher stability against thermal and oxidative degradation

Deploying CESAR1 systems requires robust models

Predicting performance for industrial applications

Design, optimisation and scale-up of CESAR1 plants

High-fidelity CESAR1 models are required in commercial softwares (Aspen Plus,…)

Limited information in the literature regarding comprehensive modelling of CESAR1

Objective

Develop and validate a comprehensive and robust CESAR1 model in Aspen Plus to predict performance for various industrial applications

Robust model over a wide range of operating conditions (inlet CO_2 fraction, regeneration pressure)

Pilot plant scale validation: TCM Mongstad unit

Simulations at varying inlet CO_2 contents (from 4 to 20 vol.%)

Outline

Development of the model

Validation of the model

Application to industrial cases

Conclusions

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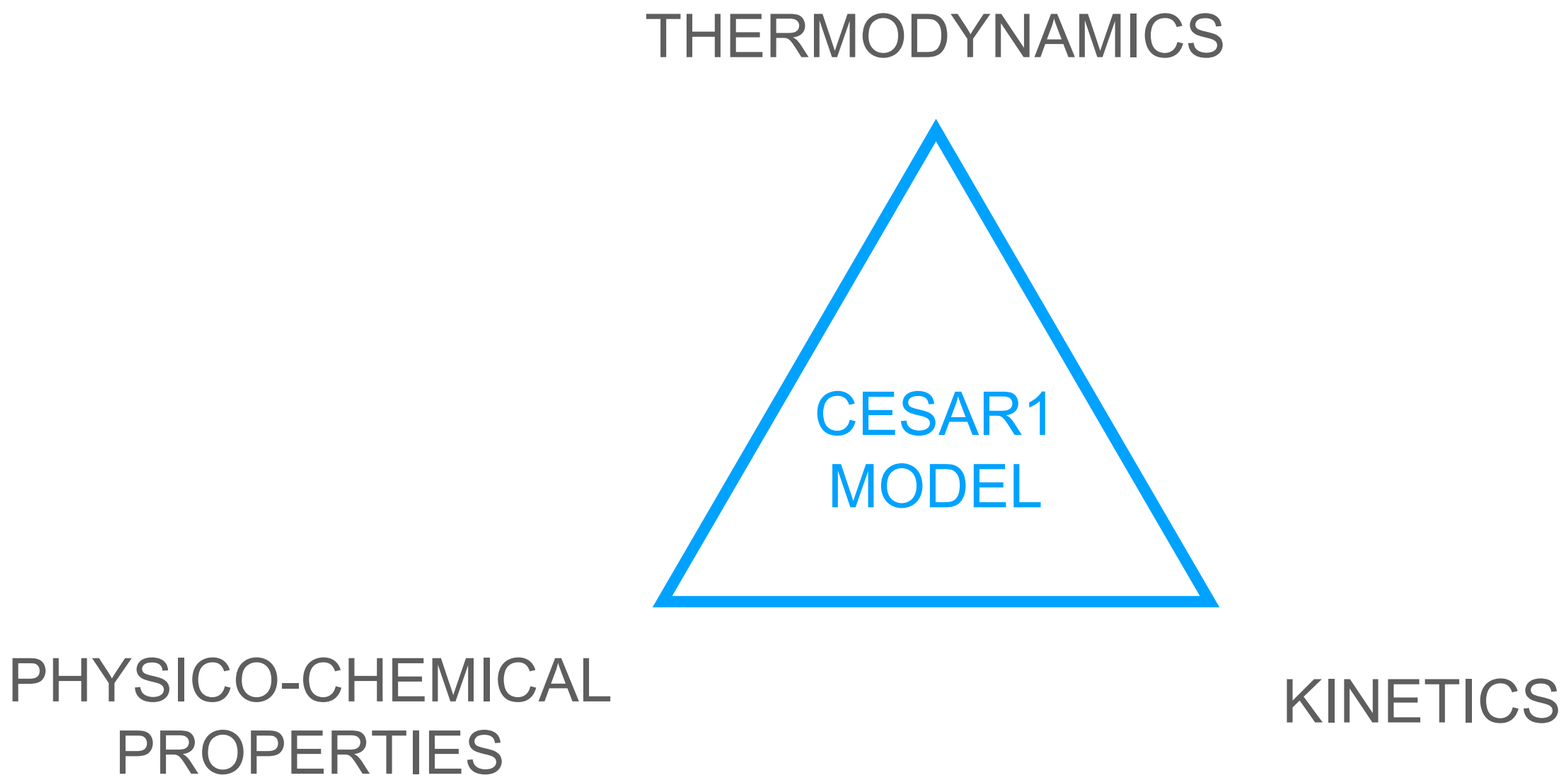
A robust model requires accurate sub-models



