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Implementation of Langmuir-Hinshelwood Kinetics in CFD Modeling of Entrained Flow Gasification

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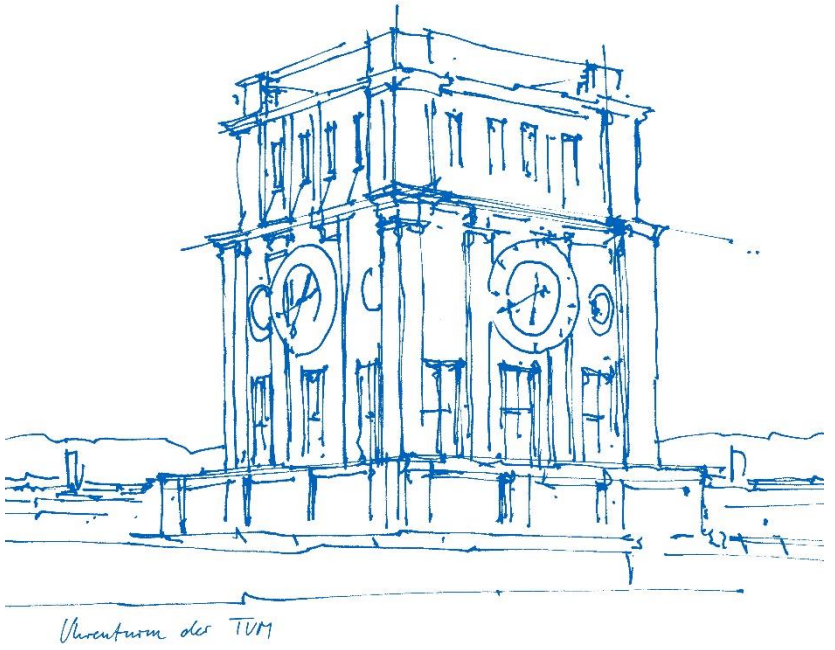
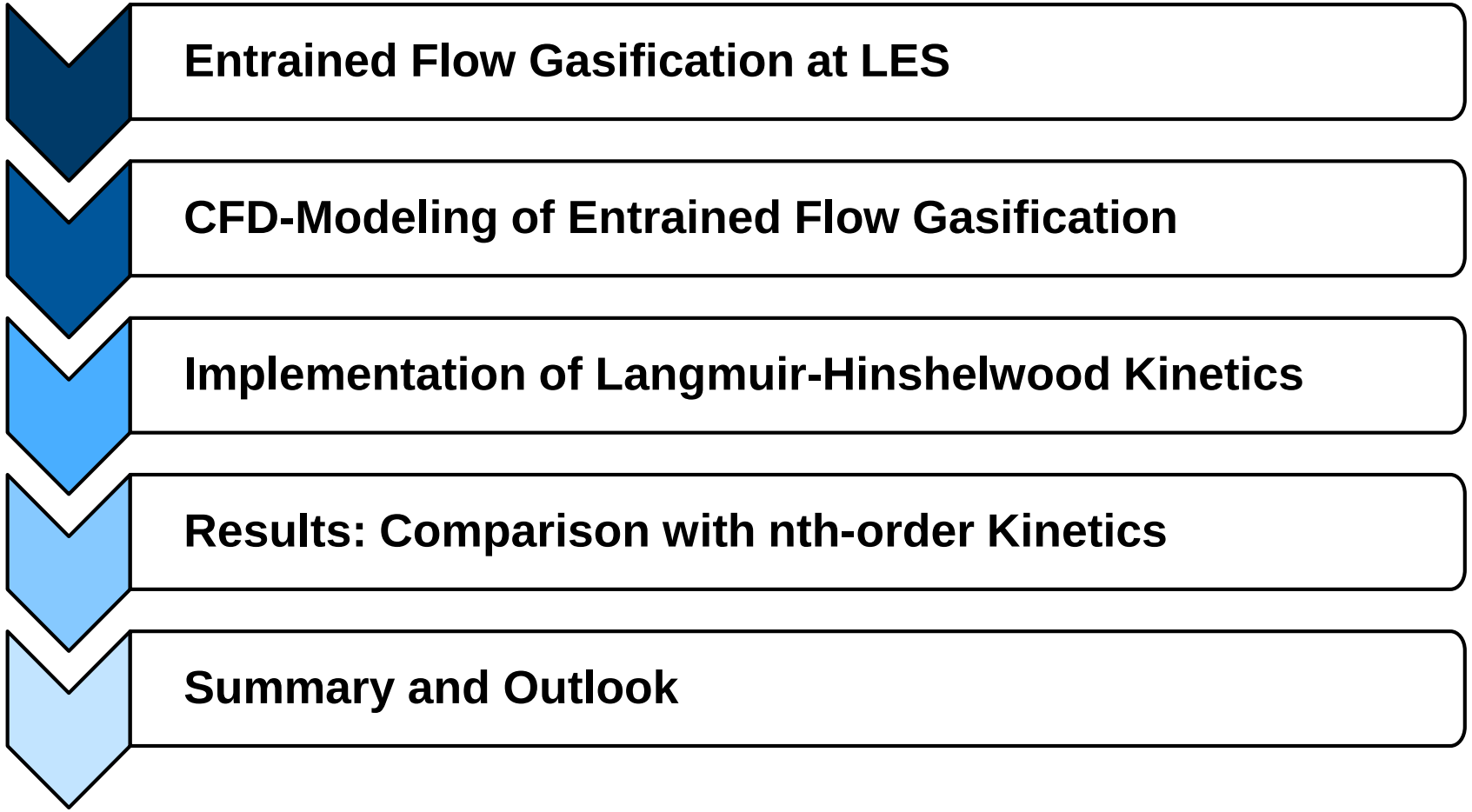
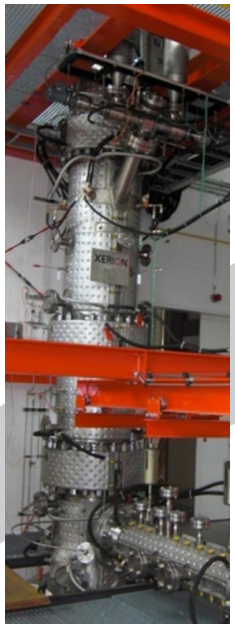


