ETH zürich

Optimal Process design of MDEA CO_2 Capture Plant for Low-Carbon Hydrogen Production

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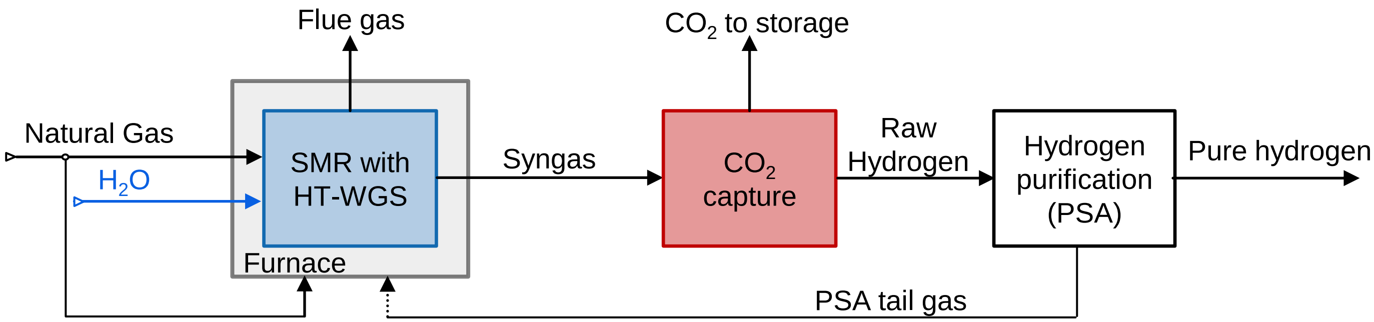
Hydrogen production with CCS

- ELEGANCY Enabling a Low-Carbon Economy via Hydrogen and CCS

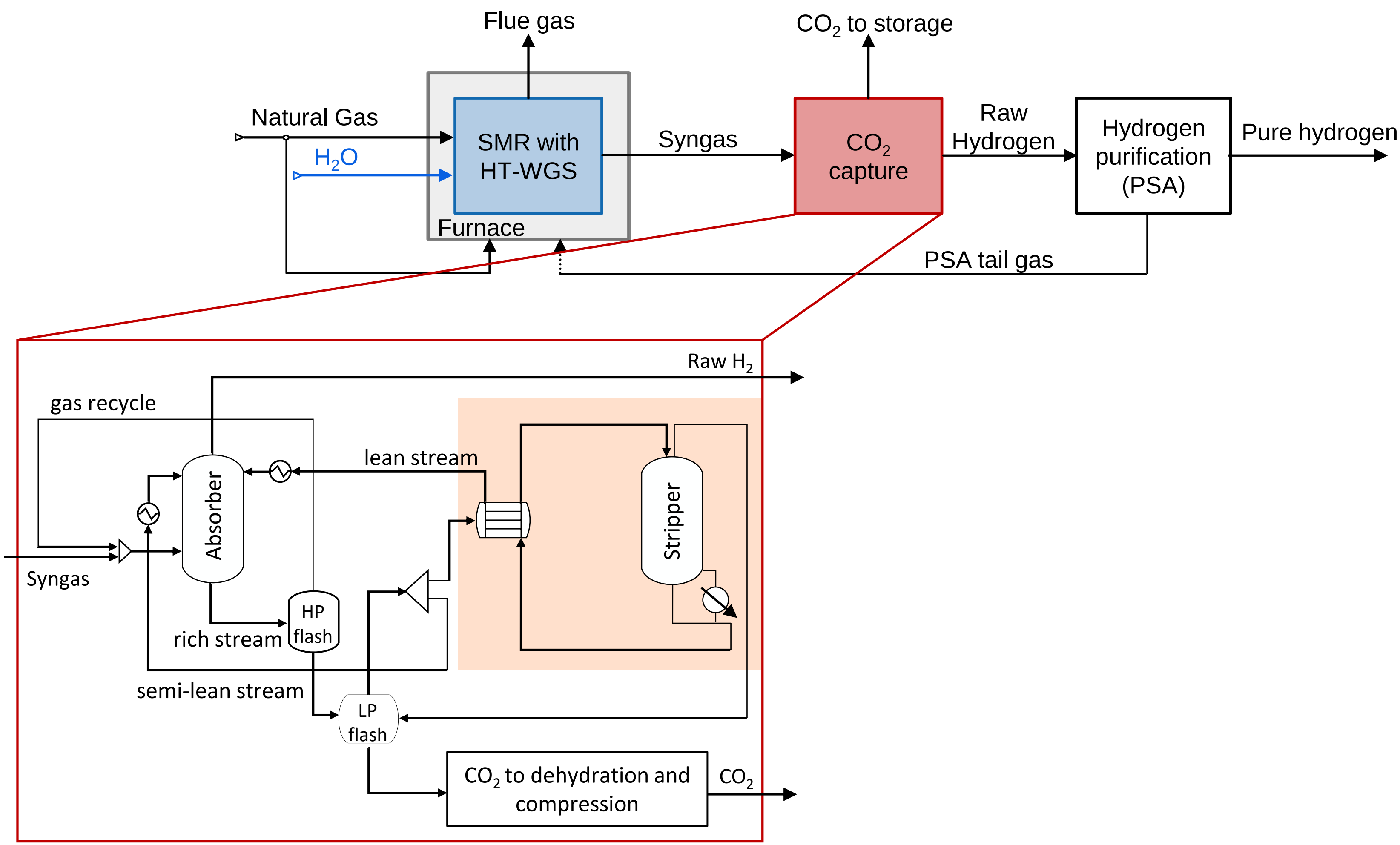
- State-of-the-art low carbon H_2 production
  - → Steam Methane Reforming with pre-combustion carbon capture (solvent: Methyl diethanolamine, MDEA)

- Goals
  - → developing a methodology to optimize H_2 production with CCS
  - → testing on a case study with existing technologies
  - → applying this methodology to new technologies (e.g. Vacuum Pressure Swing Adsorption)