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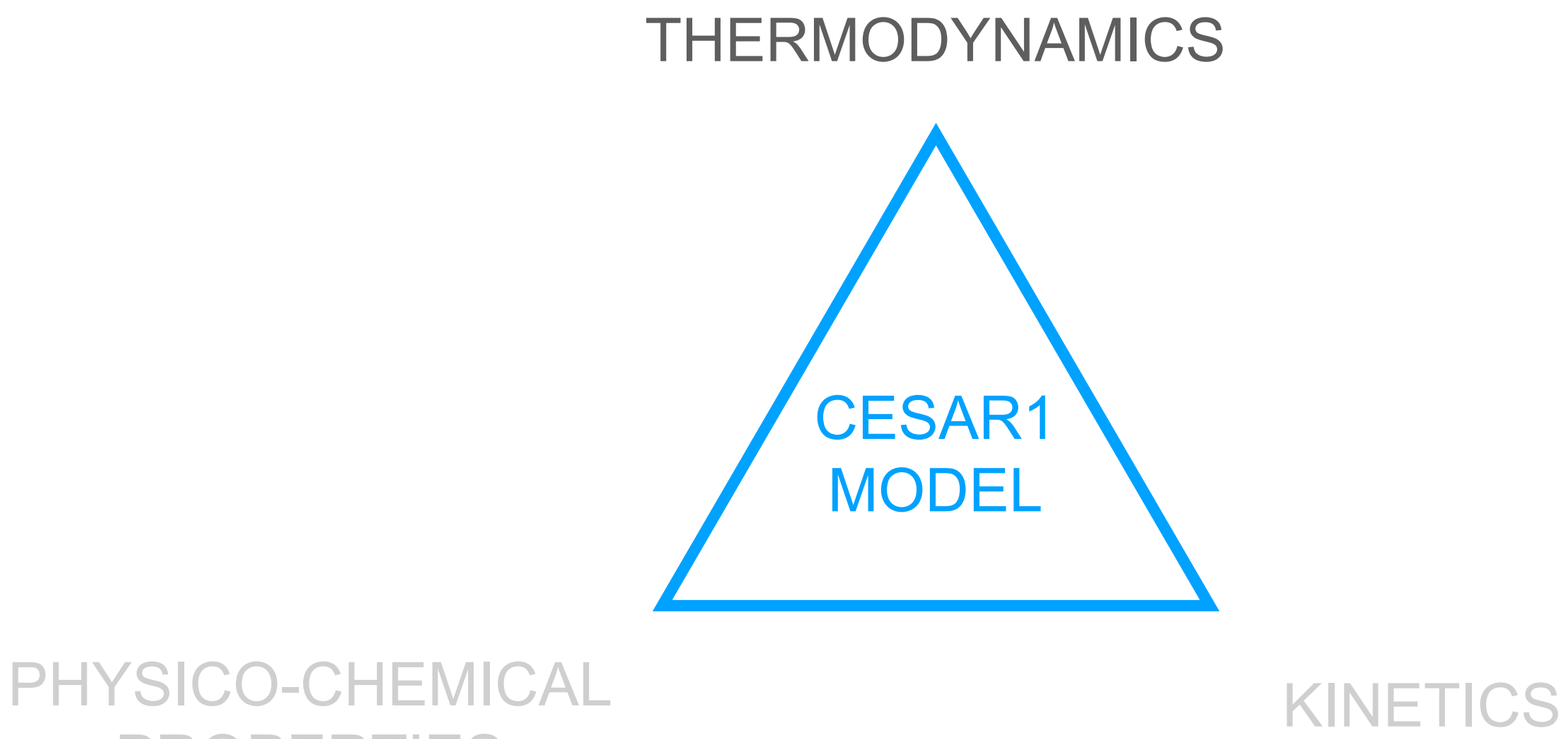

An open-access consistent Aspen Plus thermodynamic model is available in litterature

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

Open access, thermodynamically consistent, electrolyte NRTL model for piperazine, AMP, water, CO_2 systems on Aspen Plus

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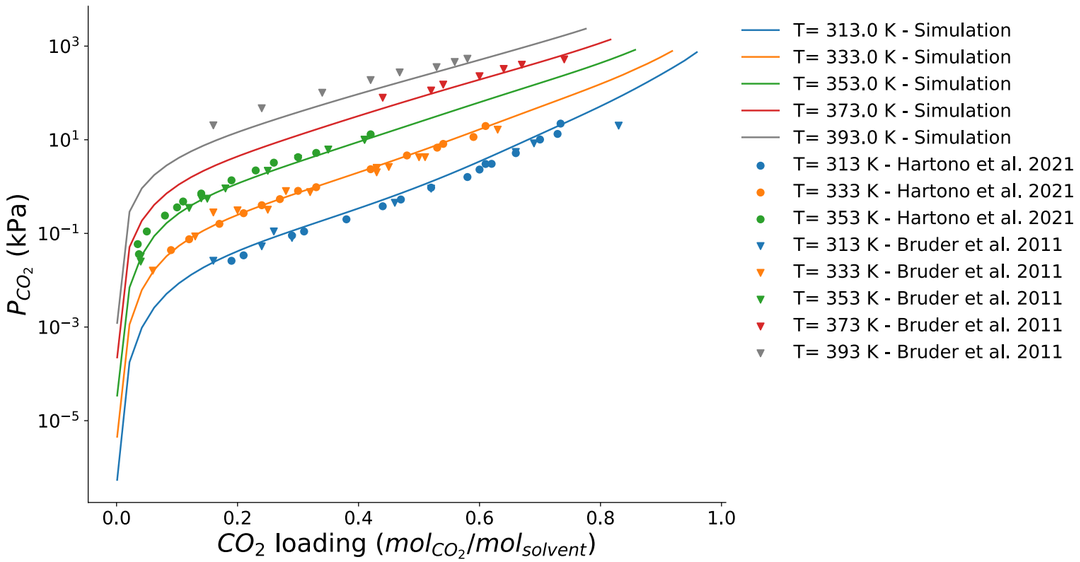
[a] Qingshanhu Energy Research Center, Zhejiang University, Hangzhou 310027, China
[b] Research Centre for Carbon Solutions, School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh, United Kingdom



ELECNRTL for liquid electrolyte

Redlich-Kwong-Soave for vapor phase

Sequential regression of model parameters using VLE and calorimetry data

Validated on a wide range of conditions:

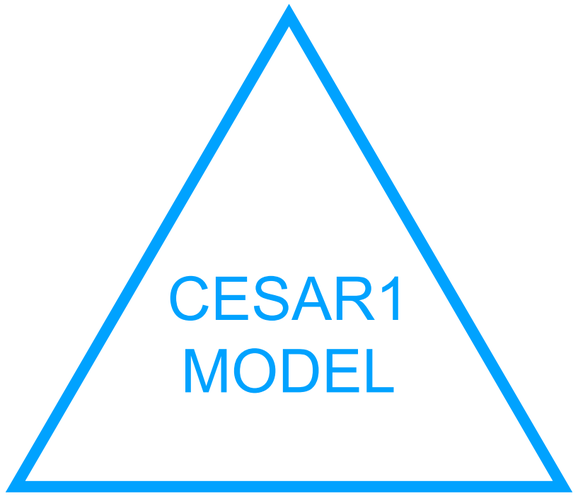
- **AMP**: 0-35.7 wt.% / **PZ**: 0–32.8 wt.%
- **Temperature**: 20-160°C
- **CO_2 loading**: 0.04 – 1.07 mol_{CO2}/mol_{amines}

