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DEVELOPMENT AND VALIDATION OF A REDUCED ONE-DIMENSIONAL MODEL FOR ACCELERATED SIMULATION OF COAL GASIFICATION

Mathias Hartwich, André Bader, Andreas Richter, Bernd Meyer

REDUCED ORDER MODEL

Nowadays, numerical models are more and more used to optimize high-temperature conversion processes and to develop new technologies, e.g. for more efficient, low CO_2 conversion processes. Despite its promising capabilities, the high computational costs for CFD prevents its use for comprehensive parameter studies or for a fully automated process optimization. The application of reduced order models can solve these issues and enables:

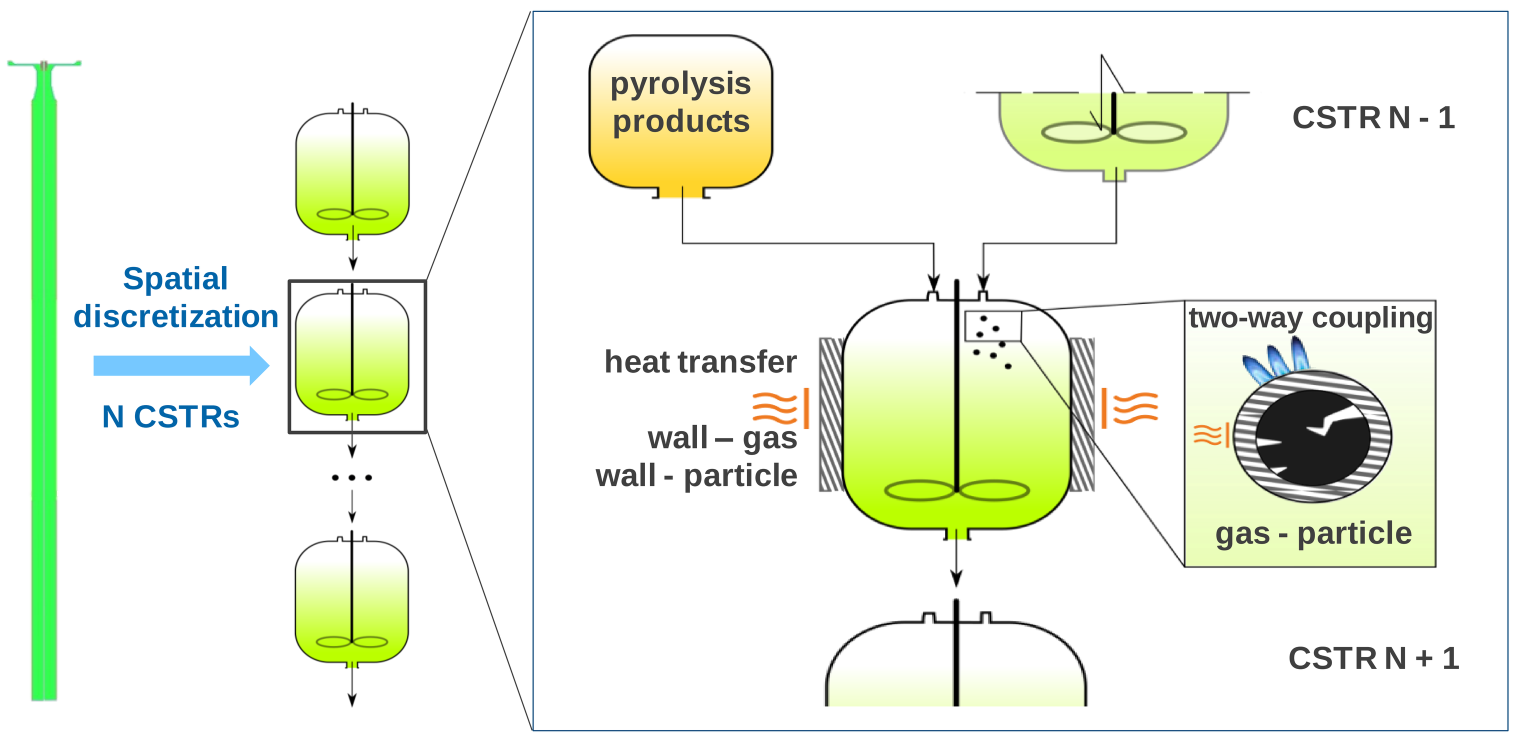
- comprehensive parameter studies
- fully automated process optimization
- advanced analysis of experiments.

Combining reduced order models, experimental validation and detailed CFD-models, the reliable and efficient development of new technologies within defined confidence intervals is feasible.

