Carbon2Chem®

Modeling the Catalytic Conversion of Steel Mill Gases

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Carbon2Chem® - 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

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







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/CO₂)
- 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

	1		
		1 22 scenario 1a 00d schlumph (met)	
	gss A	Global Definitions	
073	0	P: Barameters	
		Materials	
Þ		R1 - Methanol Synthesis (comp. R1)	
Þ	10	(2CData (c2cdata)	
Þ		R1P1 - Compressor R1P1 (comp R1P1)	
Þ		R1P2 - Compressor R1P2 (comp_R1P2)	
Þ	2	H1 - Hütte (comp H1)	
Þ		B1 (comp B1)	
Þ		B2 (comp B2)	
Þ		B3 (comp B3)	
Þ		B4 (comp B4)	
Þ	12	B5 (comp B5)	
Þ		E1 - Electrolysis (comp E1)	
Þ	 a) 	E1P1 (comp_E1P1)	
Þ	- 29	S1 (comp_S1)	
Þ		S2 (comp_S2)	
Þ		S3 (comp_S3)	
Þ		S4 (comp_S4)	
⊳		S5 (comp_S5)	
Þ		SP1 (comp_SP1)	
Þ	: 15	SP2 (comp_SP2)	
Þ	< 10 ¹	SP3 (comp_SP3)	
Þ	-	SP4 (comp_SP4)	
Þ	•	SP5 (comp_SP5)	
Þ	. 10	G1 (comp_G1)	
Þ	- 43	G2 (comp_G2)	
Þ		G3 (comp_G3)	
Þ		B1b - ePREOS y (comp_B1b)	
Þ	e 🕫	B1c - eSRK y (comp_B1c)	
Þ	< 10	B1d - ePREOS Pressure (comp_B1d)	
₽		B1e - eSRK Pressure (comp_B1e)	
Þ		B2b - ePREOS (comp_B2b)	
Þ	5 9 5	B2c - eSRK (comp_B2c)	
Þ		B2d - ePREOS Pressure (comp_B2d)	
Þ		B2e - eSRK Pressure (comp_B2e)	
Þ		E1P2 - Compressor E1P2 (comp_E1P2)	
Þ	1.5	SIP1 - Compressor SIP1 (comp_SIP1)	
P		S2P1 - Compressor S2P1 (comp_S2P1)	
P		S3P1 - Compressor S3P1 (comp_S3P1)	
Þ		S4P1 - Compressor S4P1 (comp_S4P1)	
Þ	10	S5P1 - Compressor S5P1 (comp_S5P1)	
P		S1P2 - Compressor S1P2 (comp_S1P2)	
P	10	SZP2 - Compressor SZP2 (comp_S2P2)	
P	1	53P2 - Compressor 53P2 (comp_53P2)	
P	-	M1 - Mixing BFG/BOFG (comp_M1)	
P	000	Study 1 - Stationary	
P	000	Study 2 - Time Dependent	
P	000	Study 3 - Time Dependent	
P	100	Study 4 - Time Dependent	
P	00	study 5 - Time Dependent	







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

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







90 Days Process Simulation – Synthesis Gas Quality at R1



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



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Carbon2Chem[®] – Further Steps

State of work

A transient flowsheet model for methanol production from steel mill gases has been successfully 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)

We wish to acknowledge the German government and the Bundesministerium für Bildung und Forschung (BMBF) for the financial support (FKZ 03EK3037D) of this work.

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Federal Ministry of Education and Research