AARD = 22.3% for VLE

AARD = 6.3% for heat of CO_2 absorption

A robust model requires accurate sub-models

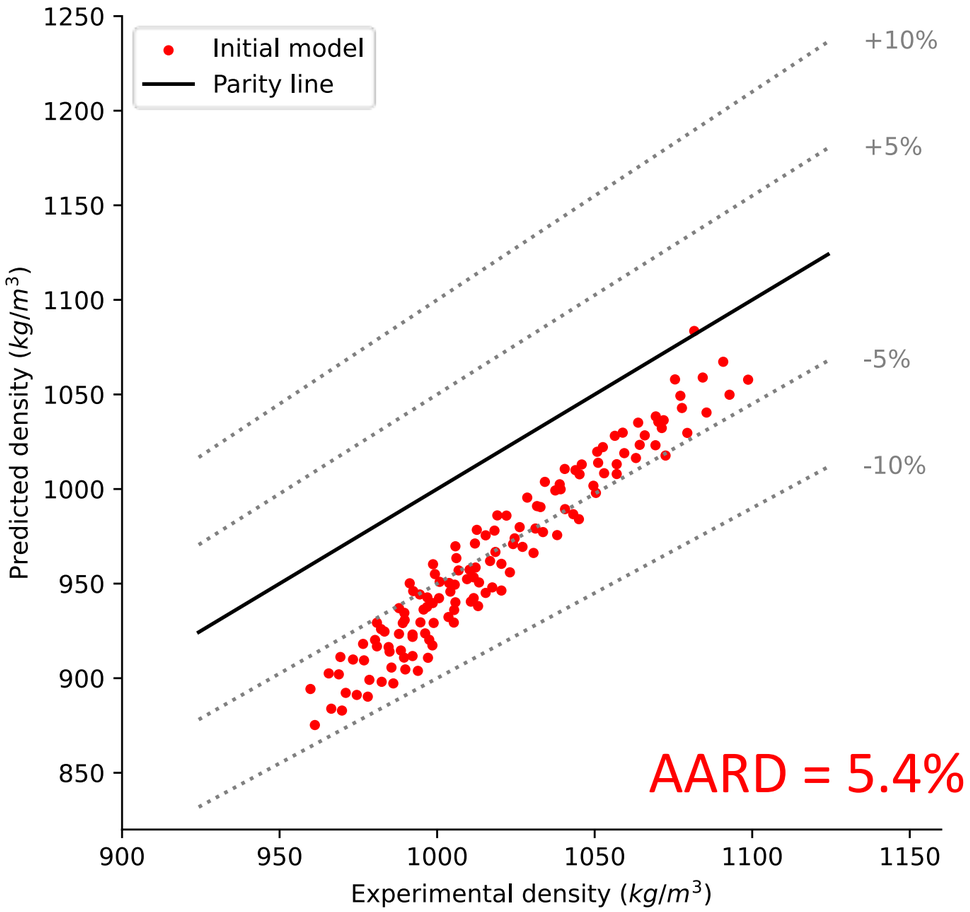
THERMODYNAMICS



PHYSICO-CHEMICAL
PROPERTIES

KINETICS

Initial density model with default parameters slightly underestimates predictions

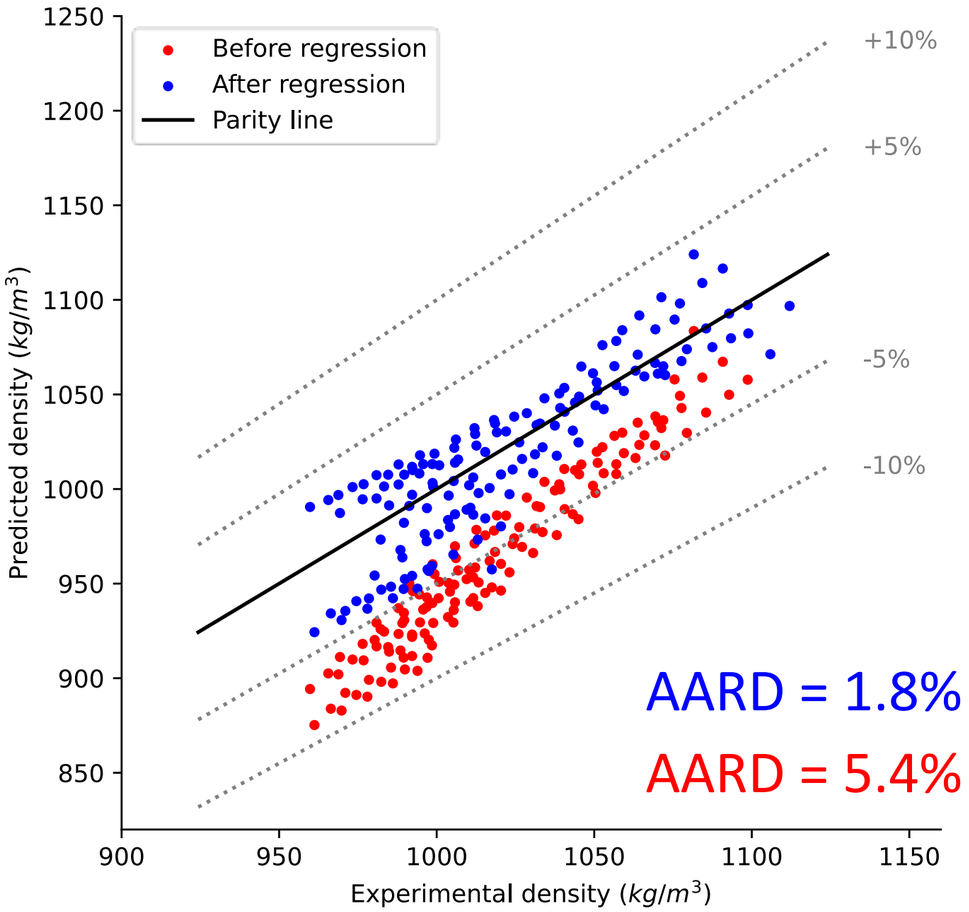


Clarke model: $V_{sol} = V_m + V_{el}$

Rackett equation — Redlich and Meyer

Missing parameters related to PZ and AMP ions (default values)