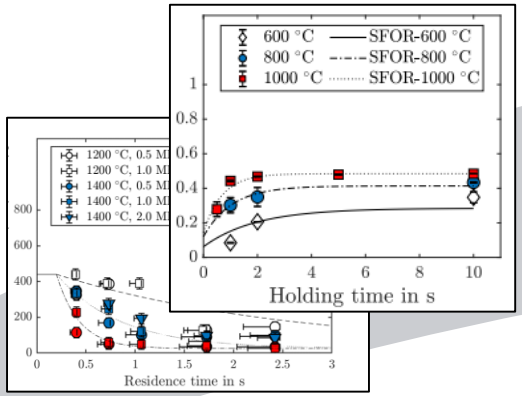
Structure


Entrained Flow Gasification at LES
CFD-Modeling of Entrained Flow Gasification
Implementation of Langmuir-Hinshelwood Kinetics
Results: Comparison with nth-order Kinetics
Summary and Outlook

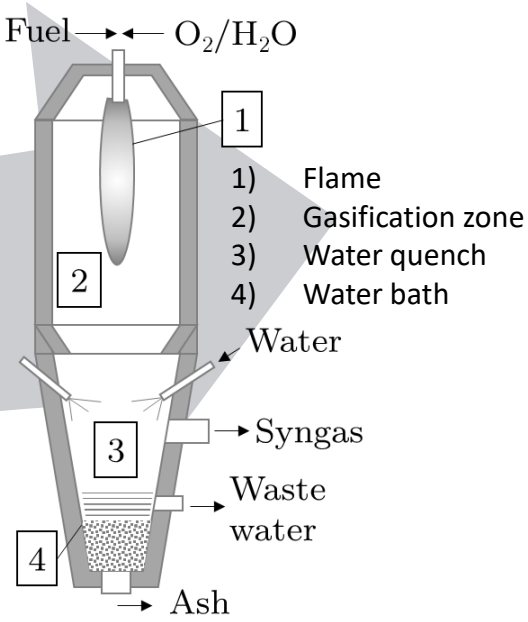
Overview

Model validation





$$r_{obs} = \frac{\eta \cdot S \cdot k_{0,1} \exp\left(-\frac{E_{A,1}}{RT}\right) p_{VM}}{1 + k_{0,a} \exp\left(-\frac{E_{A,a}}{RT}\right) p_{VM} + k_{0,b} \exp\left(-\frac{E_{A,b}}{RT}\right) p_{PG}}$$



