Carbon2Chem®

Modeling the Catalytic Conversion of Steel Mill Gases

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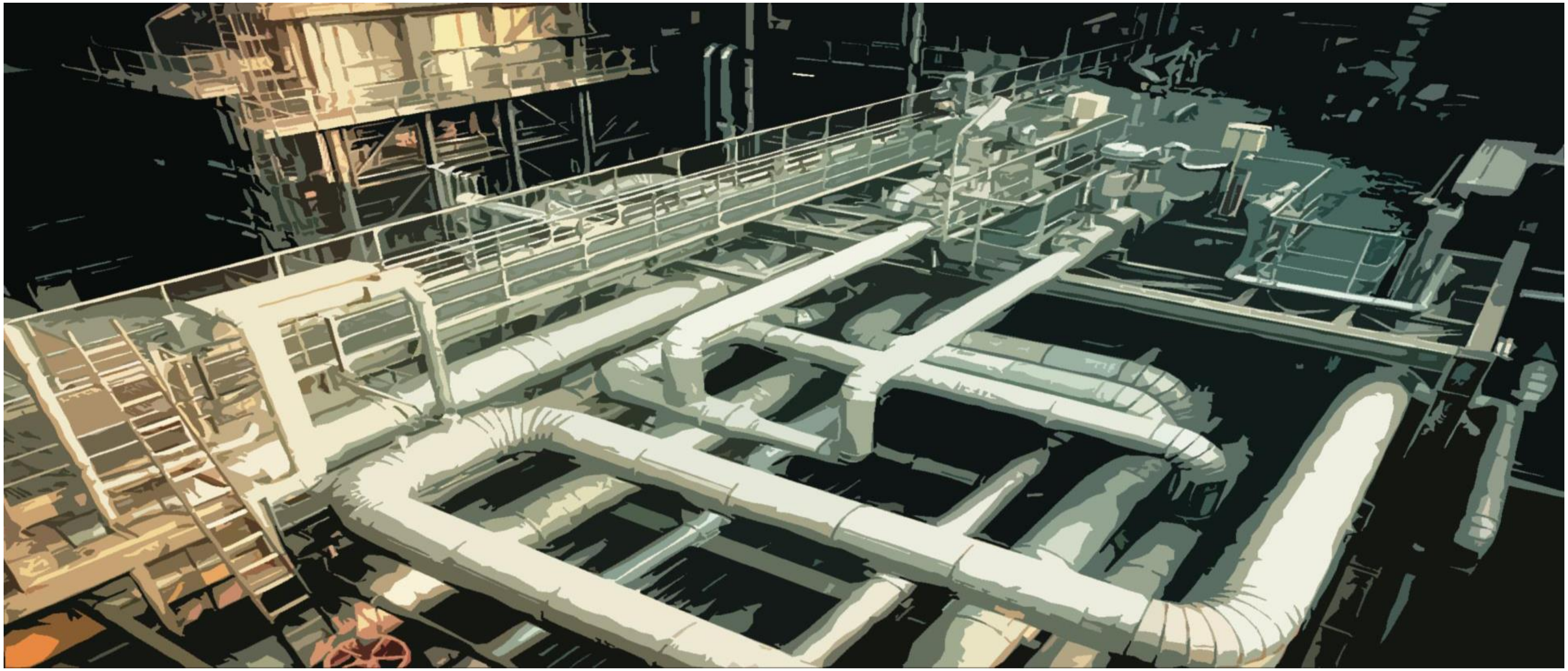