Regressing ions related parameters allows to improve density prediction



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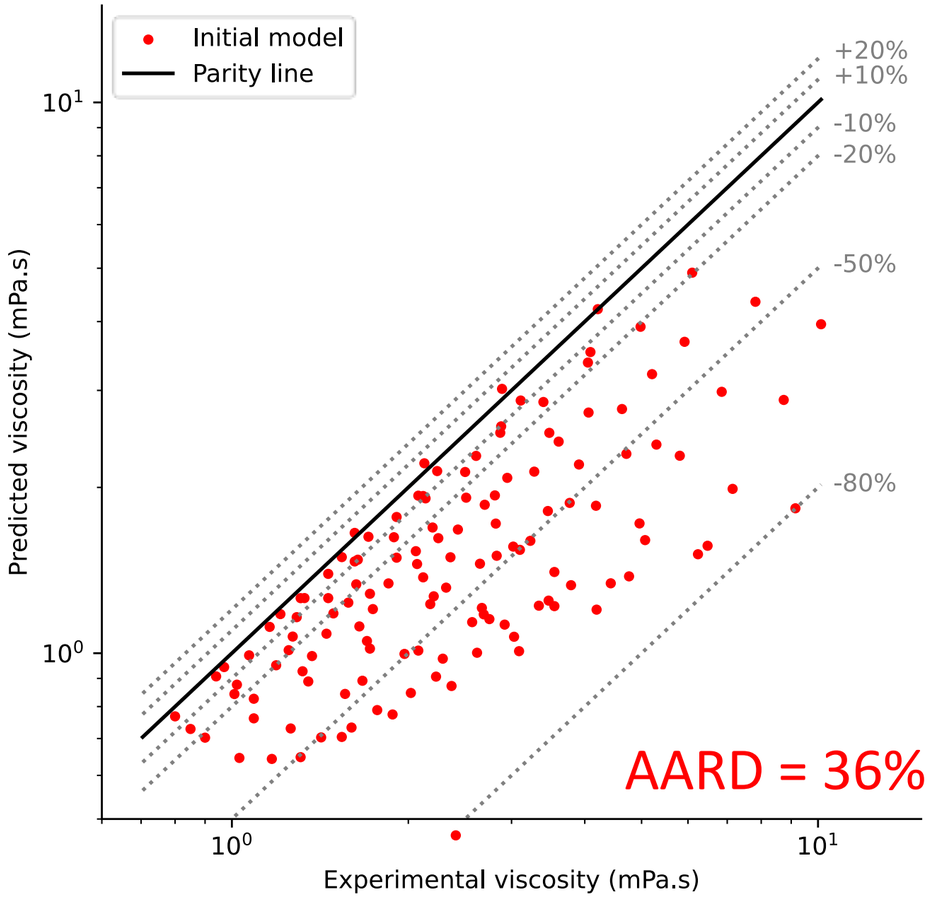
Regression of the missing parameters with density data of *Morlando et al.*

AMP: 17.8-35.5 wt.% / **PZ**: 8.6–12.9 wt.%
Temperature: 20-80°C
CO_2 loading: 0 – 0.86 mol_{CO2}/mol_{amines}

Initial viscosity model with default parameters performs poorly



Jones-Dole model:

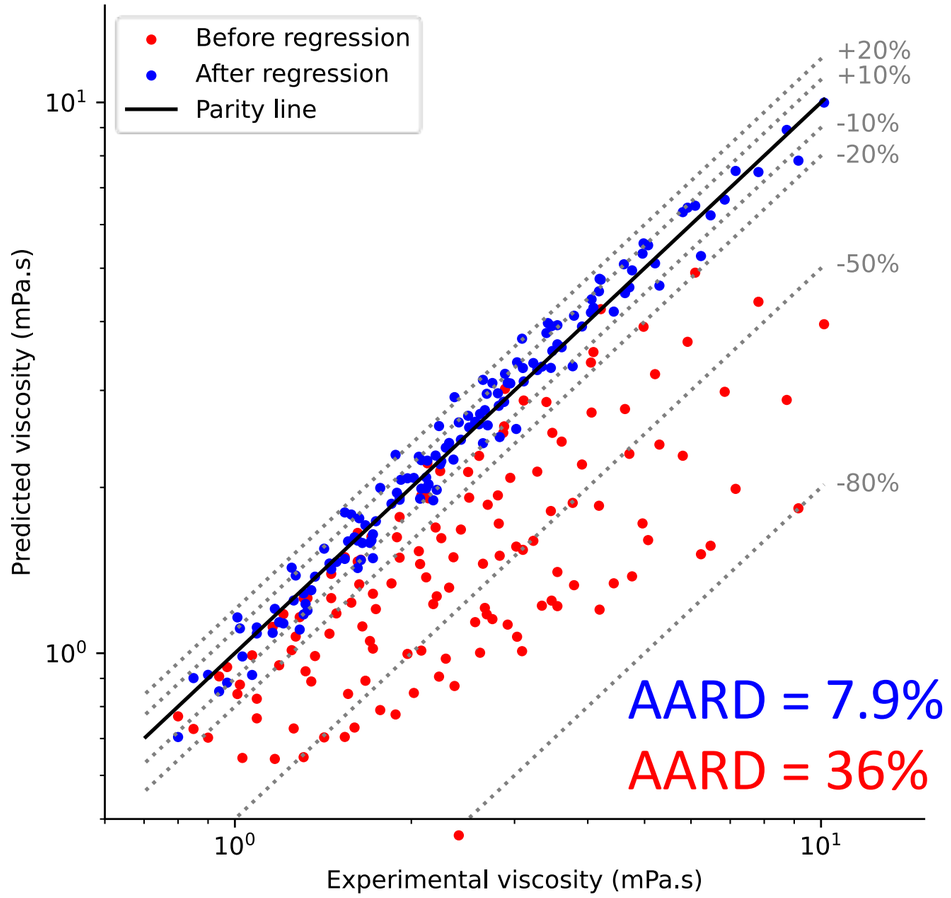
$$\eta_{sol} = \eta_m \left(1 + \sum_{ca} \Delta\eta_{ca}\right)$$