Low-Carbon Hydrogen Production

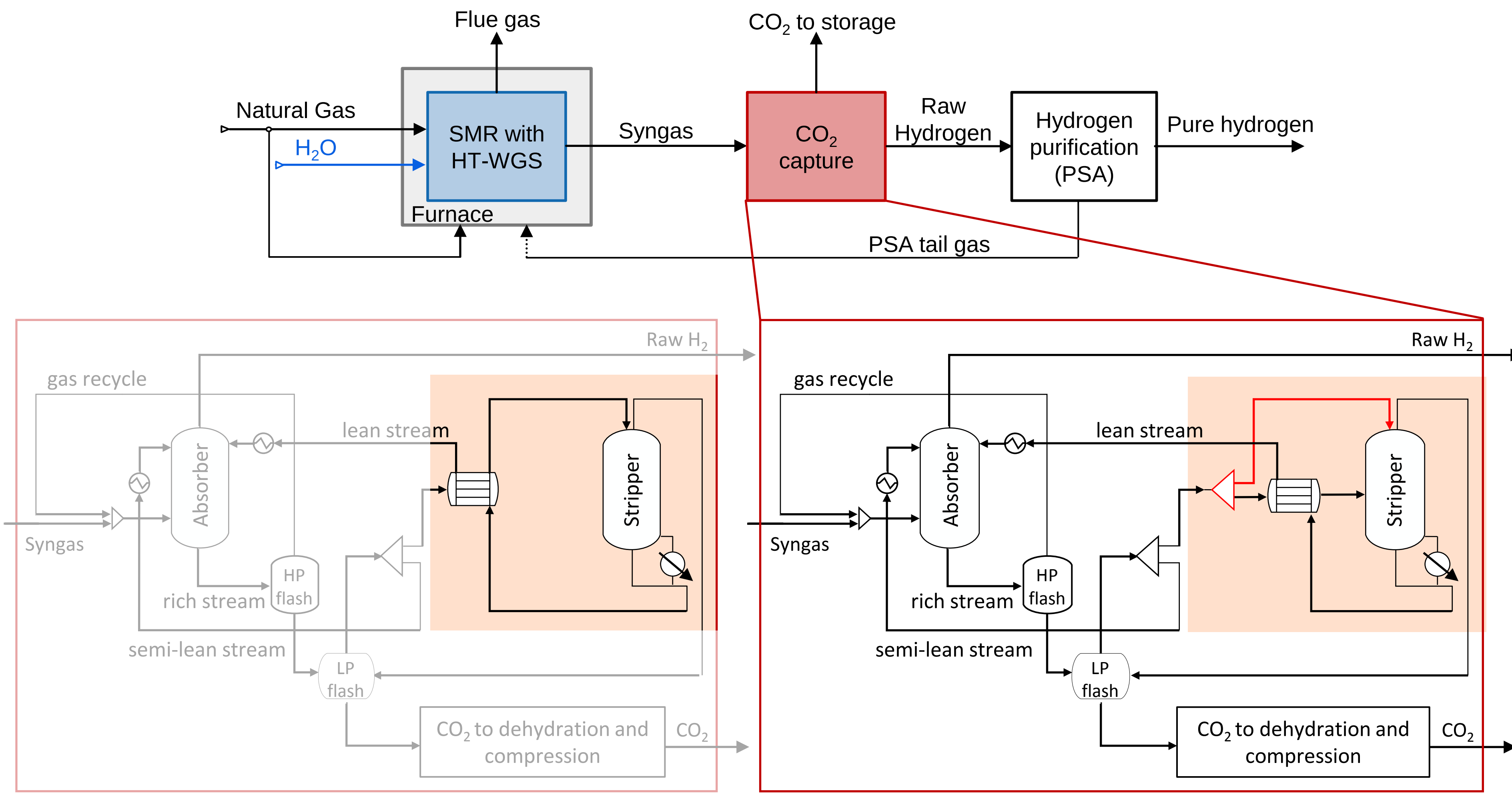


MDEA capture process: benchmark



[1] Romano, M. C., Chiesa, P., & Lozza, G. (2010). Pre-combustion CO2 capture from natural gas power plants, with ATR and MDEA processes. *International Journal of Greenhouse Gas Control*, *4*(5), 785-797.

This study: advanced MDEA process configuration



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MDEA process simulation

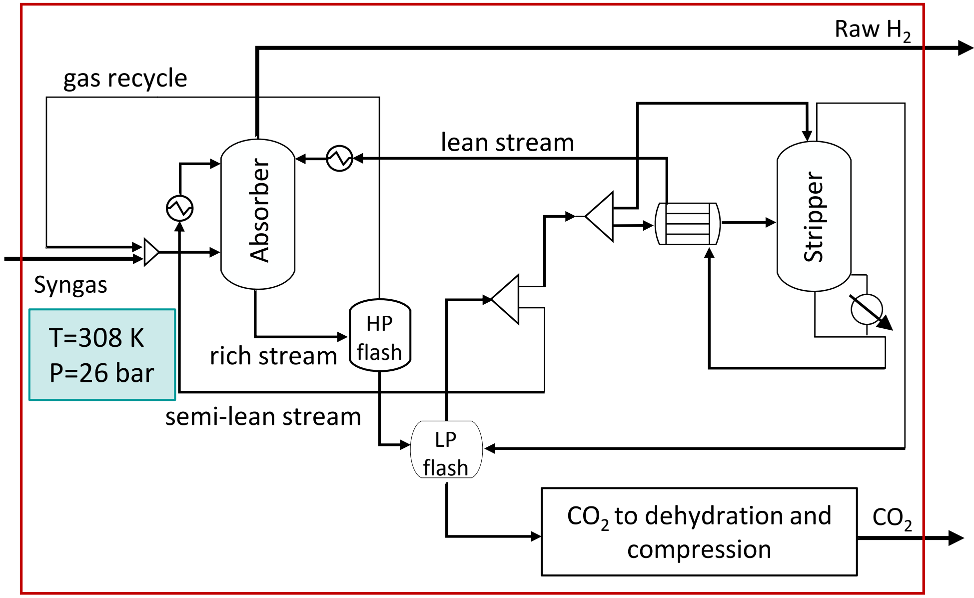
- The process is simulated in Aspen Plus®
  - RadFrac model with equilibrium stage calculations used for the columns

- The liquid phase is described by the Electrolyte NRTL model, while for the vapour phase Redlich-Kwong equation of state is used.

  → for CO_2 compression the Peng-Robinson equation of state is selected

Mole flow [kmol/hr]	Syngas	Raw H_2	Pure CO_2
H_2	4985	4985	0.0003
CO_2	1070	107	963
CO	304	304	ppm
CH_4	200	200	ppm
N_2	13	13	ppm
Total flow [kmol/hr]	6572	5609	963
Purity		**88.8%**	**99.9%**