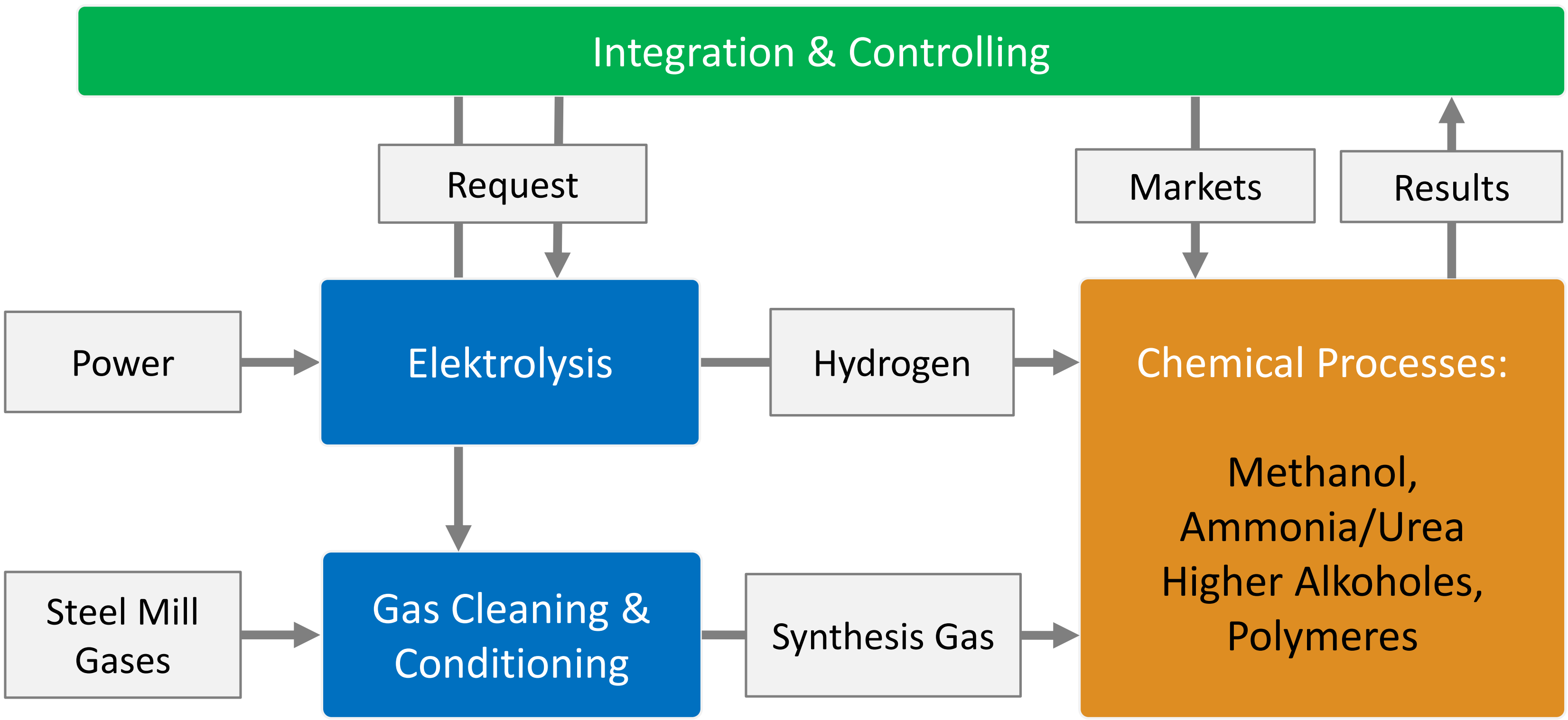
Carbon2Chem® - Steel Mill Gases

Table 1. Molar composition [mol/mol] of steel mill gases.

Component	Coke Oven Gas	Blast Furnace Gas	Basic Oxygen Furnace Gas
Hydrogen	0.63	0.04	0.05
Carbon Monoxide	0.07	0.25	0.64
Carbon Dioxide	0.02	0.23	0.17
Methane	0.22	0	0
Nitrogen	0.06	0.48	0.14

Carbon2Chem® – CCU Model Concept