MODEL DESCRIPTION

In this study, a Python based reduced order model was developed. It includes

- detailed gas-phase chemistry (via Cantera)
- detailed intrinsic char conversion models
  - different particle evolution models
  - representation of kinetically controlled and diffusion controlled regimes
- two-way coupling of fluid and solid phase
- heat transfer between the two phases and to the wall



The governing equations for the solid phase can be formulated as follows:

$$\frac{\partial T_p}{\partial t} = \frac{1}{m_p c_p} \cdot hA_p \cdot (T_{gas} - T_p) + \sigma \epsilon_p A_p (T_{wall}^4 - T_p^4) - R \cdot m_C \cdot H_R$$

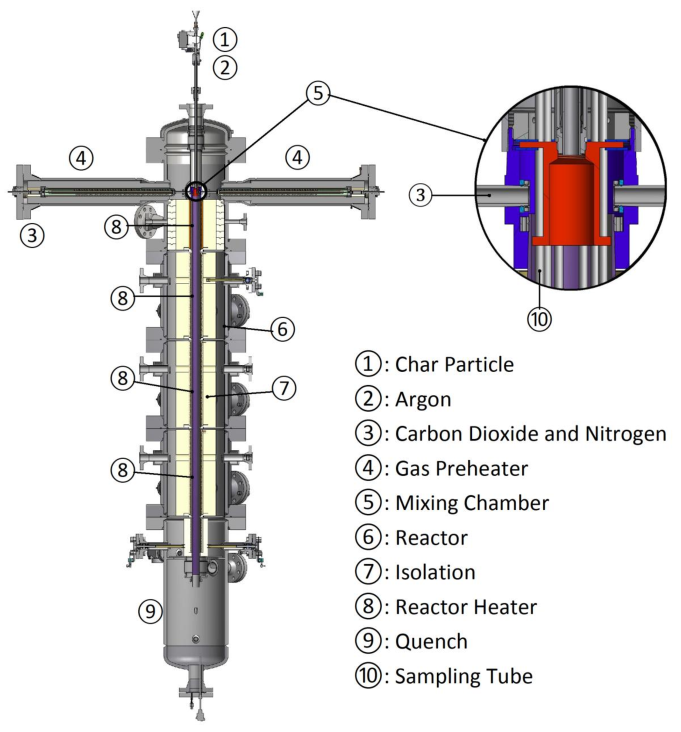
$$\frac{\partial X_C}{\partial t} = R \cdot (1 - X_C)$$

$$\frac{\partial u_p}{\partial t} = \left(1 - \frac{\rho_{gas}}{\rho_p}\right) \cdot \vec{g} + 3c_d \cdot \rho_{gas} \cdot \frac{|u_p - u_{gas}|(u_{gas} - u_p)}{8 r_p \rho_p}$$

MODEL VALIDATION

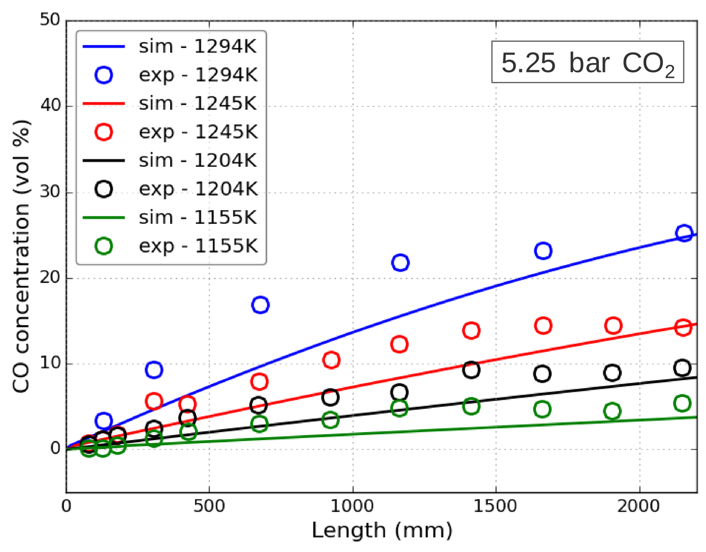
Validation of the sub models and the overall model is necessary to proof the correctness of the model. Ideally experiments for validation of the data are available.

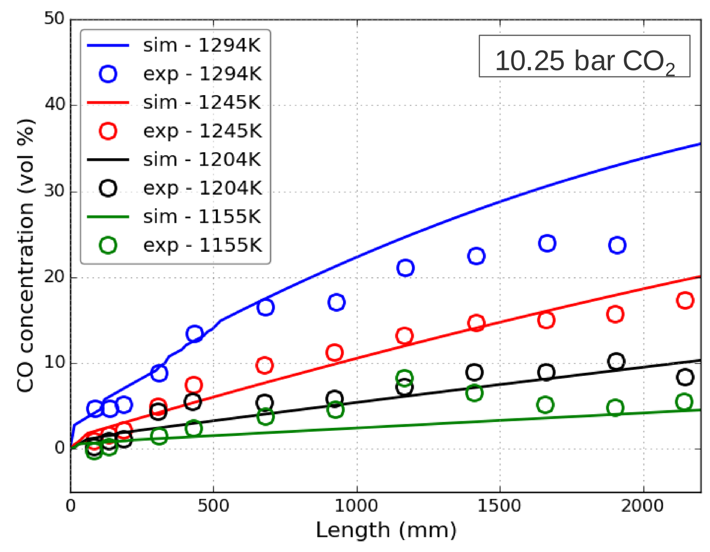
Experiments for studying the influence of the temperature and CO_2 concentration on the Boudouard reaction at a pressure of 21 bar were carried out using the pressurized drop tube reactor KIVAN[1] (at TU Bergakademie Freiberg). Some basic settings are listed in the table below.