Aspen Liquid Mixture Vicosity model

Jones-Dole correction

Missing AMP interaction and AMP ions parameters (default values)

AMP-related parameters regression leads to significantly improved viscosity prediction



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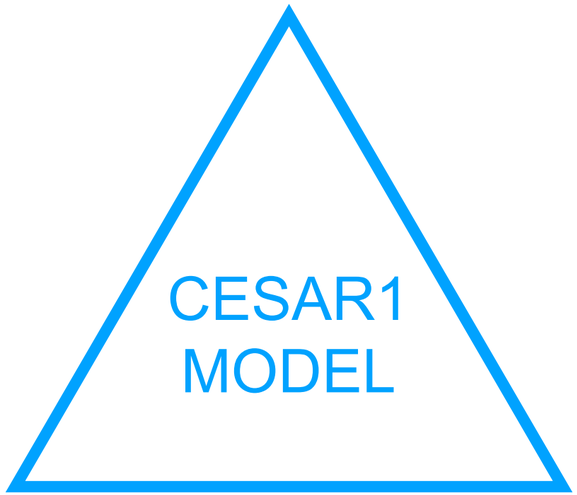
THERMODYNAMICS

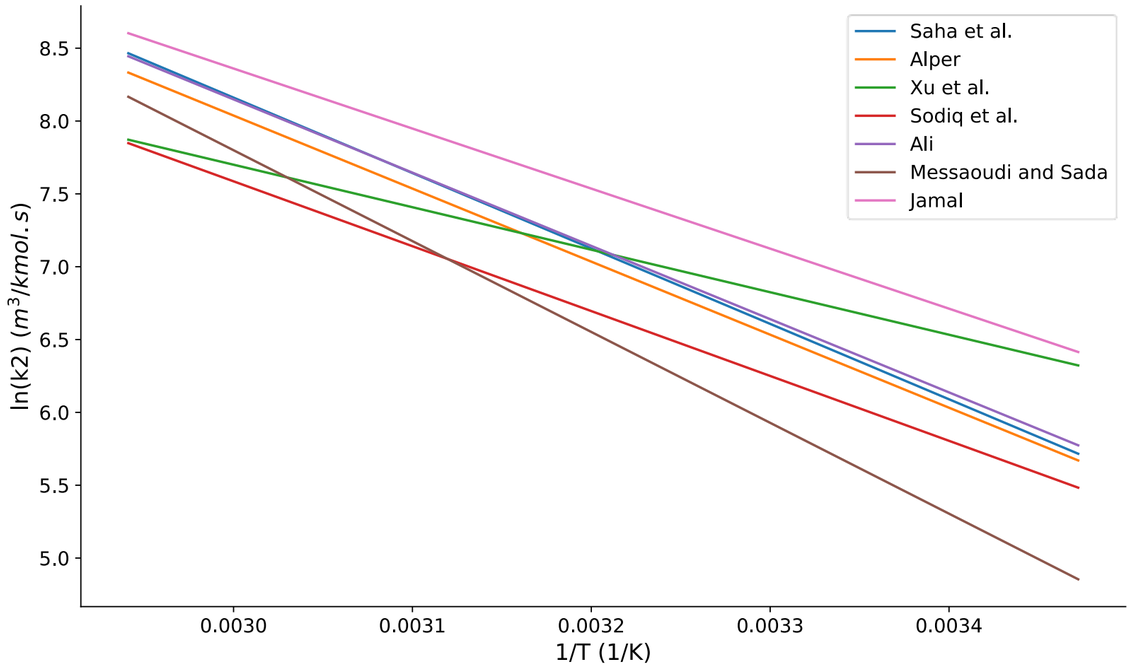


PHYSICO-CHEMICAL PROPERTIES

KINETICS

Significant differences exist among kinetics laws for AMP-CO_2 reaction in litterature

	REACTIONS	Kinetic laws
1)	CO2 + OH- --> HCO3-	
2)	HCO3- --> CO2 + OH-	
3)	PZ + CO2 + H2O --> PZCOO- + H3O+	
4)	PZCOO- + H3O+ --> PZ + CO2 + H2O	
5)	PZCOO- + H2O + CO2 --> PZCOO-2 + H3O+	
6)	PZCOO-2 + H3O+ --> PZCOO- + H2O + CO2	
7)	AMP + CO2 + H2O --> HCO3- + AMPH+	