1) Flame
2) Gasification zone
3) Water quench
4) Water bath

Biomass and Residues

Experiments

Models

Simulations

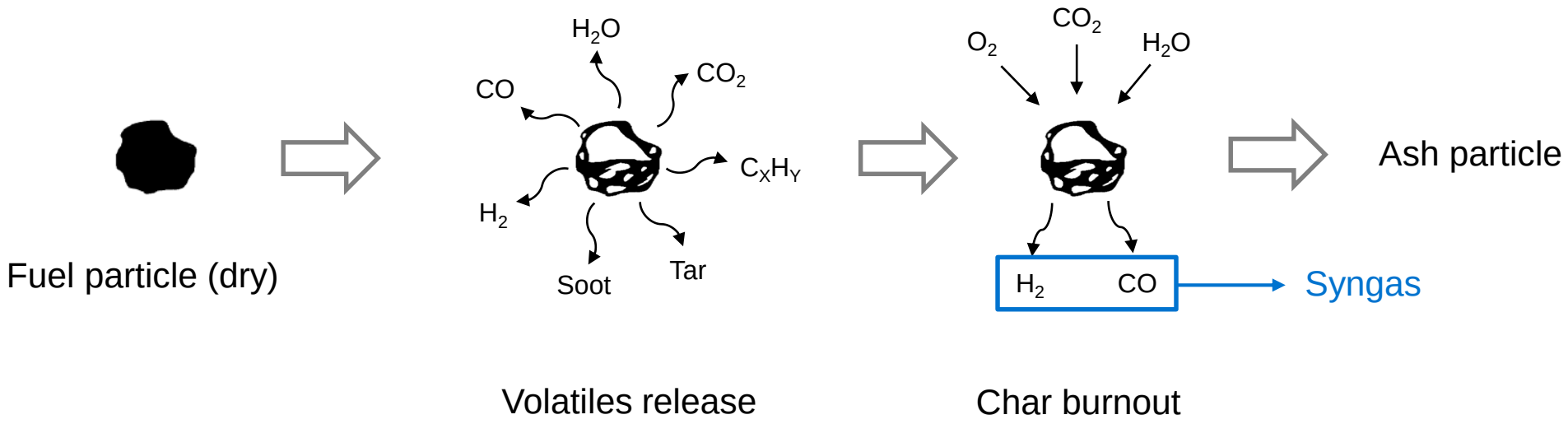
Design Optimization

Sensitivity analysis

Modeling Approach

- Entrained flow gasification conditions:
  - Temperature: 1200-1600 °C
  - Pressure: 1-40 bar
  - Fuel particle size: <300µm

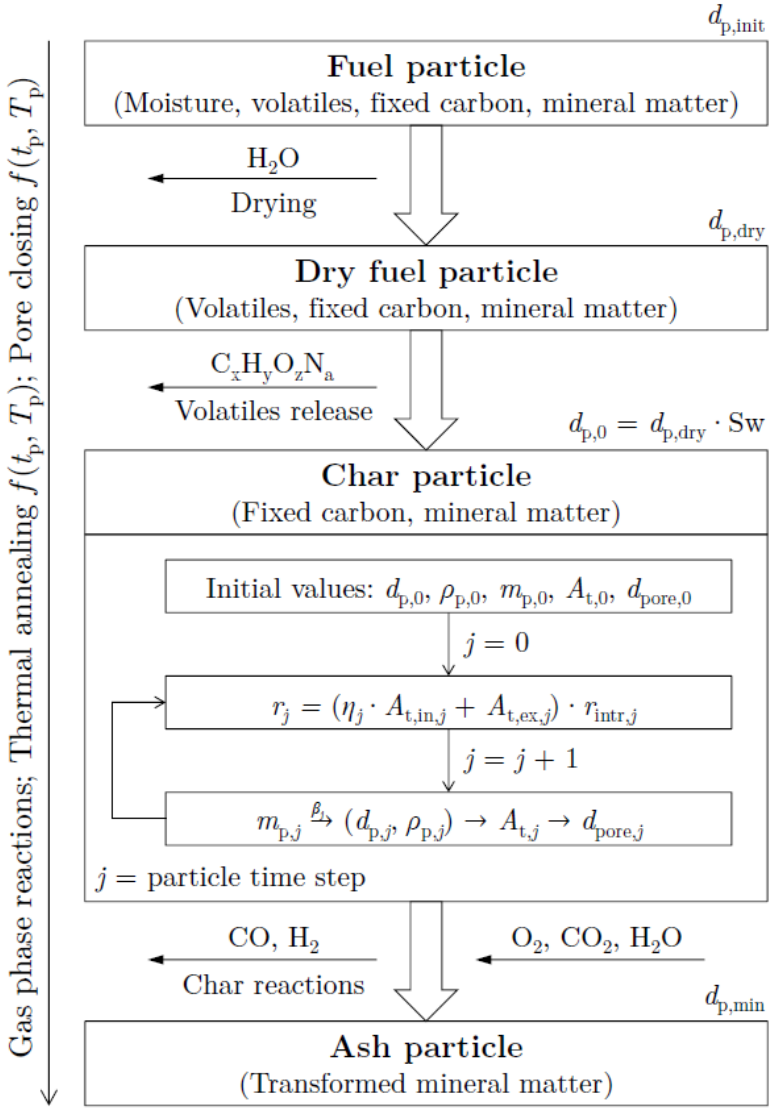
- Reduction of the gasification process on the following main steps:



Model Overview

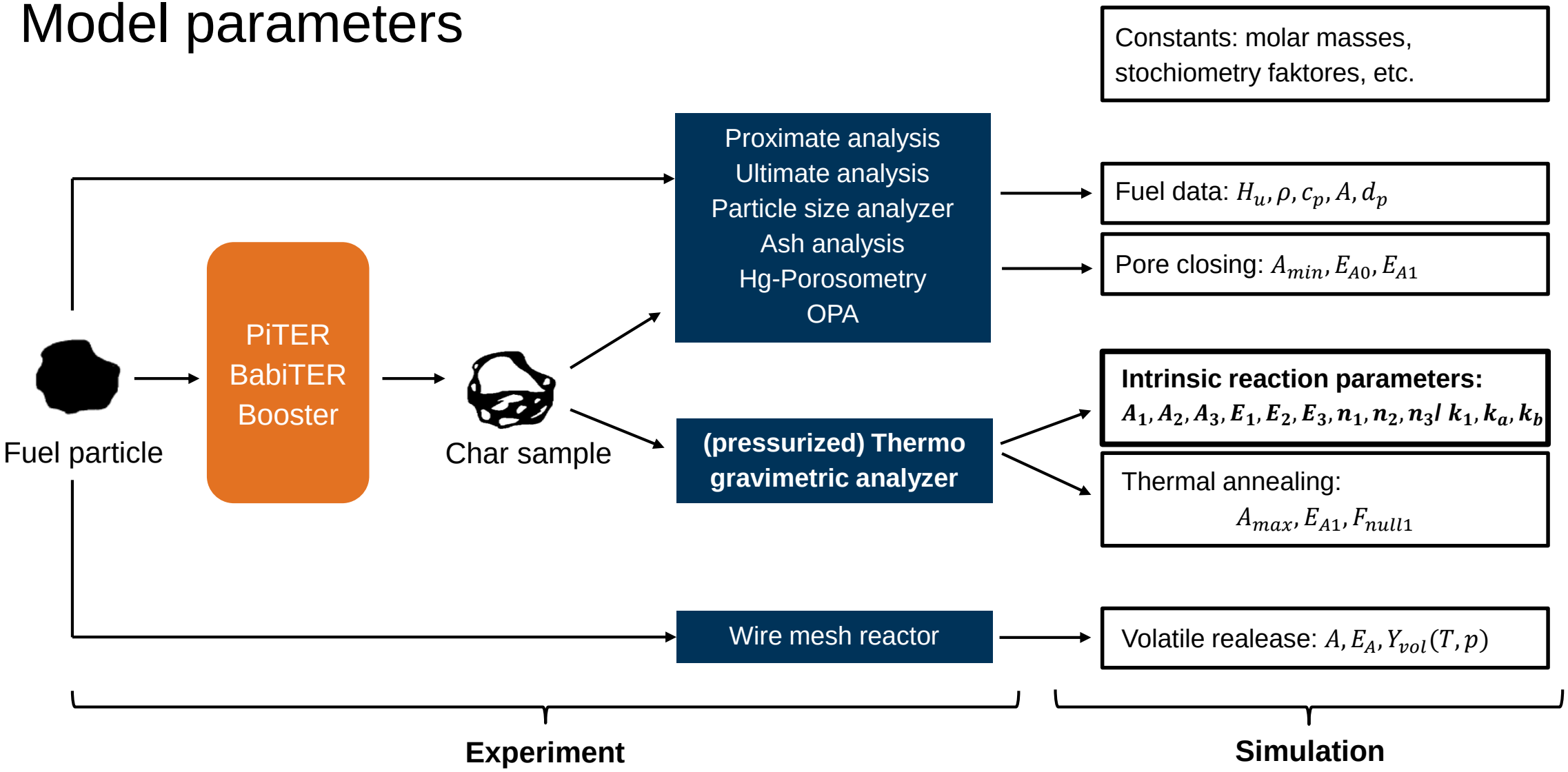
- Software: ANSYS Fluent, stationary RANS equations
- Modelling approach: DPM (discrete phase model): Eulerian-Lagrangian approach

  → Simulation of individual fuel particels as spheres
- Pyrolysis: SR-/TCR kinetic and $Y_{vol}(T,p)$ from measures
- Gas-phase reactions: Jones-Lindstedt-Mechanism
- Char reactions (O_2/CO_2/H_2O): User-Defined-Function
  - **Nth-order approach/ LH-approach with saturation and product inhibition**
  - Effectiveness factor to account for pore diffusion limitations
  - Thermal annealing submodel
  - Submodel for char structure developement
- Solution process by alternating calculation of the gas and solid phase