CO_2 capture rate: 90%



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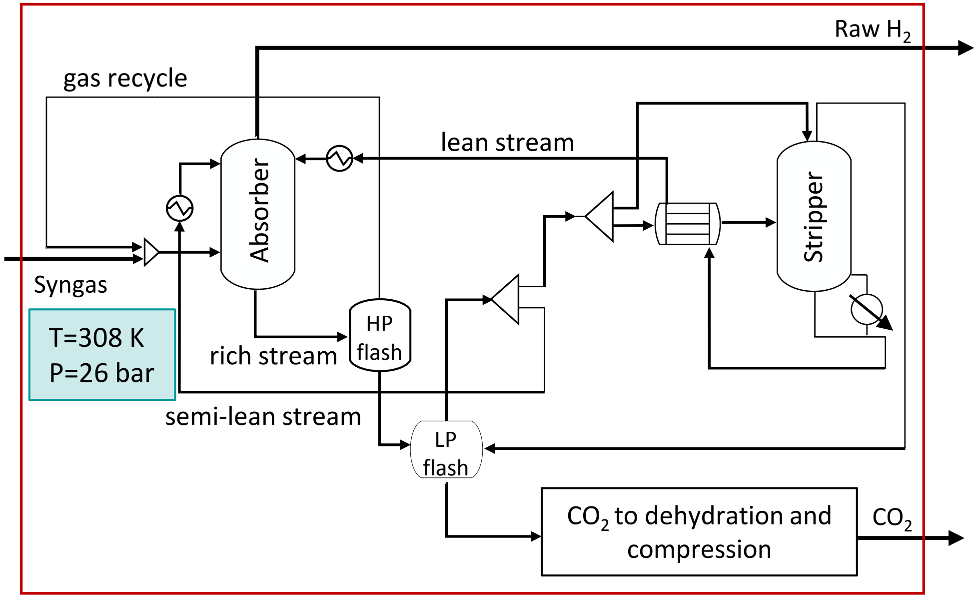
H_2	4985	4985	0.0003
CO_2	1070	32	1038
CO	304	304	ppm
CH_4	200	200	ppm
N_2	13	13	ppm
Total flow [kmol/hr]	6572	5534	1038
Purity		**89.9%**	**99.9%**

CO_2 capture rate: 97%



Description of the optimization problem

- Multi-objective optimization problem
- To minimize the total specific exergy *w* while maximizing the capture rate *Ψ*: $\min \left[w, \frac{1}{\Psi} \right]$

$$w = \frac{W_{tot}}{\dot{m}_{CO_2 \text{ captured}}} \qquad W_{tot} = \eta_P \sum_i W_{pump_i} + \eta_C \sum_j W_{compr_j} + Q_R \left(1 - \frac{T_{amb}}{T_{reb} + \Delta T_{min}} \right)$$

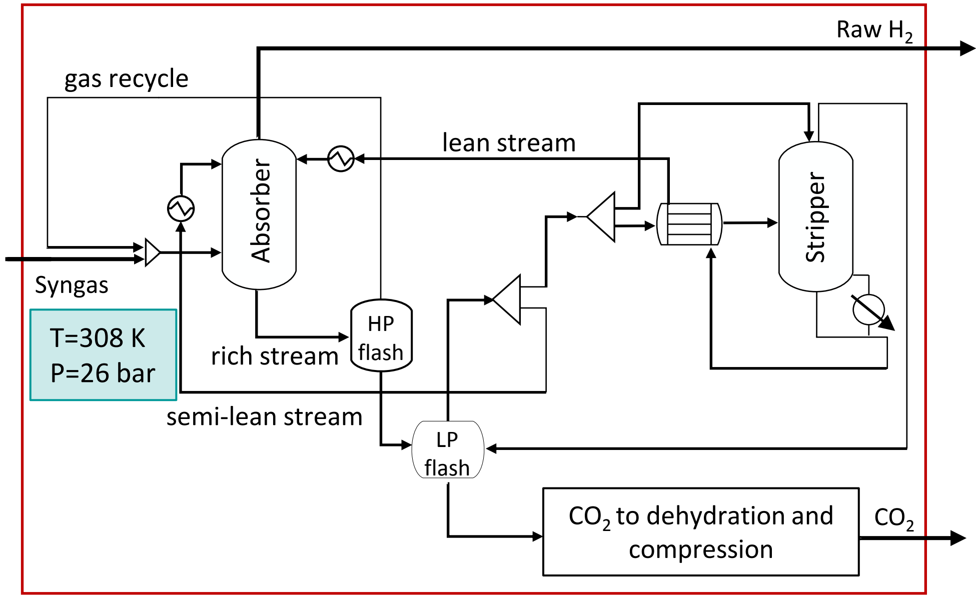
$T_{amb} = 282$ K, $\Delta T_{min} = 10$ K

- All process variables, such as flowrates and column conditions, could be tuned to optimize the process

  → time demanding

- Faster systematic approach

  → define the Key Process Variables, which will then become the decision variables in the optimization problem



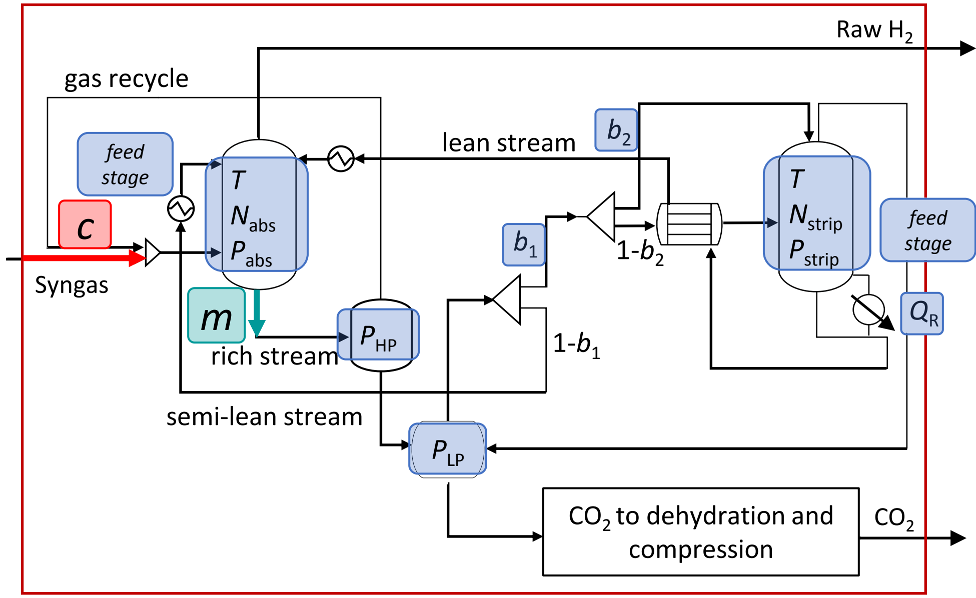
Process variables

- Pressure and temperature of the units
- Size of the columns
- Split fractions
- Reboiler duty and feed stages
- Liquid to gas mass flow ratio (*L*/*G*)