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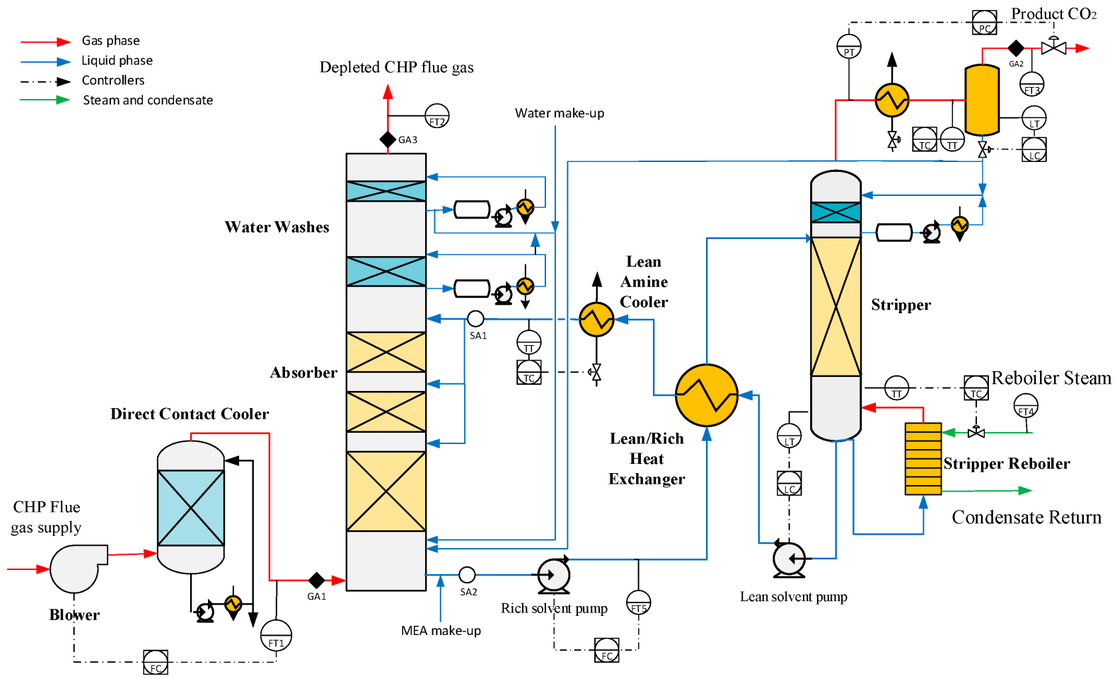
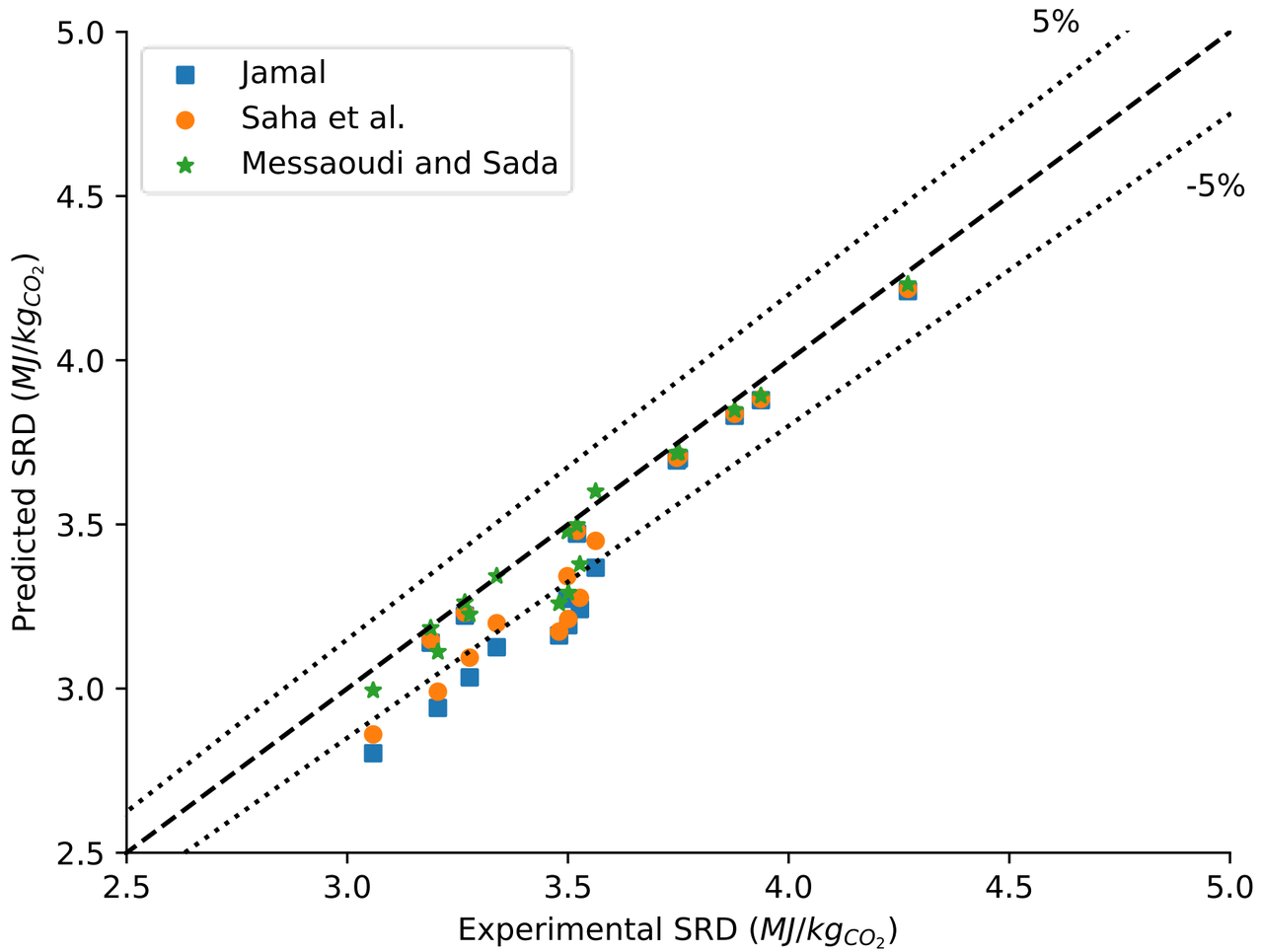
The amine plant unit at TCM Mongstad has been modelled in Aspen Plus



Absorber height	24 m
Stripper height	8 m
Absorber diameter	Rectangular 3.55*2 m
Stripper diameter	1.3 m
Packing type	Koch FLEXIPAC 2X
Stripper pressure	1.9 bar
CO_2 content in gas	3.4 vol.%
Gas flow rate	50000 l/h
Solvent composition	27 wt.% AMP - 13 wt.% PZ
Capture rate	90-98%
L/G (kg/Sm^3)	0.6-1.2