Source: Stefan DeYoung

Model parameters



Char Reaction Kinetics: Regime Dependent Reaction Rate

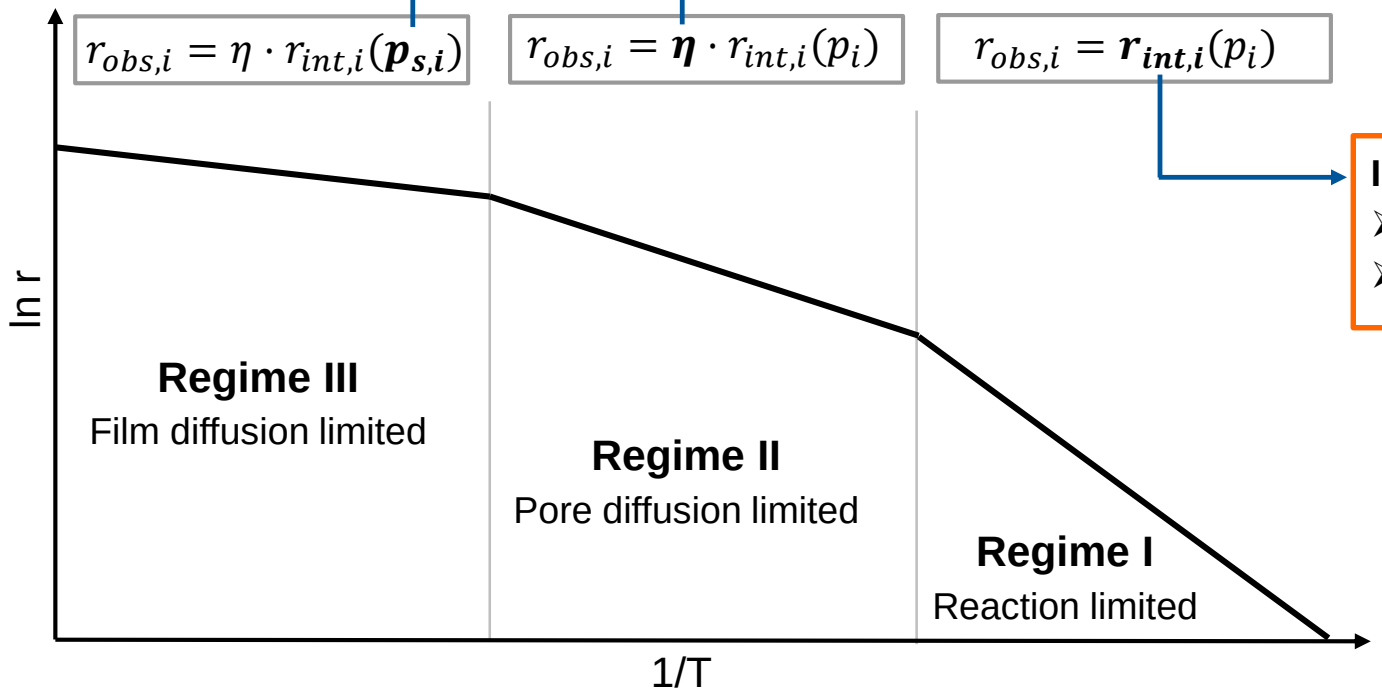
Partial pressure at particle surface

- Film diffusion in the particle boudary layer: $p_{s,i} < p_i$

Effectiveness factor:

- Function of Thiele Modulus $\phi_i(p_i)$
- Accounts for concentration gradient inside the particle

$r_{obs,i} = \eta \cdot r_{int,i}(\boldsymbol{p_{s,i}})$ $r_{obs,i} = \boldsymbol{\eta} \cdot r_{int,i}(p_i)$ $r_{obs,i} = \boldsymbol{r_{int,i}}(p_i)$



Intrinsic reaction rate:

- Nth order approach
- Langmuir Hinshelwood

Char Reaction Kinetics: Intrinsic Reaction Rate

Nth-order Approach

Intrinsic reaction rate:

$$\boldsymbol{r_{int,i} = k \cdot p_i^n = k_0 e^{-\frac{E_A}{RT}} \cdot p_i^n}$$

- 3 kinetic parameters (orange)
- Partial pressure of reactant gas p_i

Langmuir-Hinshelwood Kinetics

Intrinsic reaction rate:

$$\boldsymbol{r_{int,i} = \frac{k_1 \cdot p_i}{1 + k_a \cdot p_i + k_b \cdot p_j} = \frac{k_{0,1} e^{-\frac{E_{A,1}}{RT}} \cdot p_i}{1 + k_{0,a} e^{-\frac{E_{A,a}}{RT}} \cdot p_i + k_{0,b} e^{-\frac{E_{A,b}}{RT}} \cdot p_j}}$$

- 6 kinetic parameters (orange)
- Partial pressure of reactant gas p_i and product gas p_j
- Additional effects: Saturation and product gas inhibition

Observed reaction rate: $r_{obs,i} = \eta \cdot r_{int,i}(p_{s,i})$

- Partial pressure at particle surface → film diffusion limitation
- Effectiveness factor → pore diffusion limitation