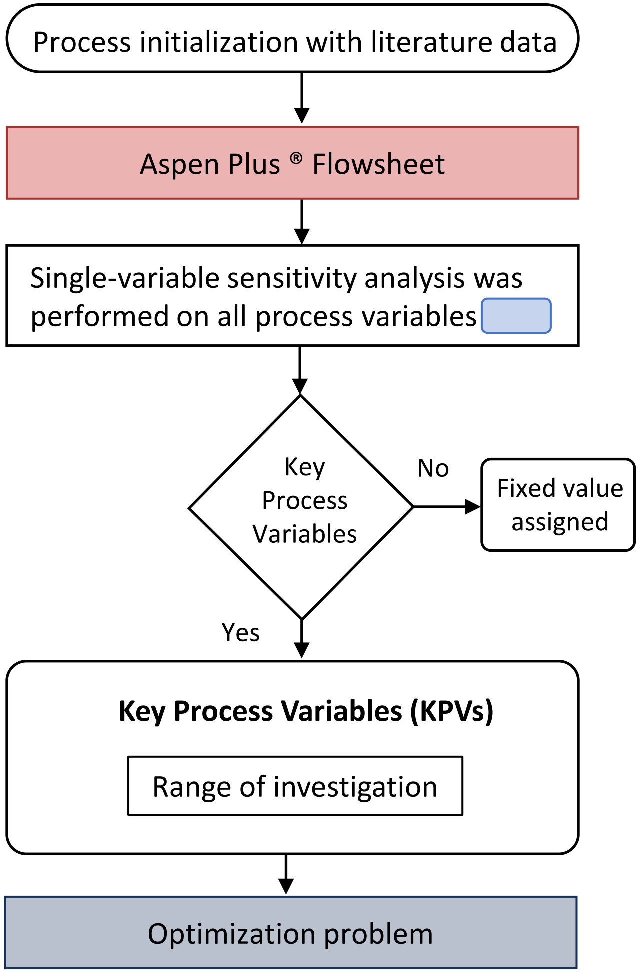
  → CO_2 to MDEA molar ratio (*c*/*m*)

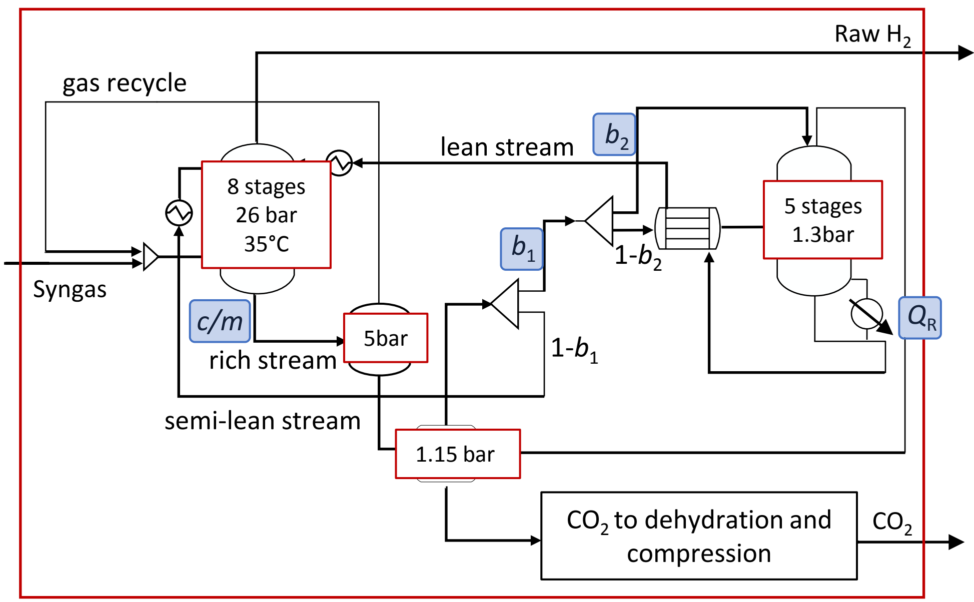
$$\frac{c}{m} = \frac{CO_2 \text{ syngas}}{\text{MDEA rich stream}}$$

→ *c*/*m* depends on the MDEA concentration (here: 40 wt%, CO_2 free)