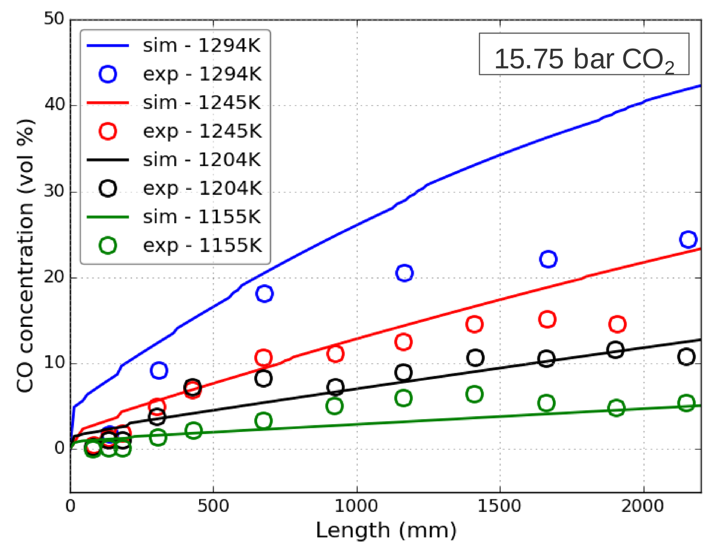


	Value	Unit
Reactor tube heated length	2.7	m
Reactor tube diameter	0.06	m
maximum pressure	100	bar
maximum temperature	1420	K
coal feed stream	11	g/min
gas feed mass flow (CO_2, N_2)	100	L/min STP
particle diameter	63-200	µm

Once the sub models are validated, the overall model can be validated. Therefore, integral quantities from experiments have to be used, for example the molar concentration of CO along the reactor can be compared for the different temperature and pressure conditions. As can be seen, for lower partial pressure of CO, the reduced order model predicts the gas phase composition quite well. Especially the final CO concentration at the outlet meet the experiments. For higher CO partial pressure and temperature, the model over predicts the conversion at the end of the reactor.[1]







CONCLUSION

In combination with a systematic model assessment by means of CFD and test facilities, reduced order models can be reliably employed in a defined confidence interval. Thereby it can be used for further efficient development of gasification technology, rapid prototyping and experimental data analysis.[2,3,4,5,6,7] Reduced order models can be a substantial link between detailed process modeling using CFD and experimental validation of new technology approaches.

REFERENCES

[1] Gonzalez, V. et al. 2018. "Experimental Investigations on Lignite Char Gasification Kinetics Using a Pressurized Drop Tube Reactor." Fuel 224: 348–56.
[2] Safronov, D. et al. 2017. "Numerical study on entrained-flow gasification performance using combined slag model and experimental characterization of slag properties." Fuel Process Technology 161: 62–75
[3] Förster,,T. et al. 2017. "3D Numerical Study of the Performance of Different Burner Concepts for the High-Pressure Non-Catalytic Natural Gas Reforming Based on the Freiberg Semi-Industrial Test Facility Hp Pox." Fuel 203: 954–63.
[4] Voloshchuk, Y. et al. 2017. "Numerical Study of Natural Gas Reforming by Non-Catalytic Partial Oxidation Based on the Virtuhcon Benchmark." Chemical Engineering Journal 327: 307–19.
[5] Rößger, P. et al. 2018. "Performance of Different Optimization Concepts for Reactive Flow Systems Based on Combined CFD and Response Surface Methods." Computers & Chemical Engineering 108: 232–39.
[6] Schulze, S. et al. 2017. "Heat and Mass Transfer Within Thermogravimetric Analyser: From Simulation to Improved Estimation of Kinetic Data for Char Gasification." Fuel 187: 338–48.
[7] Bader, A., M. Hartwich, A. Richter, and B. Meyer. 2018. "Numerical and Experimental Study of Heavy Oil Gasification in an Entrained-Flow Reactor and the Impact of the Burner Concept." Fuel Processing Technology 169: 58–70.

Mathias Hartwich, M. Sc.
TU Bergakademie Freiberg · Institute of Energy Process Engineering and Chemical Engineering · Chair of Energy Process Engineering and Thermal Waste Treatment
Reiche Zeche · Fuchsmuehlenweg 9 · 09599 Freiberg, Germany · Phone: +49 3731 39-4511 · Fax: +49 3731 39-4555 · www.iec.tu-freiberg.de