Char Reaction Kinetics: Pore Diffusion

Observed reaction rate: $r_{obs,i} = \boldsymbol{\eta_i} \cdot r_{int,i}(p_{s,i})$

$$\eta_i = \frac{1}{\phi_i}\left(\frac{1}{\tanh(3 \cdot \phi_i)} - \frac{1}{3 \cdot \phi_i}\right)$$ (→ for spheres)

Nth-order

- Thiele Modulus: $\phi_i = \mathrm{f}(\mathrm{p_{s,i}})$

  Accounts for the concentration gradient inside the particle with pore diffusion

- Numerical calculation of $\mathrm{p_{s,i}}$ with a mass balance at particle surface:

$$reaction\ rate\ (p_{s,i}) = diffusion\ rate\ (p_{s,i})$$

Langmuir Hinshelwood

- Thiele Modulus: $\phi_i = \mathrm{f}(\mathrm{p_{s,i}}, \mathrm{p_{s,j}})$

- Calculation of $p_{s,j}$

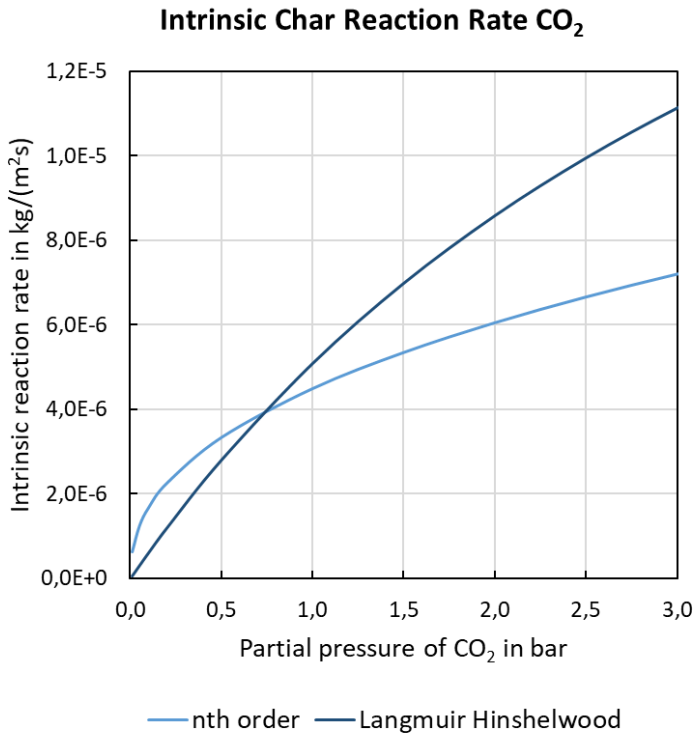
  Level 1: $\boldsymbol{p_{s,j} = p_j}$

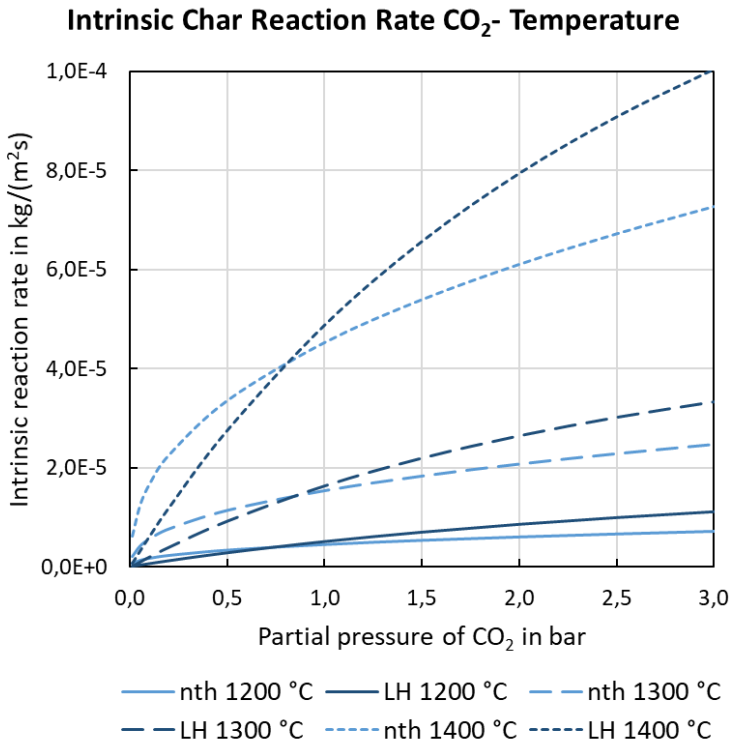
  Level 2: $p_{s,j}$ with film diffusion