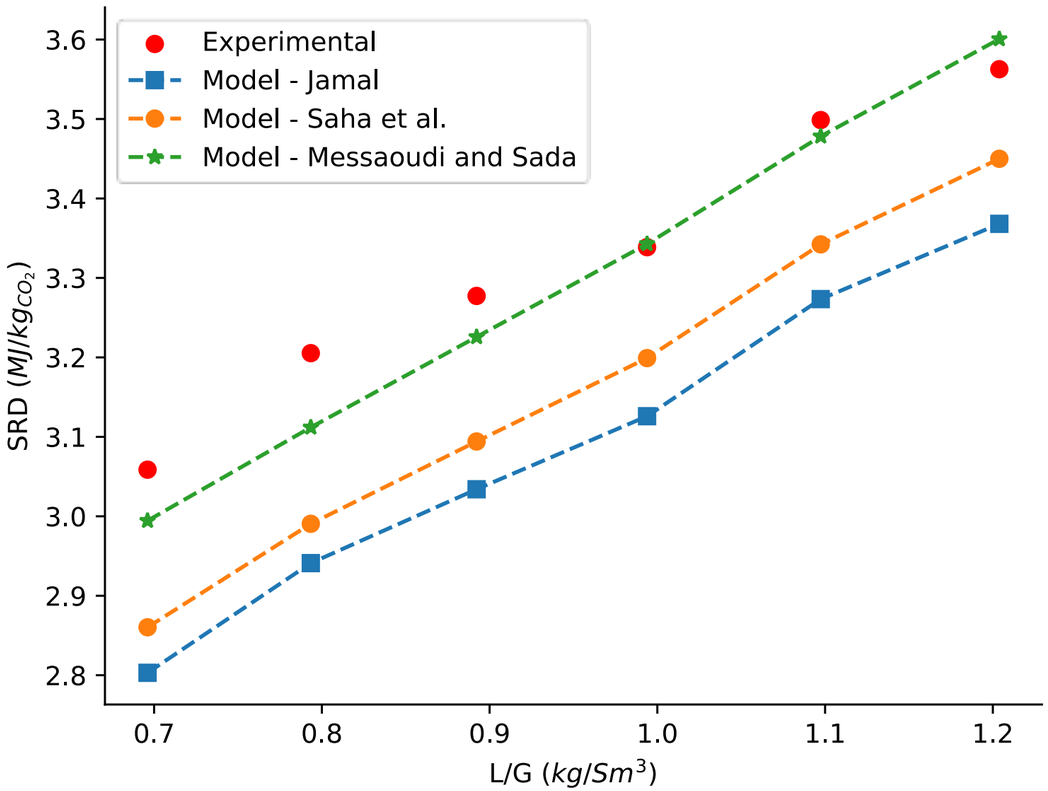
The CESAR1 model matches TCM Mongstad unit performance

Kinetic law AMP-CO_2	AARD (%)
Jamal	4.62
Saha et al.	3.88
Messaoudi and Sada	2.08