CCU = Carbon Capture and Utilization



Carbon2Chem® – Elements of CCU Simulation

Base chemical syntheses

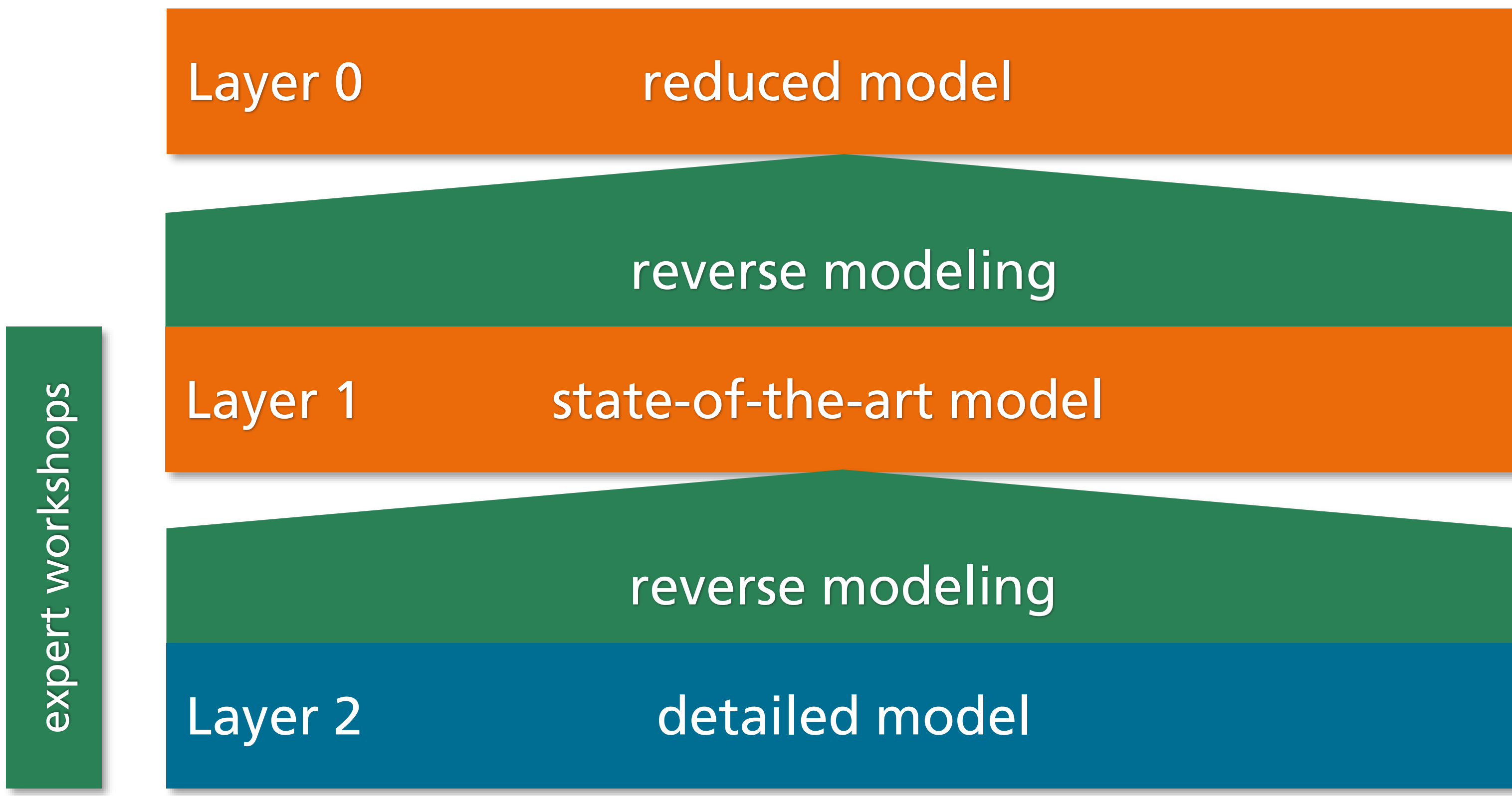
- Ammonia – heterogeneous catalytic gas phase synthesis
- Methanol – heterogeneous catalytic gas phase synthesis
- Higher alcoholes – heterogeneous catalytic gas phase synthesis
- Polymeric syntheses

