INITIATE

A STEPWISE PROJECT

Webinar - CCU MODELLING APPROACH FROM MICRO TO MACRO ASSESSMENT

Micro Model Reaction: How to Model the Process at Micro Level Identifying the Most Relevant Aspects

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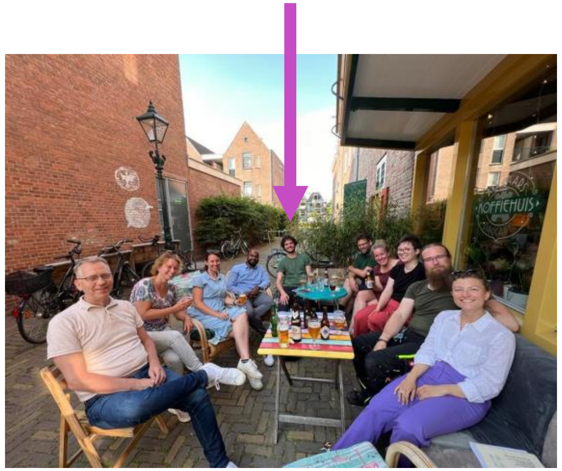
PUBLIC

Introduction

Hi I am **Francesco**, Process Technology Researcher of the **Gas Process Technology Team** at TNO.



Team

15 people, 6 nationalities.

Scientists, engineers, operators, consultants and business developers.

Activities

Adsorption and catalysis science.

Process and reactor engineering.

System analysis.

Laboratory and pilot testing.

Location: The Netherlands

TNO innovation for life

Netherlands Organization for Applied Scientific Research.

Micro Level Modelling of a Process

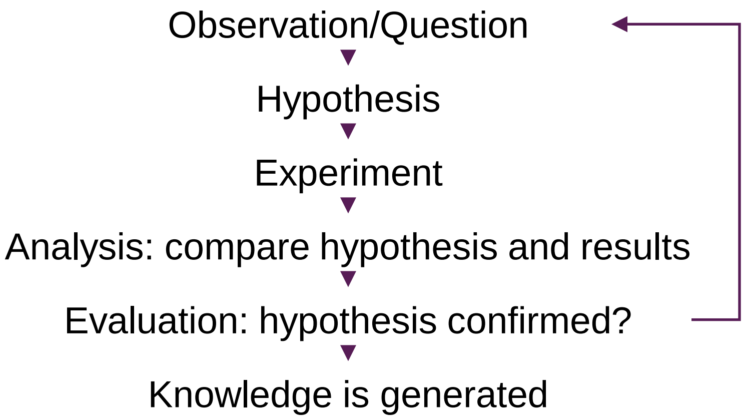
What is Modelling? Modelling is a research activity that generates knowledge.

Why Modelling? Knowledge can be used to design technology that generates value at reduced risks.

Research

Objective: Generate Knowledge

Approach: Scientific method

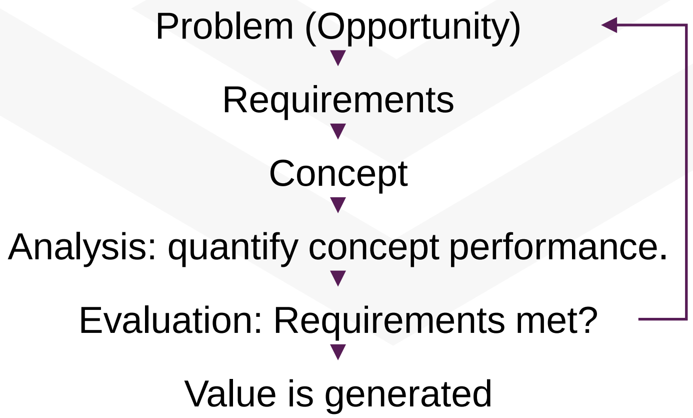


Observation/Question
▼
Hypothesis
▼
Experiment
▼
Analysis: compare hypothesis and results
▼
Evaluation: hypothesis confirmed?
▼
Knowledge is generated

Design

Objective: Generate Value

Approach: Design Methodology



Problem (Opportunity)
▼
Requirements
▼
Concept
▼
Analysis: quantify concept performance.
▼
Evaluation: Requirements met?
▼
Value is generated

Micro Level Modelling of a Process

How to **Model** the Process at **Micro Level** Identifying the **Most Relevant Aspects**?

Why building and running a model?

- To generate knowledge.
- To validate a value proposition at reduced risks (e.g. plant revamp, grassroots design, etc…).