Decision variables and ranges of investigation



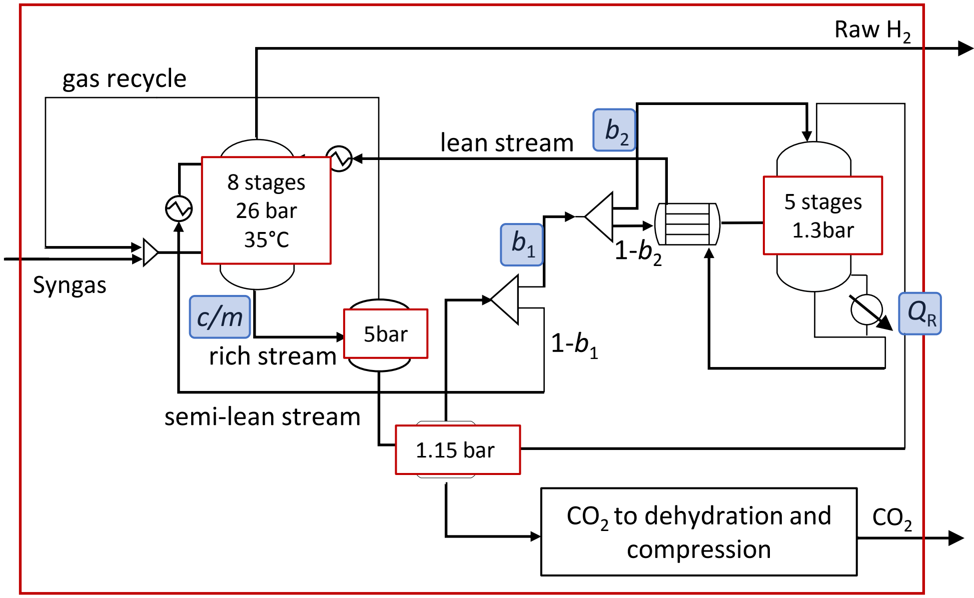


Specific optimization problem

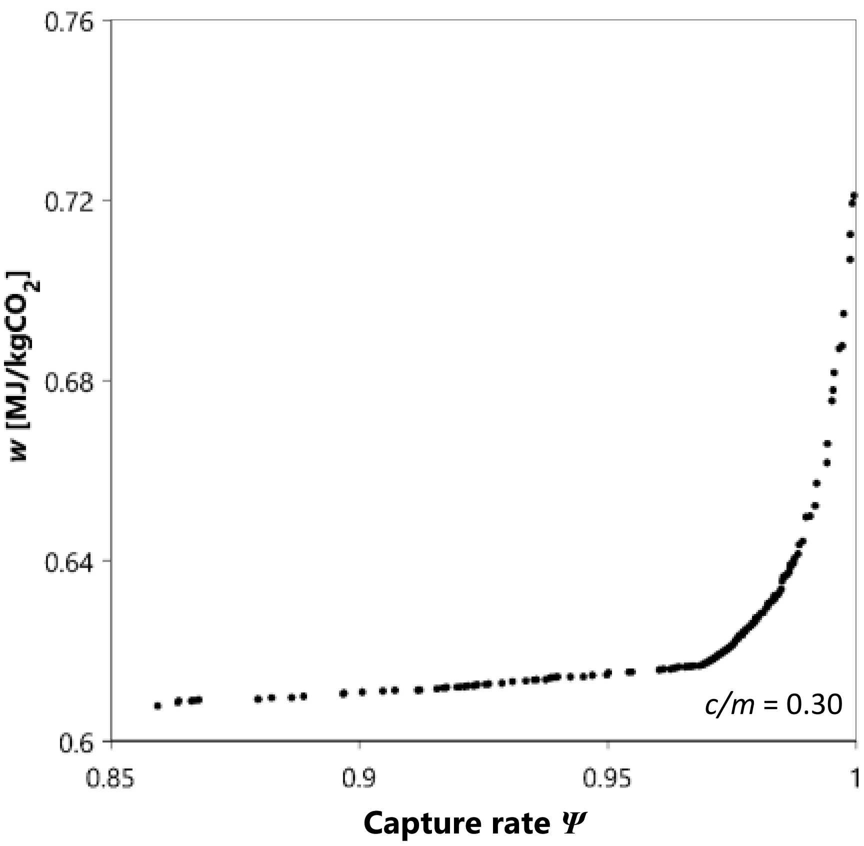
- To minimize the total specific exergy *w* while maximizing the capture rate Ψ
- Genetic algorithm

$$\min_{c/m, b_1, b_2, Q_R} \left[w, \frac{1}{\Psi} \right]$$

$$\begin{aligned} \text{subject to} \quad & c/m = [0.30, 0.40, 0.50] \\ & 0.20 \leq b_1 \leq 0.65 \\ & 0 \leq b_2 \leq 0.20 \\ & 0.65\ \text{MW/kg}_{\text{CO}_2} \leq Q_R \leq 1.2\ \text{MW/kg}_{\text{CO}_2} \end{aligned}$$