Utility processes

- Water electrolysis
- Gas tanks, gasometers, compressors, heat exchangers, separators …
- Controlling loops

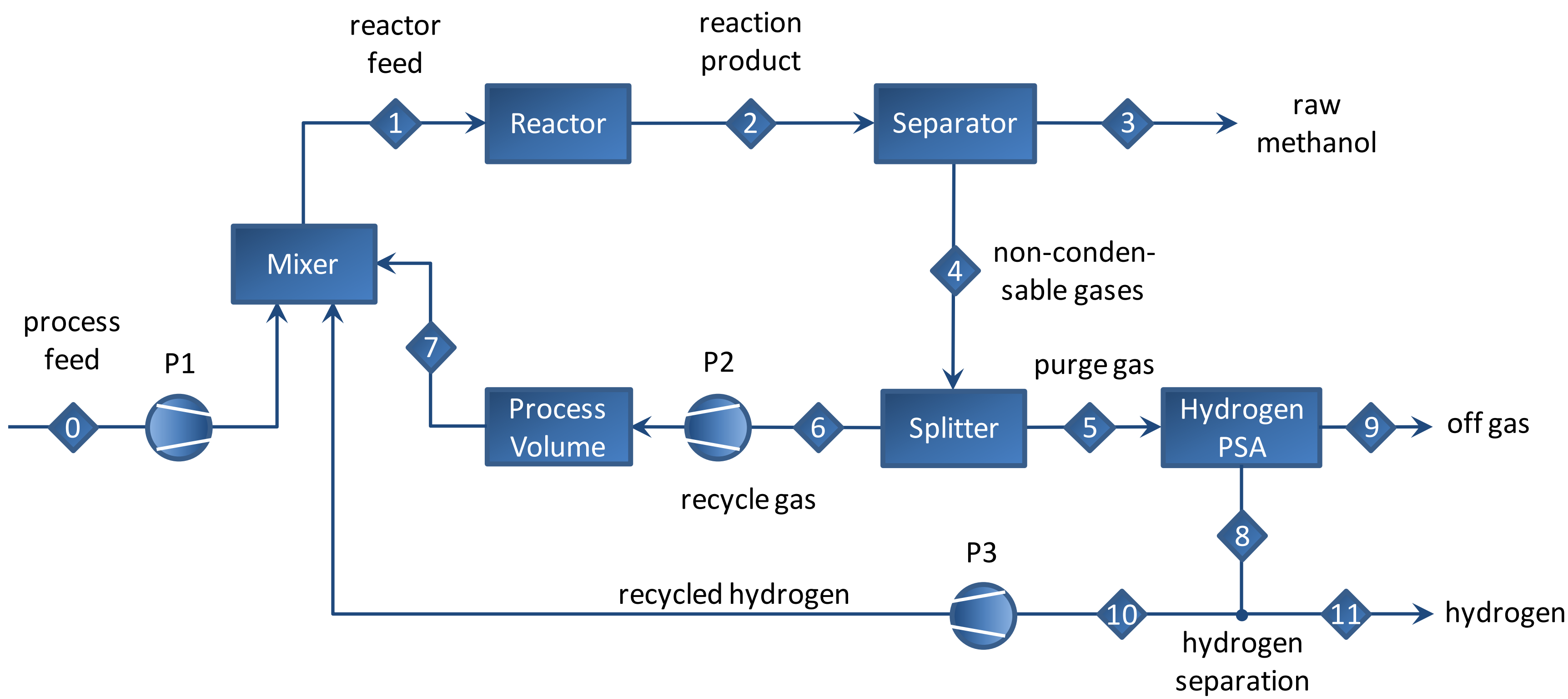
Carbon2Chem® – Model Levels

Reverse Modeling couples models at different levels of detail



Example: Methanol Synthesis Process – Reaction Model

Process Model – Layer 1/2



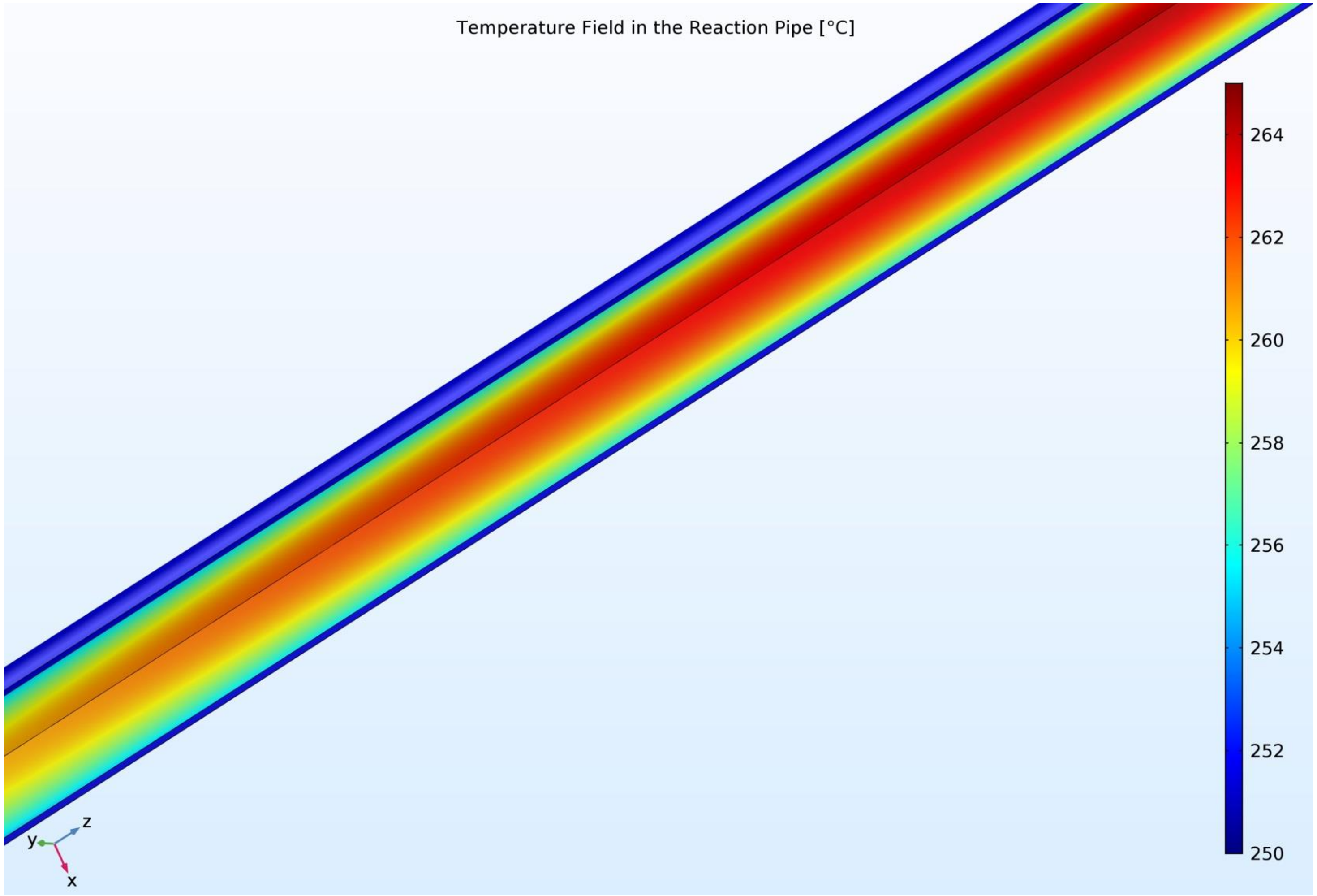
Methanol Synthesis Reaction Model

Model features – Level 1/2

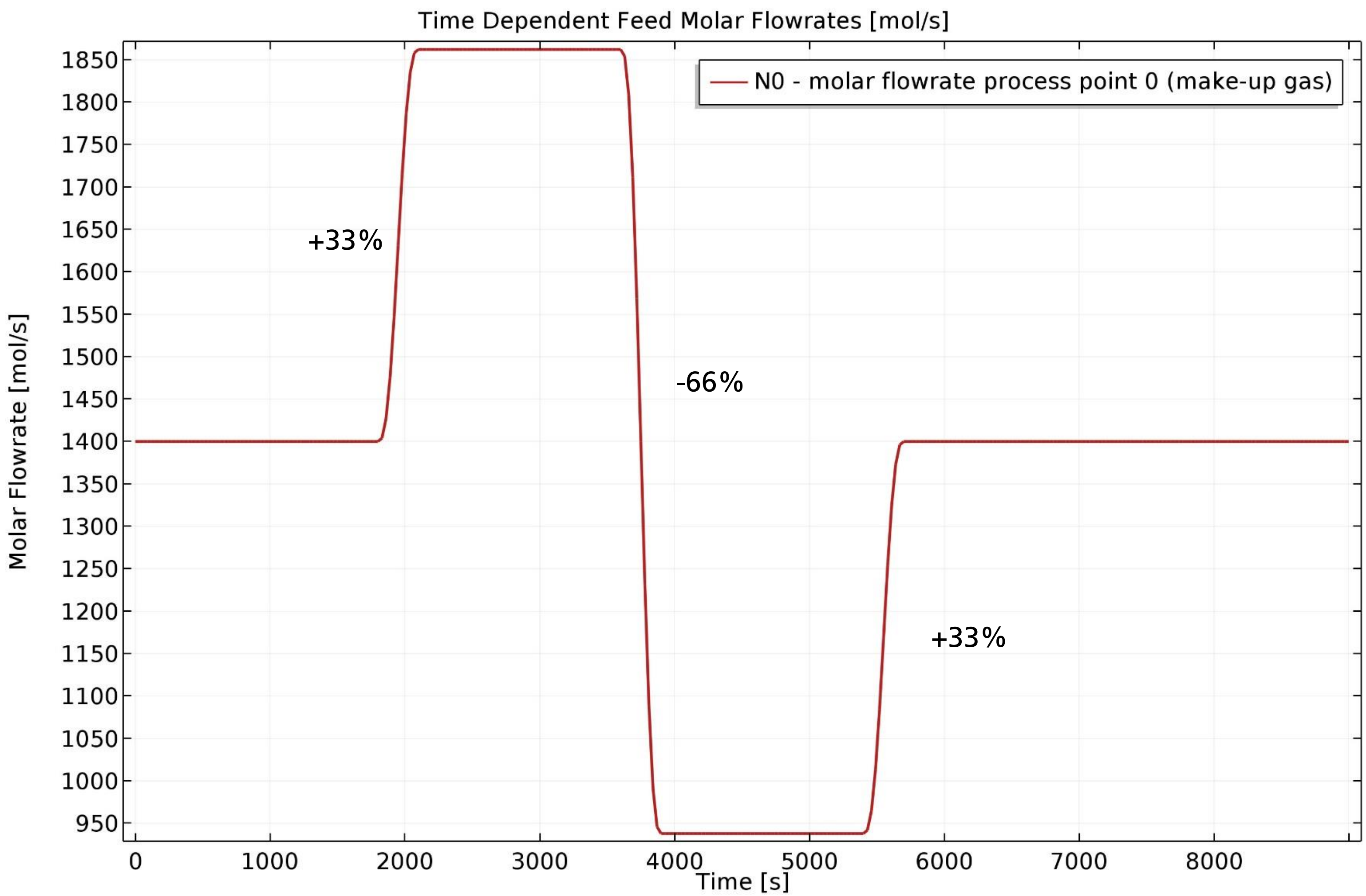
- 1-d / 2-d rigorous time dependent models, pipe geometry
- Model type: porous media non-isothermal reactive flow
- Set with the General Form PDE from the Mathematics module
- Enhanced reaction models with up to 3 kinetic expressions
- Fugacities from cubic equations of state (ePR, eSRK)
- Process loop with thermodynamic separator model (methanol/water/CO_2)
- Validation with data of Graaf/Beenackers from literature*

*) G.H. Graaf, A.A.C.M Beenackers; Comparison of two-phase and three-phase methanol synthesis processes; Chem. Eng. Proc. 35 (1996) 413-427