Why modelling on a “micro” level?

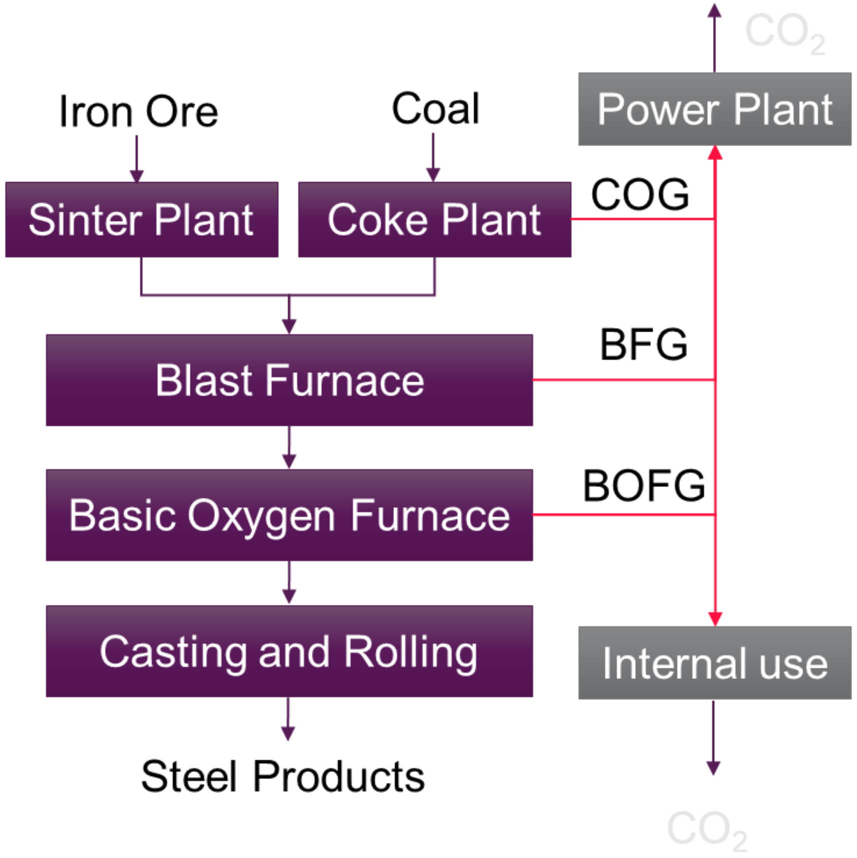
- To match the required accuracy.
- To reduce the required amount of (experimental, plant) data that are needed to build the model.

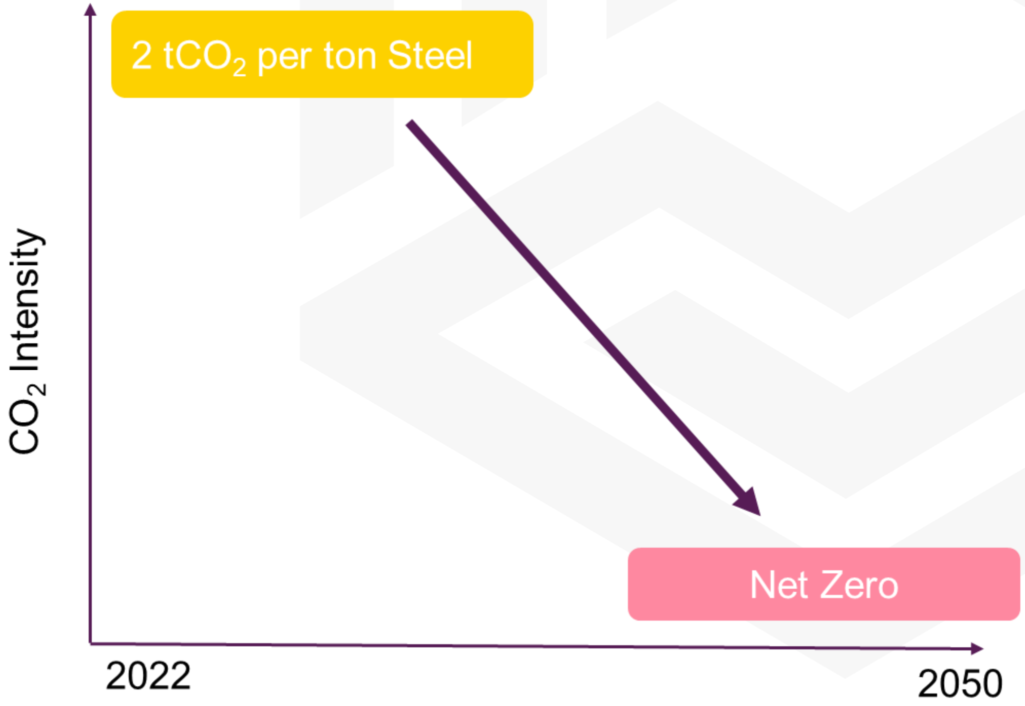
How to identify the most relevant (process) aspects?