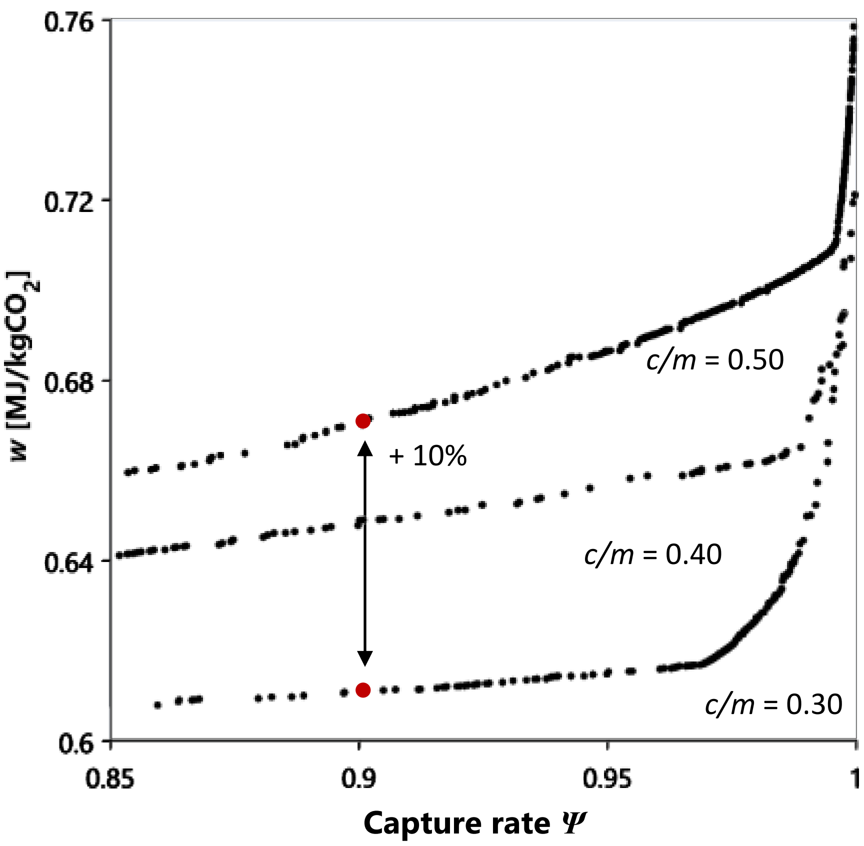


Key process variables analysis – *c/m*

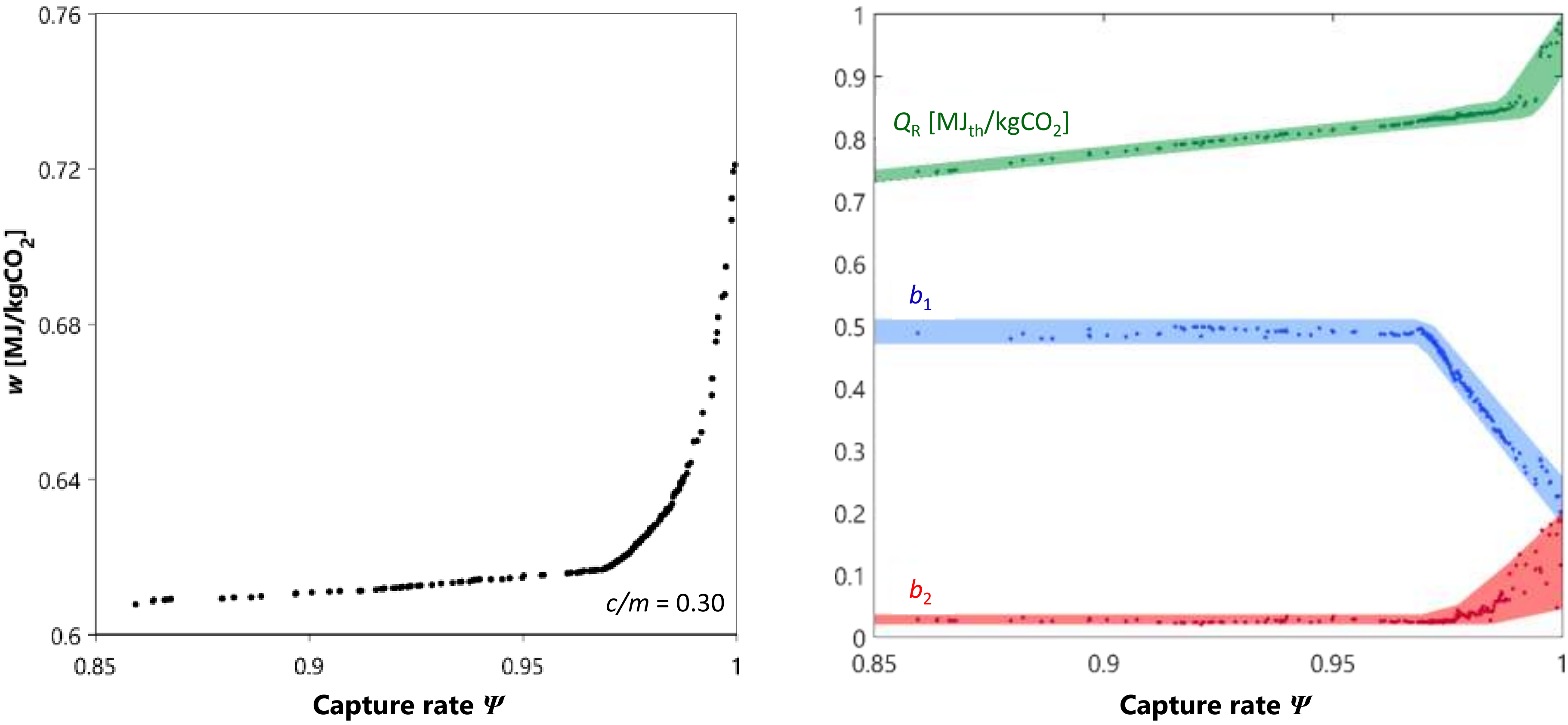


Key process variables analysis – *c/m*

Ψ = 90%



Analysis of the optimization results



Analysis of the optimization results

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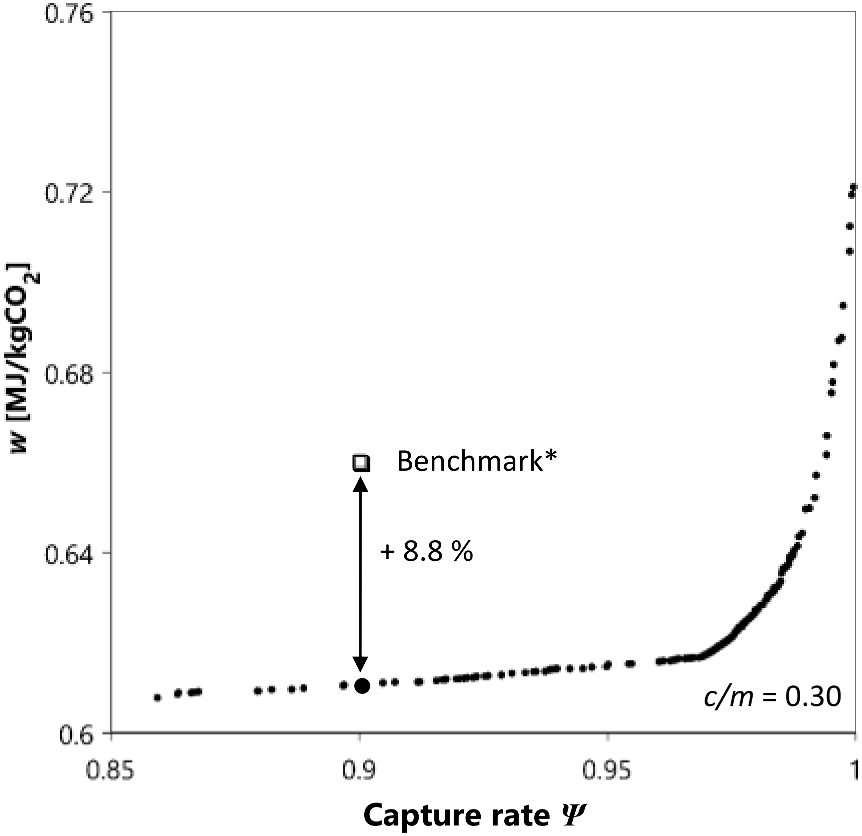

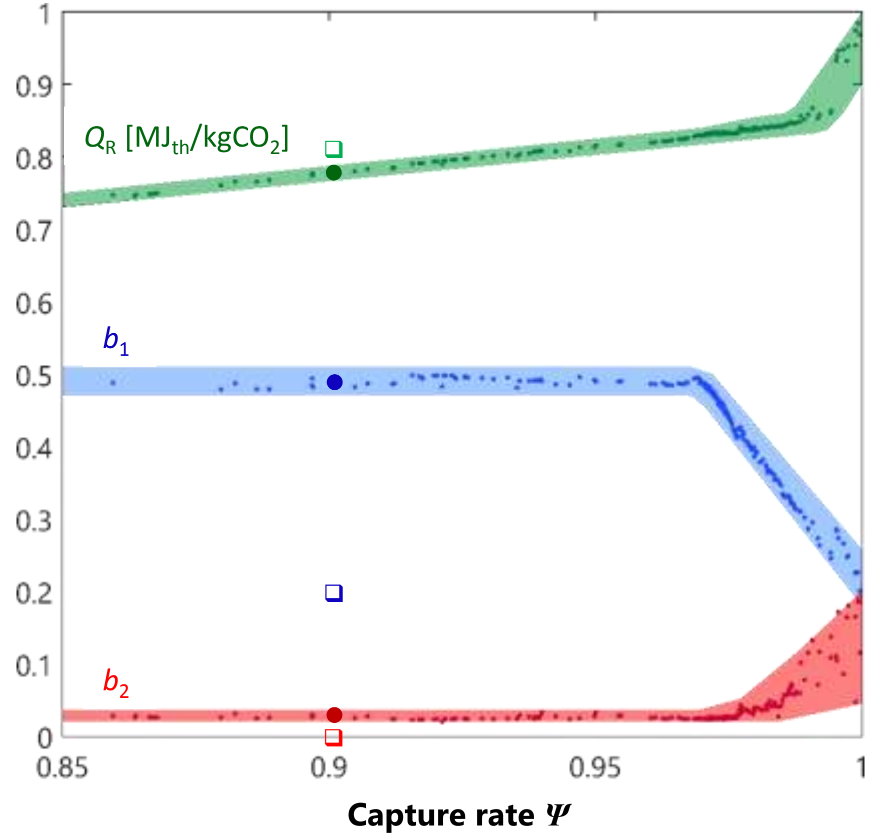

*Results taken from an MDEA plant optimization work[1]