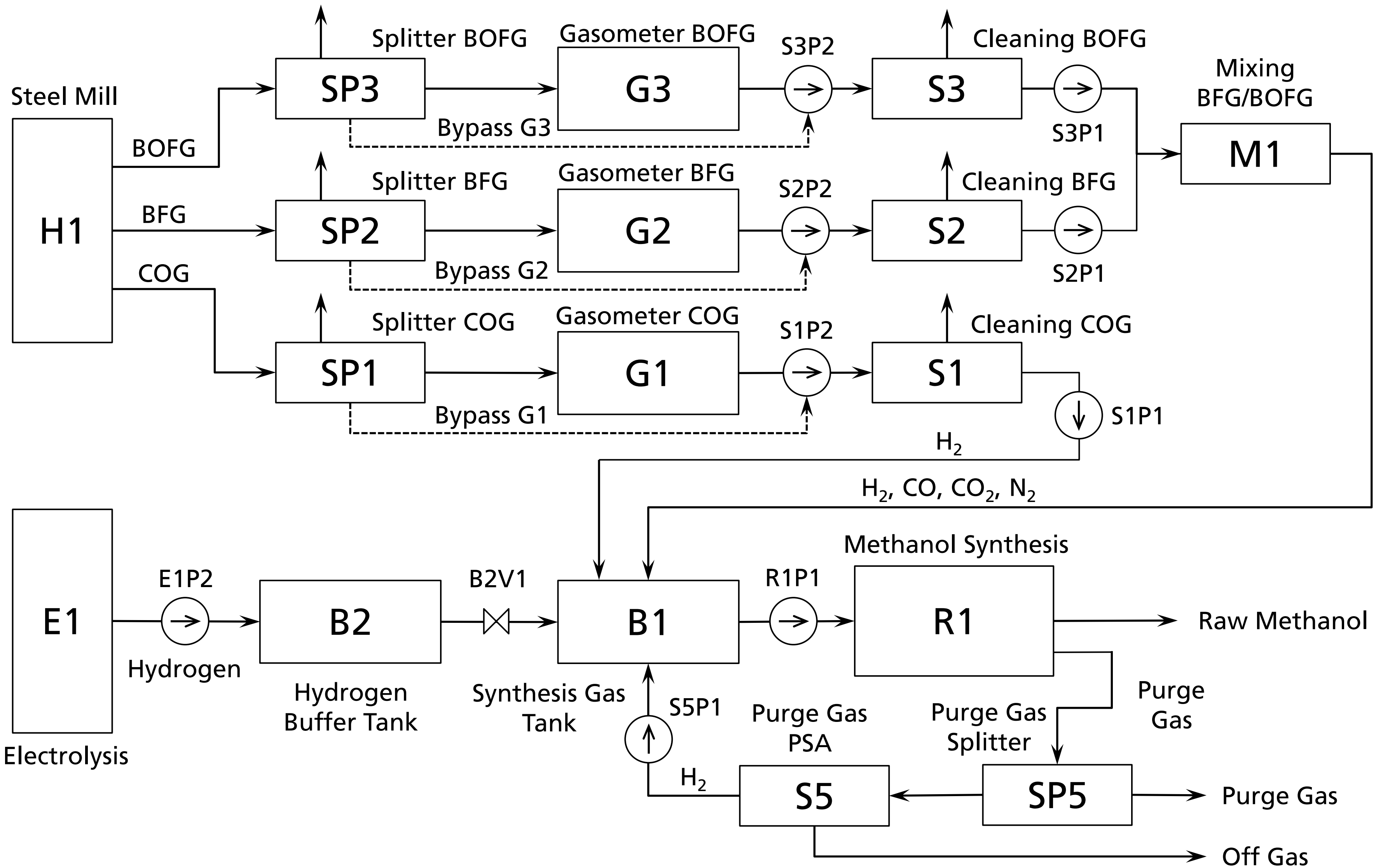
2D-Simulation of Tubular Reactor – Temperature Field



Time Dependent Simulation – Methanol Production



Prozess Flow Sheet – Methanol Production Scheme



Carbon2Chem® – Control Concepts

1. Hydrogen driven scenario

- Available hydrogen is the set point variable for carbon usage
- Hydrogen sources are COG and electrolysis (power input)
- Availability of „green power“ drives the chemical routes

2. Carbon driven scenario

- Available carbon (steel mill gas) is the set point variable for hydrogen
- Hydrogen is produced as requested ---> power input as requested

3. Chemical driven scenario

- Chemical production is set point for carbon usage & hydrogen production

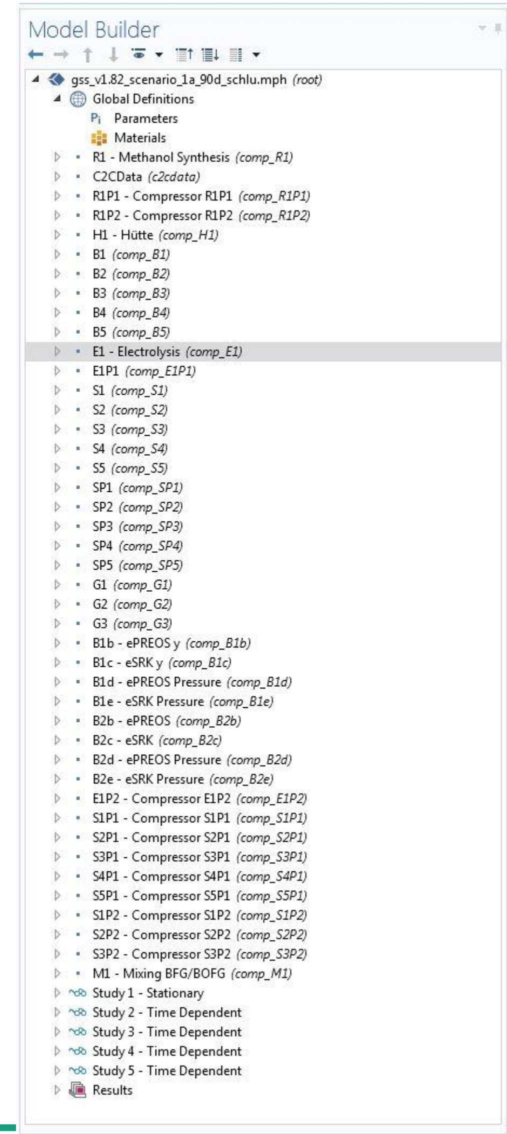
Carbon2Chem® – Implementation in COMSOL®