- Check the “experimental conditions” that the model needs to predict and desired accuracy.
- Check the stakeholders’ requirements that enables to generate value.

An Example: SEWGS Design in the INITIATE Process

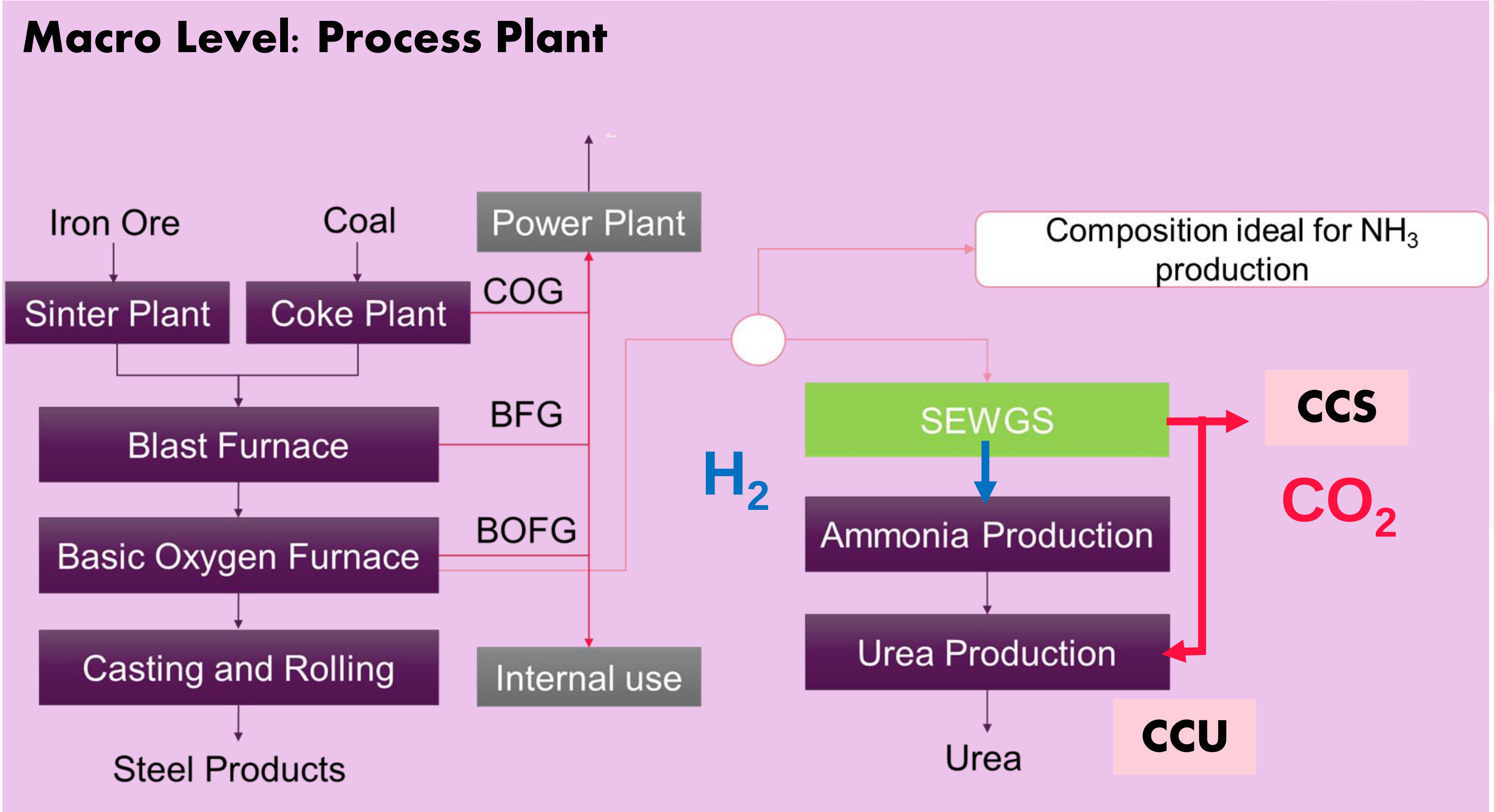
Problem: Enable achieve cost-effective CO2 neutral steelmaking by 2050.