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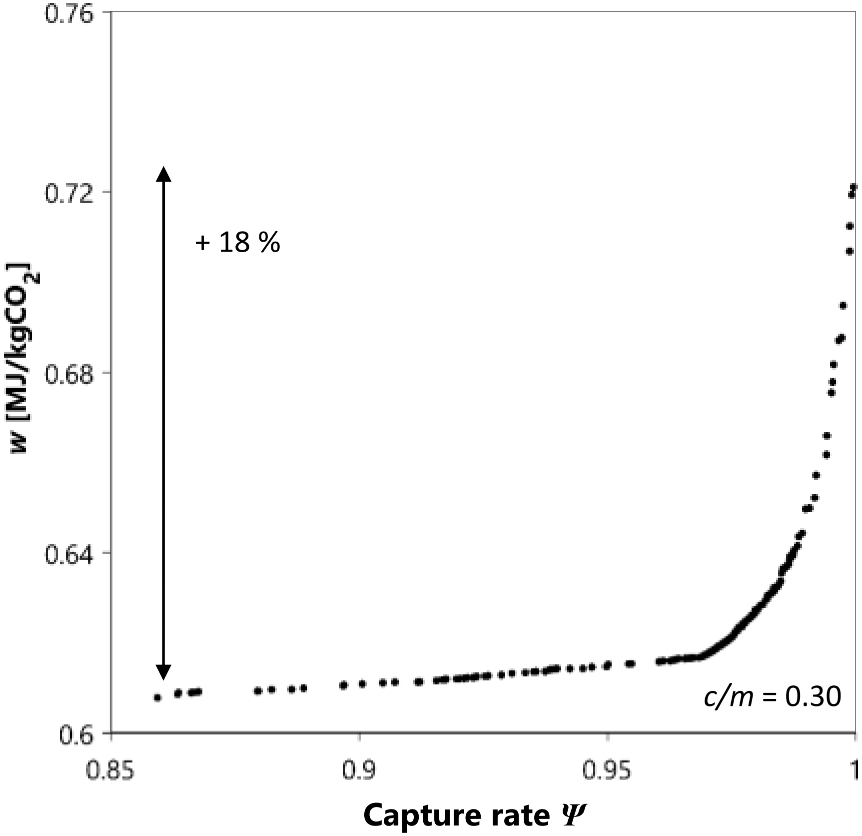
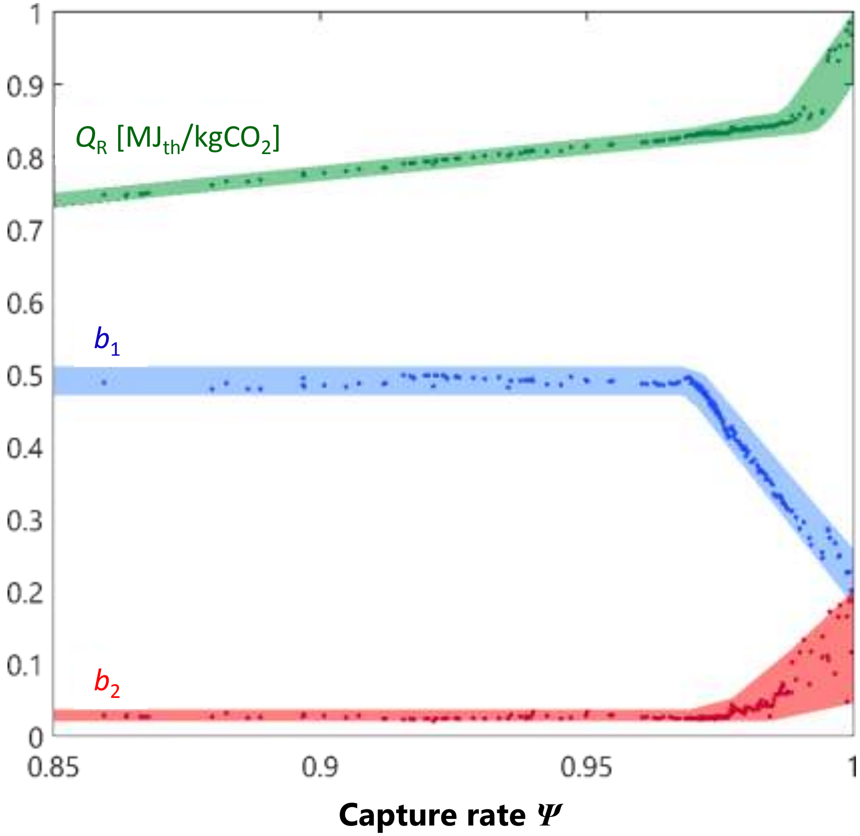
Analysis of the optimization results

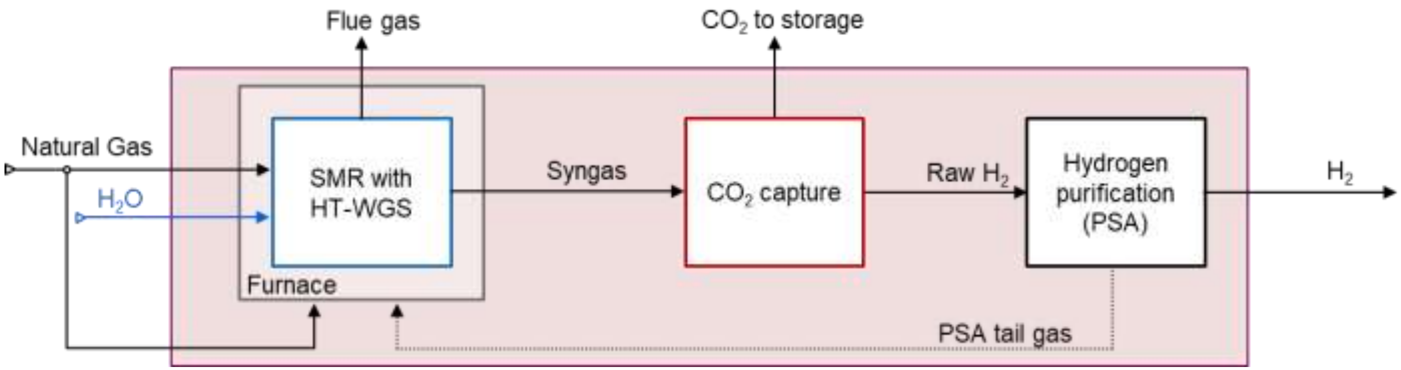
- At $\Psi > 97\%$ the w exponentially increases
- The contribution of b_2 becomes more important to reach higher capture rates more efficiently





Conclusions

- A rigorous approach was developed with the goal of finding the optimal operating conditions of a MDEA CO_2 capture plant
  - multi-objective optimization was used as a tool to find the Pareto Optimum between the total specific exergy and the capture rate
  - the decision variables were selected among the process variables by performing single-parameter sensitivity analysis
- The addition of a second splitter is advantageous especially while operating at high capture rates
- To decide how to operate the CO_2 capture plant, we need to look at the entire process