Flowsheet organization

- Organization of the model in 44 single components
- Coupling interfaces as variable blocks in every component (input_interface, result_interface)
- Coupling of result –> input between components

Development tasks

- Development of every component
- Testing of every component as stand-alone
- Coupling components to flowsheet model



90 Days Process Simulation – Gas Usage Scenario

Gas usage scenario

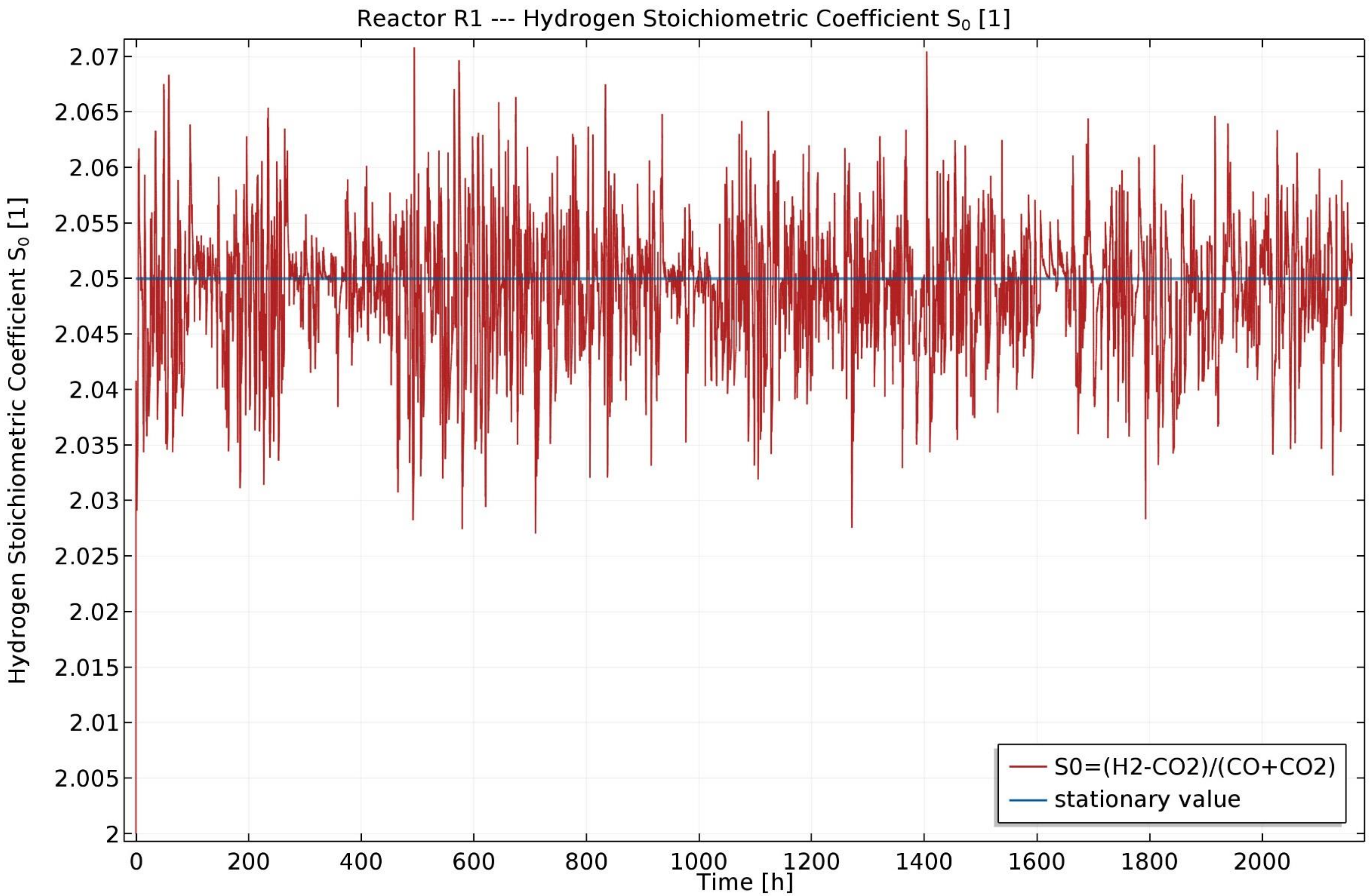
- Coke Oven Gas (COG) to gas cleaning unit S1
- Blast Furnace Gas (BFG) to gasometer G2
- Hydrogen separation from COG in gas cleaning unit S1
- BFG output at G2 is controlled by the hydrogen offer in B1

Control of blast furnace gas (BFG)