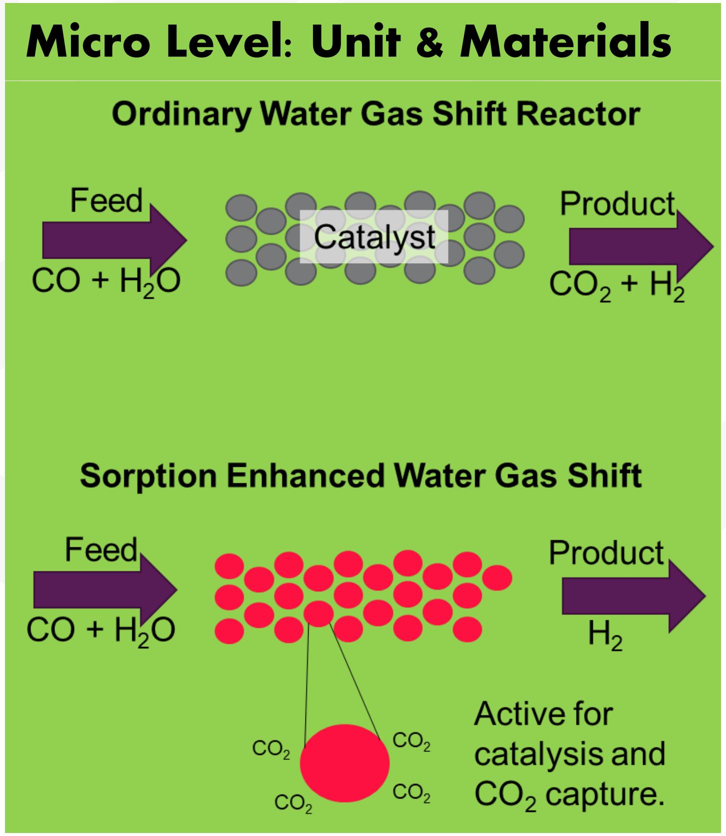




An Example: SEWGS Design in the INITIATE Process

Concept: Convert steel gases via **SEWGS** to H2 and CO2 products ready for CCS and CCU technologies.

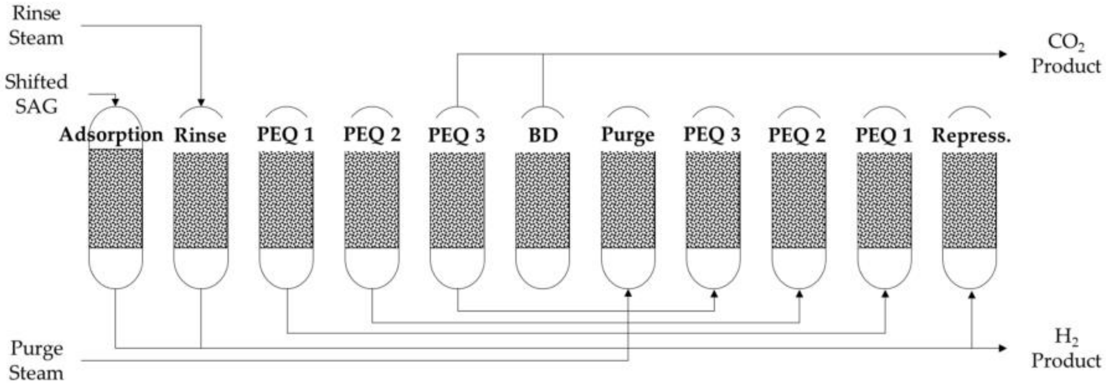


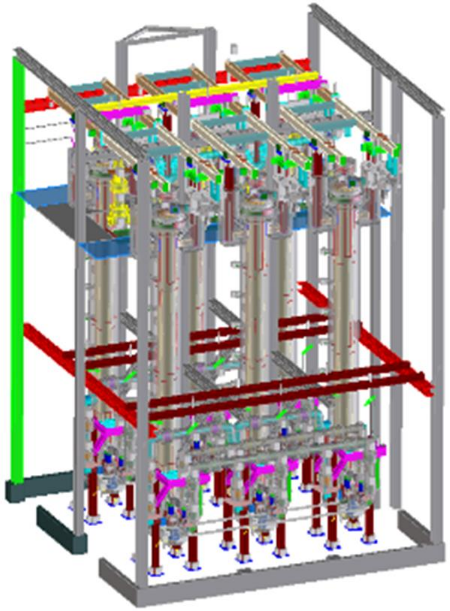


An Example: SEWGS Design in the INITIATE Process

Requirements:

- Separation and conversion (Value): CO conversion, Carbon capture rate (CCR) and Carbon Purity (CP)
- Utilities consumption (OPEX): Steam and electricity consumption
- Inventory (CAPEX): Amount of sorbent and column sizes/number





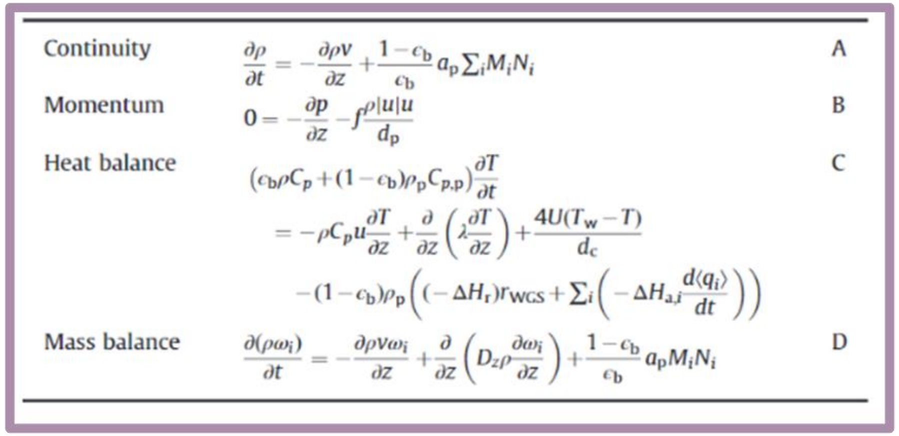
Research question (key knowledge to be generated):

What are SEWGS sizes and operating conditions that meet process requirments?

An Example: SEWGS Design in the INITIATE Process

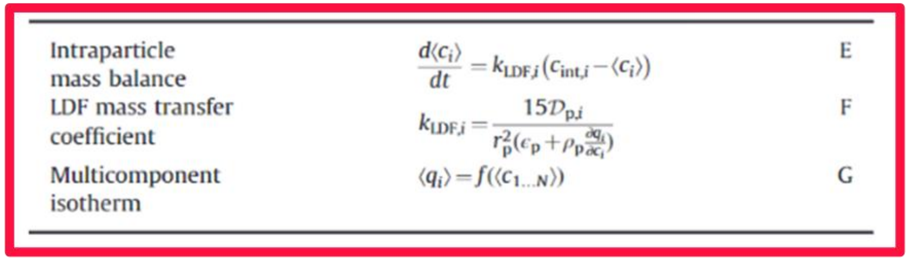
Key Aspects of the process: Column and sorbent performance to avoid running too many experiments.

Physical model of a column [1]:

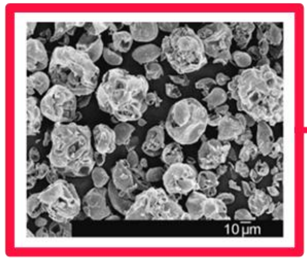


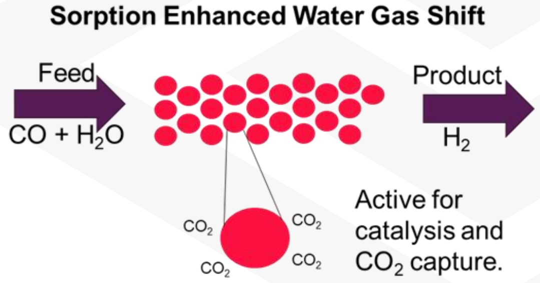
Continuity	$\frac{\partial\rho}{\partial t}=-\frac{\partial\rho v}{\partial z}+\frac{1-\epsilon_b}{\epsilon_b}a_p\sum_i M_i N_i$	A
Momentum	$0=-\frac{\partial p}{\partial z}-f\frac{\rho\lvert u\rvert u}{d_p}$	B
Heat balance	$(\epsilon_b\rho C_p+(1-\epsilon_b)\rho_p C_{p,p})\frac{\partial T}{\partial t}$ $=-\rho C_p u\frac{\partial T}{\partial z}+\frac{\partial}{\partial z}\left(\lambda\frac{\partial T}{\partial z}\right)+\frac{4U(T_w-T)}{d_c}$ $-(1-\epsilon_b)\rho_p\left((-\Delta H_r)r_{WGS}+\sum_i\left(-\Delta H_{a,i}\frac{d\langle q_i\rangle}{dt}\right)\right)$	C
Mass balance	$\frac{\partial(\rho\omega_i)}{\partial t}=-\frac{\partial\rho v\omega_i}{\partial z}+\frac{\partial}{\partial z}\left(D_z\rho\frac{\partial\omega_i}{\partial z}\right)+\frac{1-\epsilon_b}{\epsilon_b}a_p M_i N_i$	D