Acknowledgment

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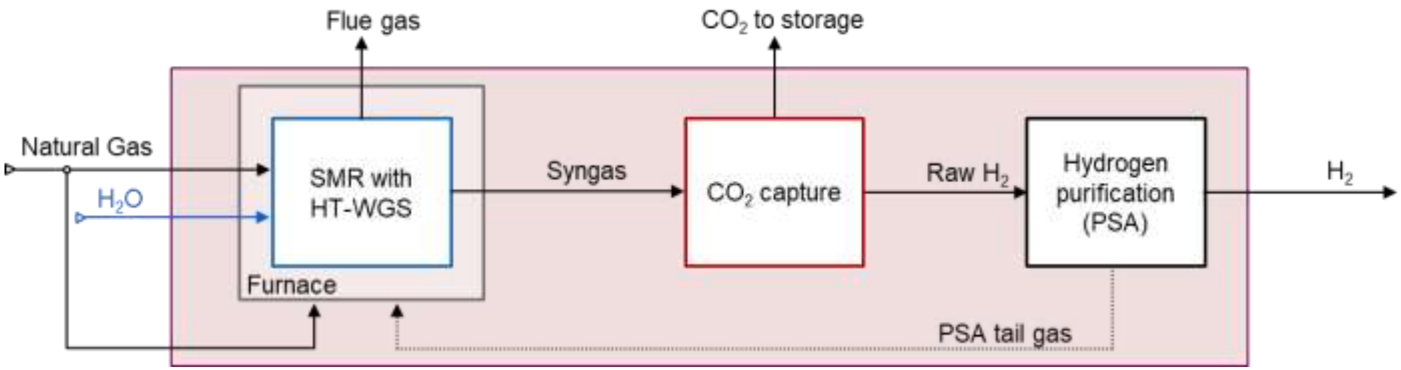
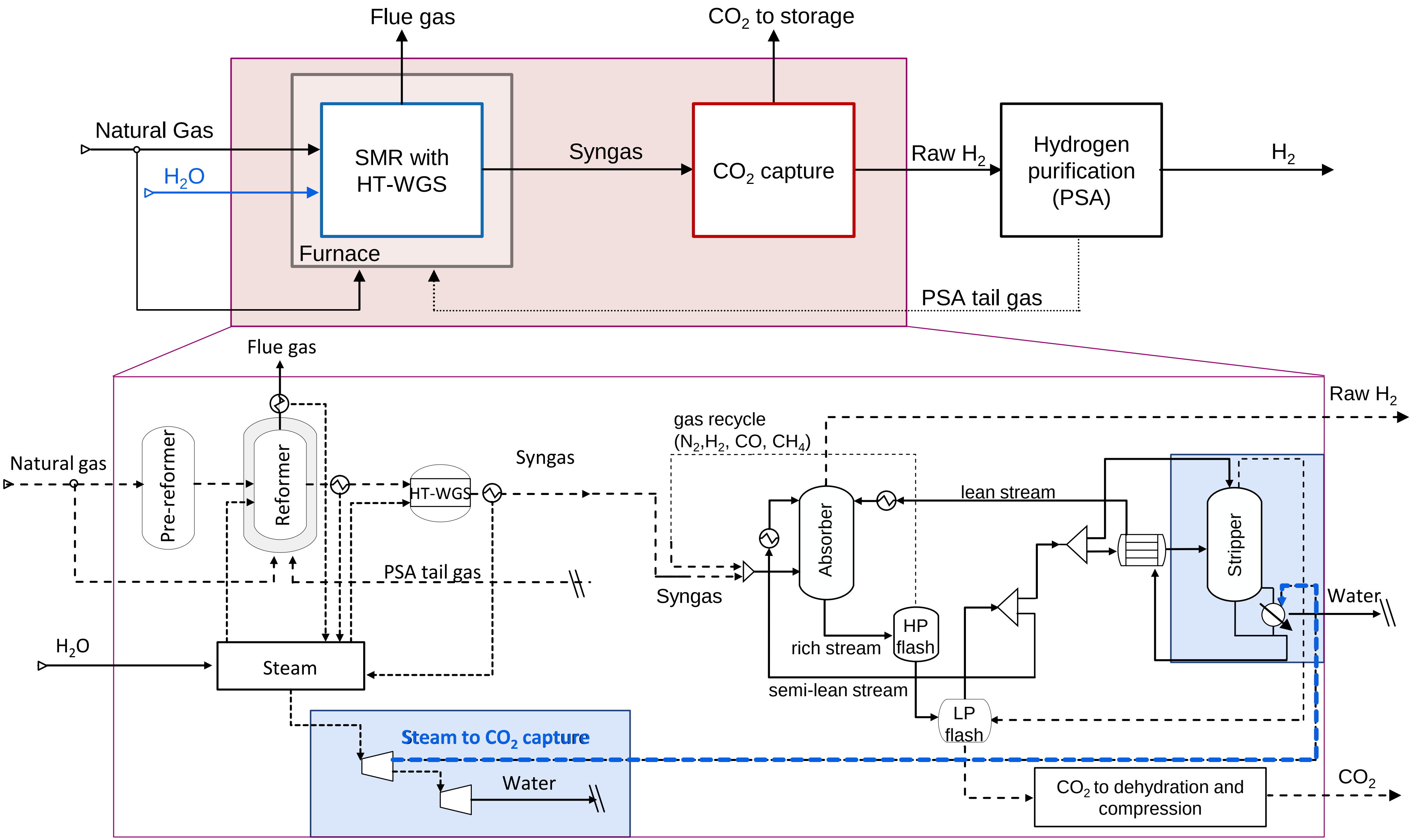


Back-up slides

Design Improving Energy Consumption



Modelling Framework

Modelling framework

Input Data

- Experimental and manufactures data from literature → Aspen Plus® modelling
- Case study data → MILP optimization

1. First principle thermodynamic models

Aspen Plus® modelling

- Equilibrium-based model
- Rate-based model

↓

2. Reduced order models for process optimization

Linear or Piece-wise affine

↓

3. MILP optimization

$$\min_{x,y} \left(c^T x + d^T y \right)$$

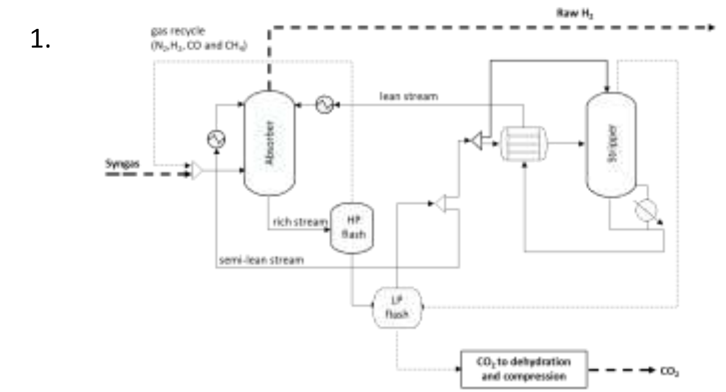
subject to

$$Ax + By \leq b$$

$$x \geq 0 \in \mathbb{R}^N, y \in \{0, 1\}^M$$

Implementation

1.



2. Energy efficiency : $E_{output} = \eta \, E_{input}$ Cost linearization : $C_i = m_i S + q_i$

3.