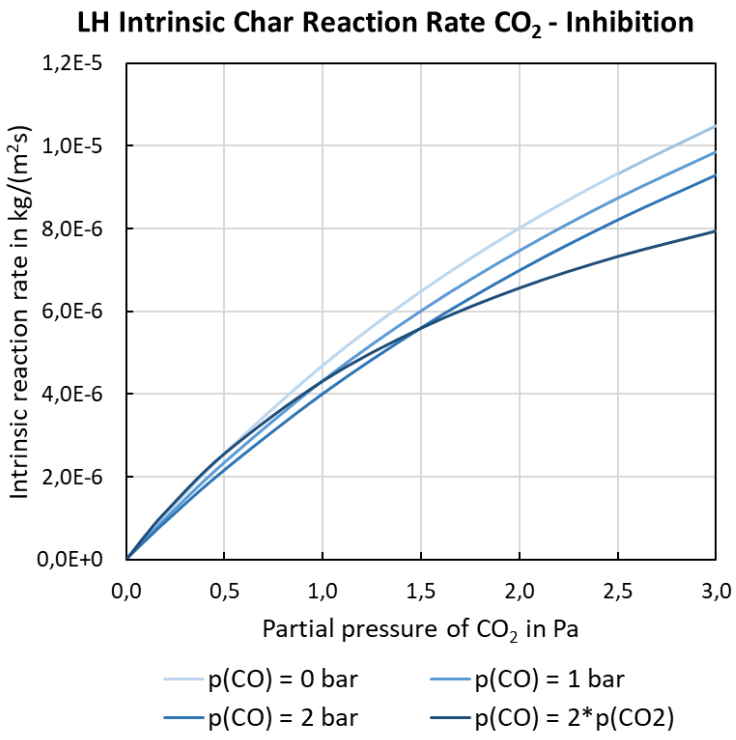
  Level 3: $p_{s,j}$ with film diffusion and concentration gradient inside the particle (e.g. with effectiveness factor for inhibition)