Semi-empirical model of the sorbent [1,2]:



Intraparticle mass balance	$\frac{d\langle c_i\rangle}{dt}=k_{LDF,i}(c_{int,i}-\langle c_i\rangle)$	E
LDF mass transfer coefficient	$k_{LDF,i}=\frac{15\mathcal{D}_{p,i}}{r_p^2(\epsilon_p+\rho_p\frac{\partial q_i}{\partial c_i})}$	F
Multicomponent isotherm	$\langle q_i\rangle=f(\langle c_{1...N}\rangle)$	G





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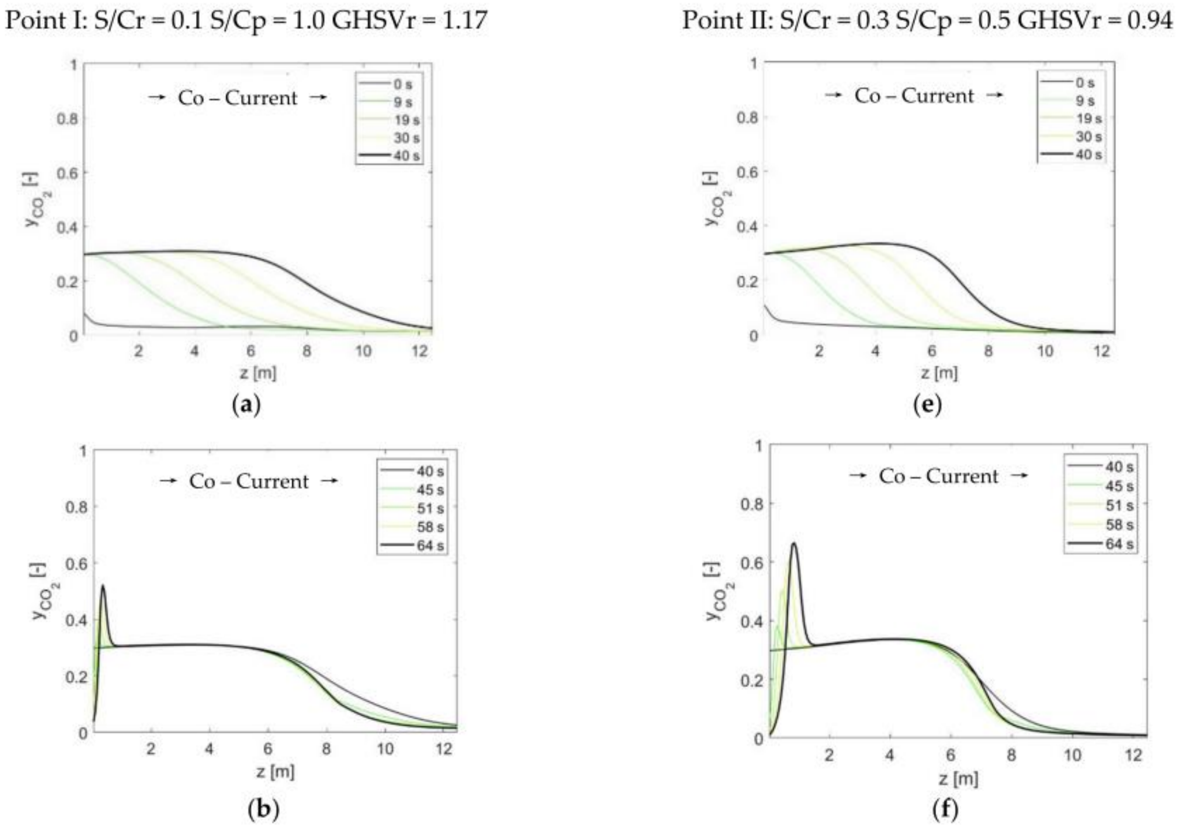
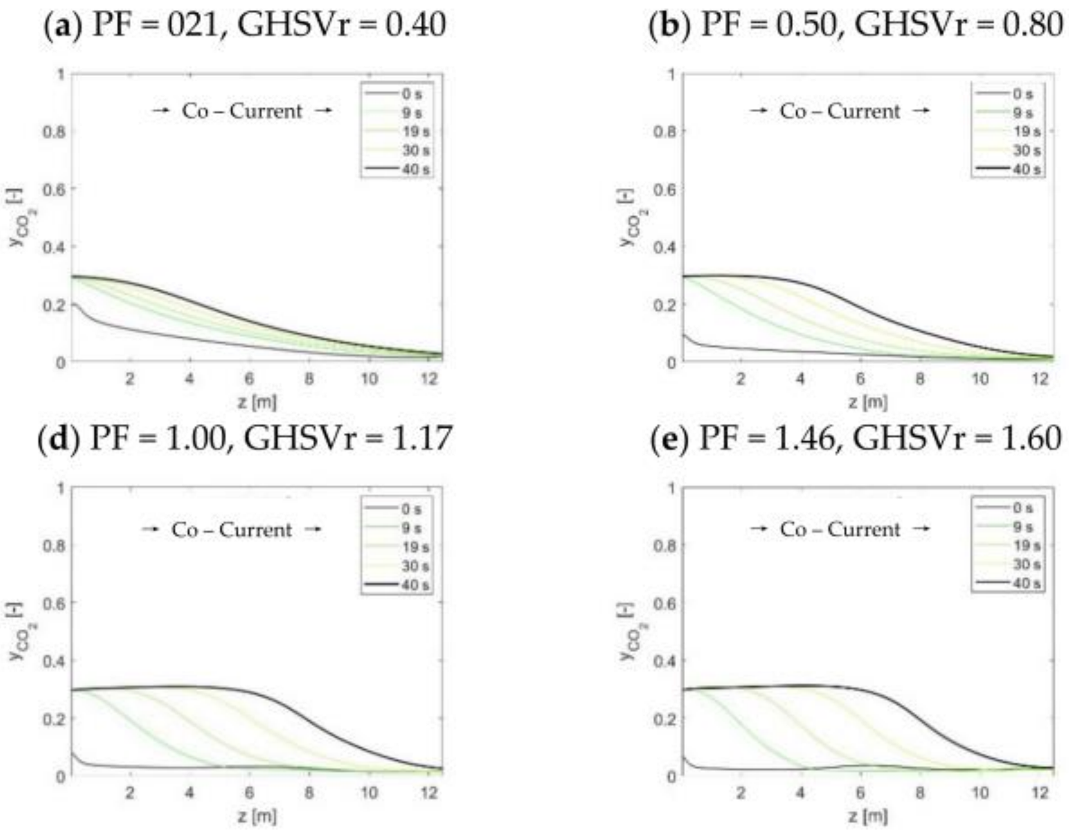
[1] Boon, Jurriaan, et al. "High-temperature pressure swing adsorption cycle design for sorption-enhanced water–gas shift." Chemical Engineering Science 122 (2015): 219-231. [2] Walspurger, Stéphane, et al. "High CO2 storage capacity in alkali-promoted hydrotalcite-based material: In situ detection of reversible formation of magnesium carbonate." *Chemistry–A European Journal* 16.42 (2010): 12694-12700.

An Example: SEWGS Design in the INITIATE Process

Generated knowledge: Understanding of column performance in every step at various conditions.