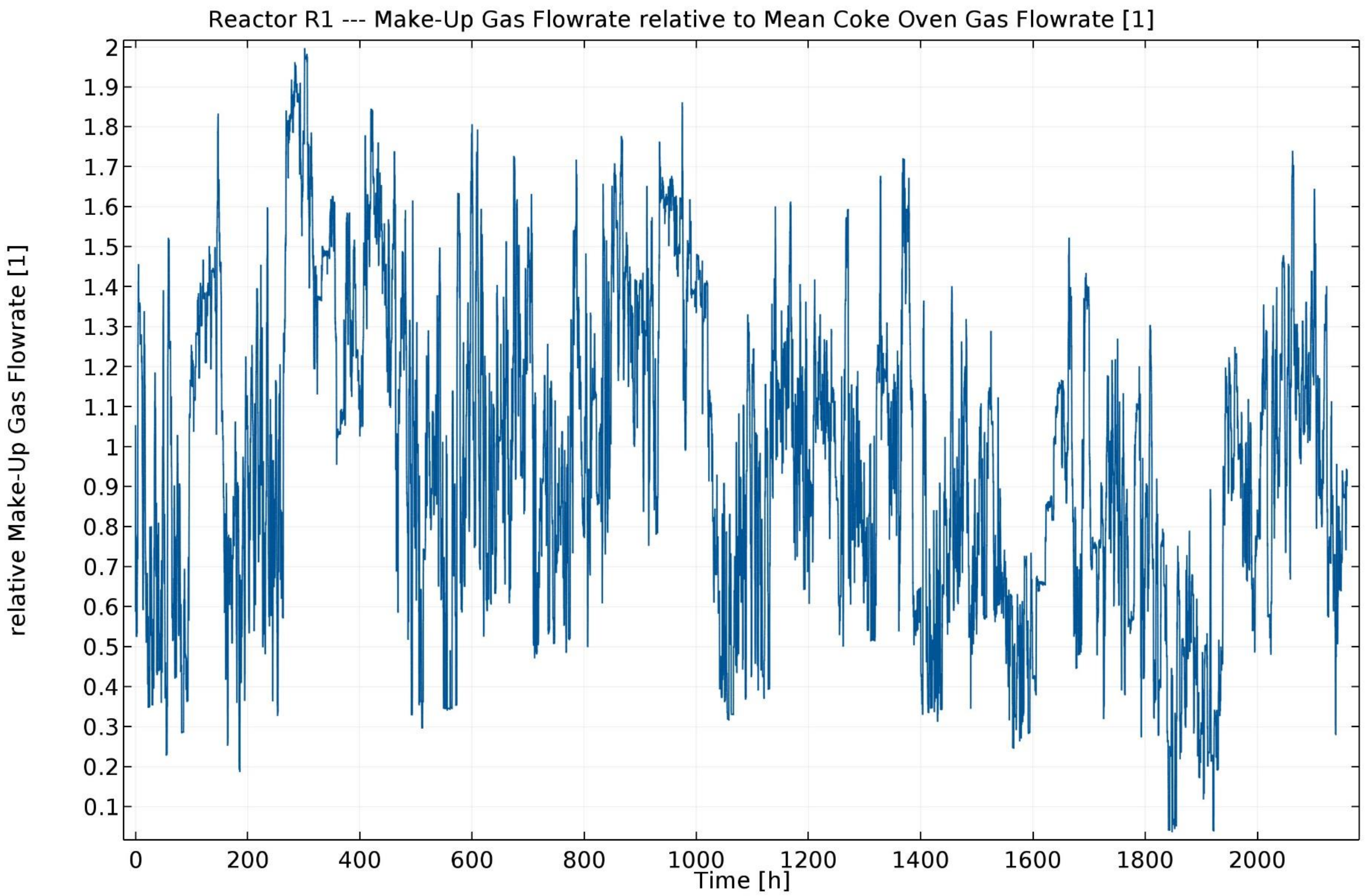
- Instantaneous mass balance of all inlets at synthesis gas tank B1
- Solve for BFG inlet with methanol stoichiometric condition

$$S = \frac{\dot{N}_{H_2} - \dot{N}_{CO_2}}{\dot{N}_{CO} + \dot{N}_{CO_2}} = 2.05 \qquad \rightarrow \qquad \dot{N}_{BFG}(t)$$

90 Days Process Simulation – Synthesis Gas Quality at R1



90 Days Process Simulation – Make-Up Gas Flowrate at R1



Carbon2Chem® – Further Steps

State of work

- A transient flowsheet model for methanol production from steel mill gases has been sucessfully developed with COMSOL Multiphysics®

Further Steps

- Simulation of different gas usage scenarios for methanol process
- Enhance model for further chemical processes
- Further development of models with experimental data from the project partners (ThyssenKrupp, Siemens, Linde, Covestro, Akzo Nobel, MPI)
- Providing of results for further optimization steps

Carbon2Chem® – Further Reading

- S. Schlüter, T. Hennig; *Modeling the catalytic Conversion of Steel Mill Gases Using the Example of Methanol Synthesis*; Chem. Ing. Tech. 2018, *90*, pp. 1541-1558, DOI: 10.1002/cite.201800021
- Chemie Ingenieur Technik, Special Edition: Carbon2Chem®, 2018, *Volume 90*, Issue No. 10 (all articles are in english language)

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