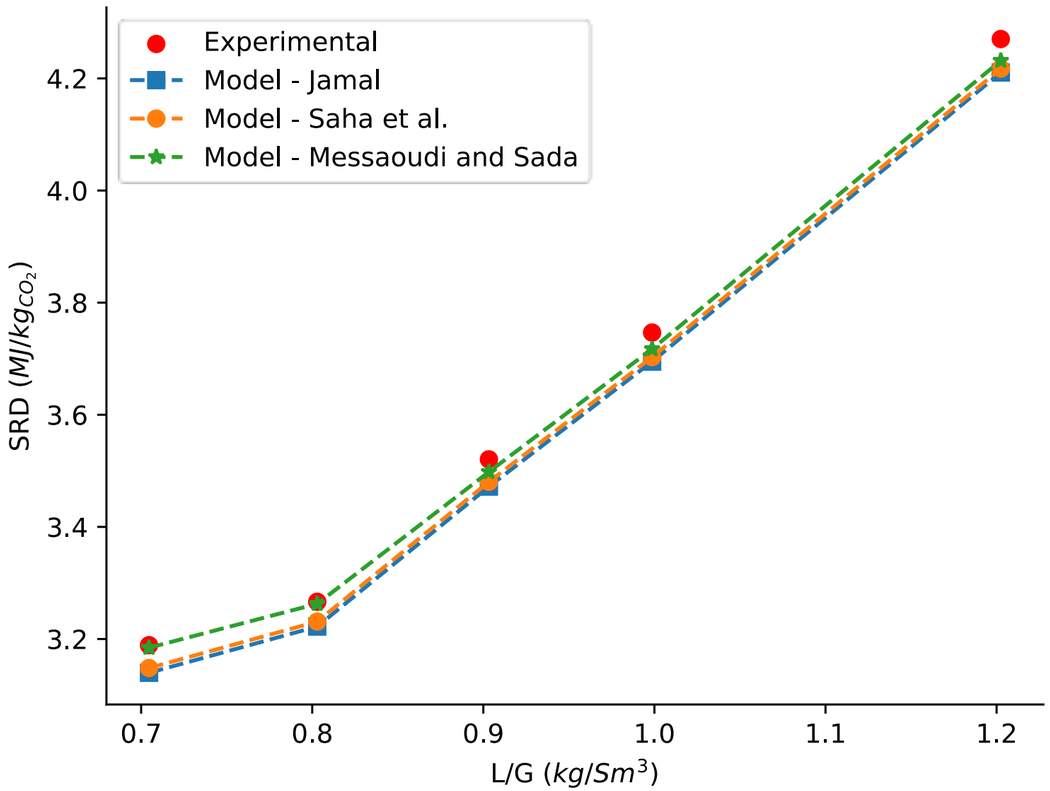


Messaoudi and Sada kinetic law best fits experimental data

capture rate ≈ 90%



capture rate ≈ 98%



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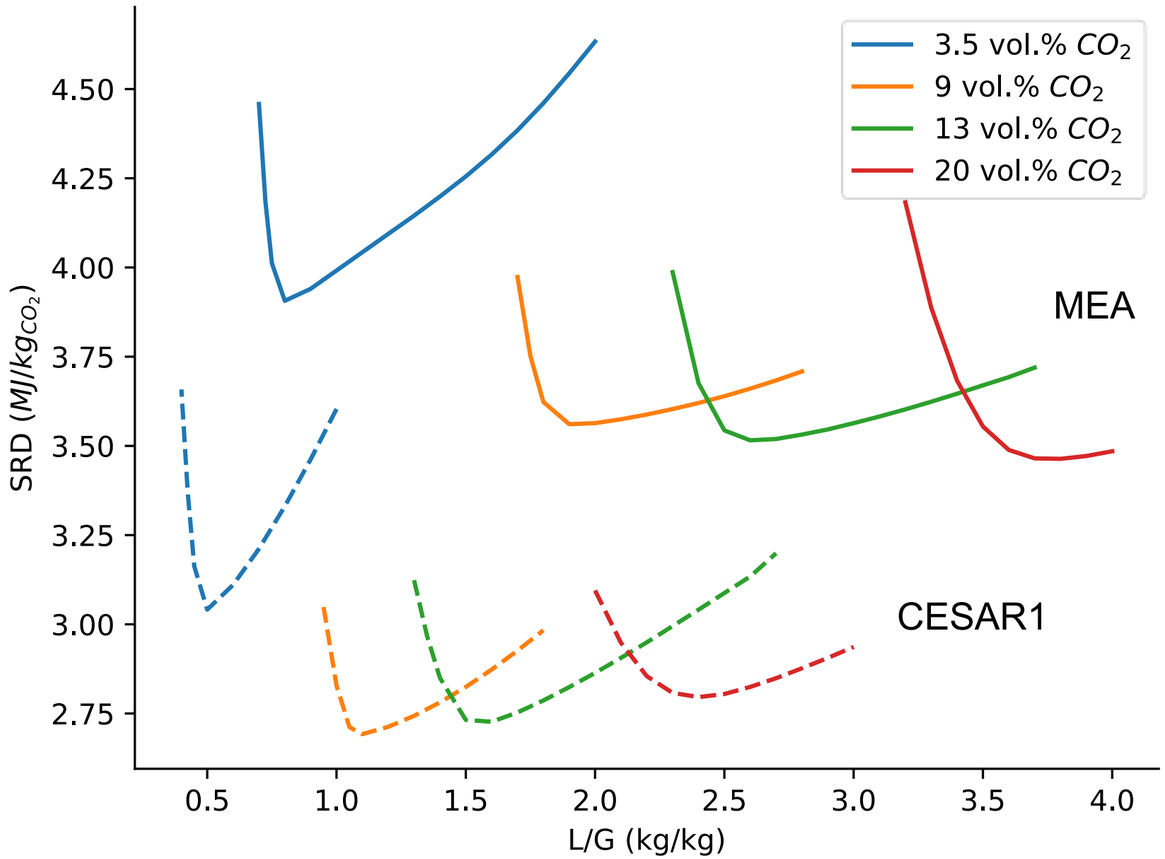
The model predicts a reduction in reboiler duty of 22% using CESAR1 instead of MEA

TCM Mongstad unit

90% capture rate

22% reduction in SRD with CESAR1

Results consistent with literature



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Development of a robust CESAR1 model in Aspen Plus

- Extension of the CESAR1 thermodynamic model of Yi et al.
- Accurate modelling of density and viscosity properties
- Study of the impact of the kinetic laws for AMP-CO_2 reaction

Validation of the model with TCM Mongstad unit data (AARD=2%)

Simulations with variable inlet CO_2 contents, providing performance prediction with CESAR1 compared to MEA (22% SRD reduction)

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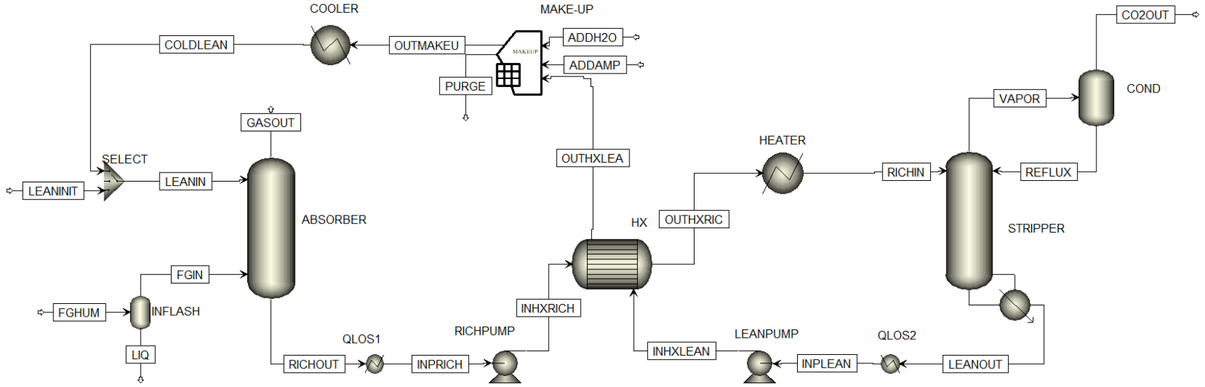
The UMONS lab-scale unit has been modelled in Aspen Plus

UMONS lab-scale unit

Aspen Plus model



Absorber height	1 m
Stripper height	0.5 m
Columns diameter	0.06 m
Packing type	Glass Raschig Ring (6*6 mm)
Pressure	1 atm

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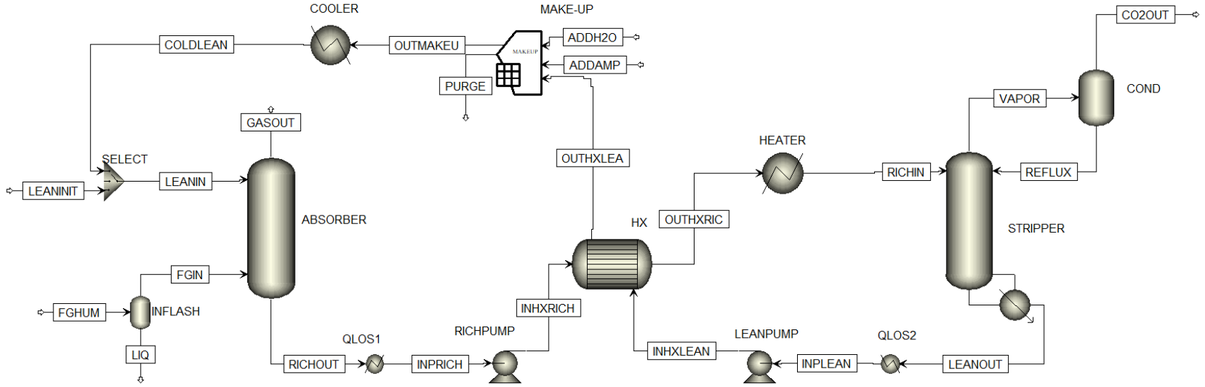
UMONS lab-scale unit

Aspen Plus model



Absorber height	1 m
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Pressure	1 atm

Good agreement with lab-scale data, but validation remains limited

Inlet gas:

$$\dot{V} = 2701\ l/h$$

$$y_{CO_2} = 20\ vol.\%$$
$$(dry\ basis)$$