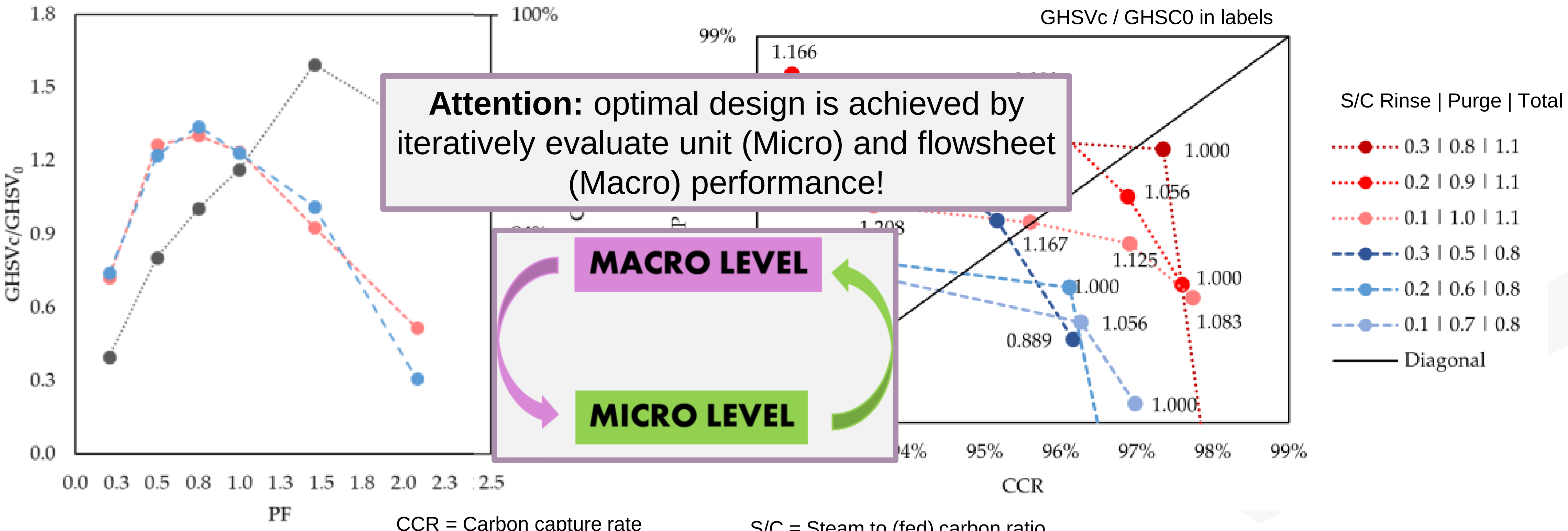
(a) (e) (b) (f)



Pictures from: Sebastiani, Francesco, et al. "Steam and Pressure Management for the Conversion of Steelworks Arising Gases to H2 with CO2 Capture by Stepwise Technology." Separations 9.1 (2022): 20.

An Example: SEWGS Design in the INITIATE Process

Generated knowledge: Overall Performance map of separation, utilities and inventory indicators for various applications.



Attention: optimal design is achieved by iteratively evaluate unit (Micro) and flowsheet (Macro) performance!

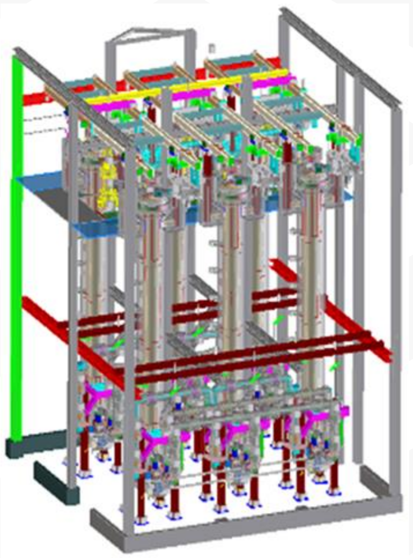
CCR = Carbon capture rate
CP = Carbon Purity
PF = Dimensionless feed pressure

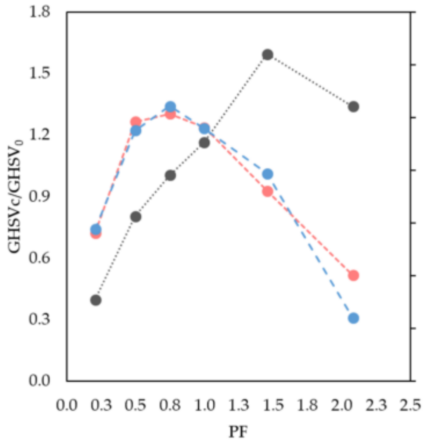
S/C = Steam to (fed) carbon ratio
$GHSV_c / GHSV_0$ = Dimensionless Carbon Gas Hourly Space Velocity

Pictures from: Sebastiani, Francesco, et al. "Steam and Pressure Management for the Conversion of Steelworks Arising Gases to H2 with CO2 Capture by Stepwise Technology." Separations 9.1 (2022): 20.

Takeaways

- Process Models generate knowledge to validate process concepts at reduced risks and costs.
- Modelling at Micro level allows to increase results accuracy and reduce the required input data to generate knowledge for various applications.
- Macro and Micro level modelling are integrated and iterative activities.





MACRO LEVEL

MICRO LEVEL

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Thank you!

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