Intrinsic Reaction Kinetics of Torrefied Wood

Influence of operating conditions for CO_2 reaction



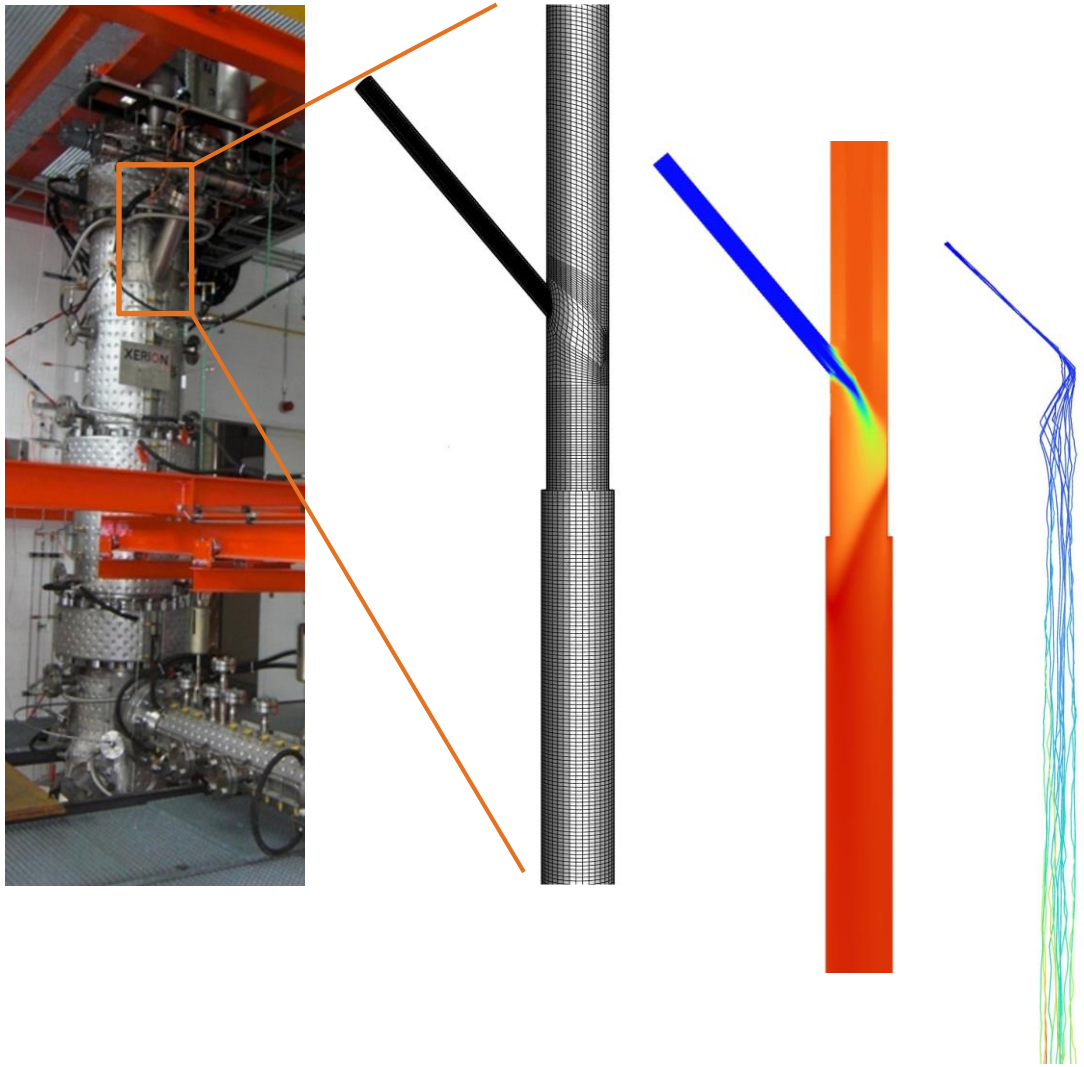




CFD Simulation of PiTER

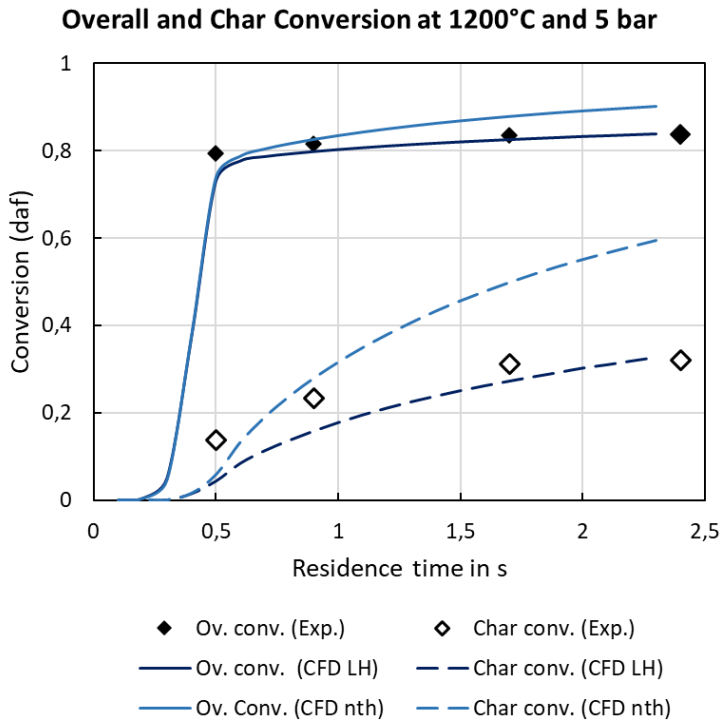
Pressurized High Temperature Entrained Flow Reactor

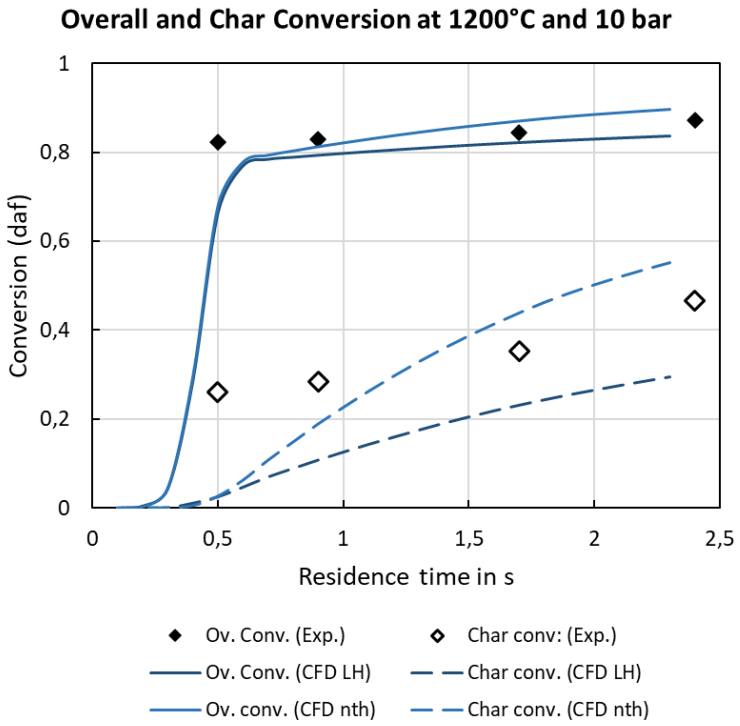
Boundary Conditions	
Fuel	Torrefied wood
Massflow	$1\ kg/s$
Particle diameter	$10\ -300\ \mu m$
Wall temperature	$1200\ -1600\ °C$
Pressure	$5/\ 10/\ 20\ bar$
O/C ratio	1 (molar)
Residence time	$2{,}4\ s$
O_2 reaction	nth order
CO_2, H_2O reaction	Langmuir Hinshelwood

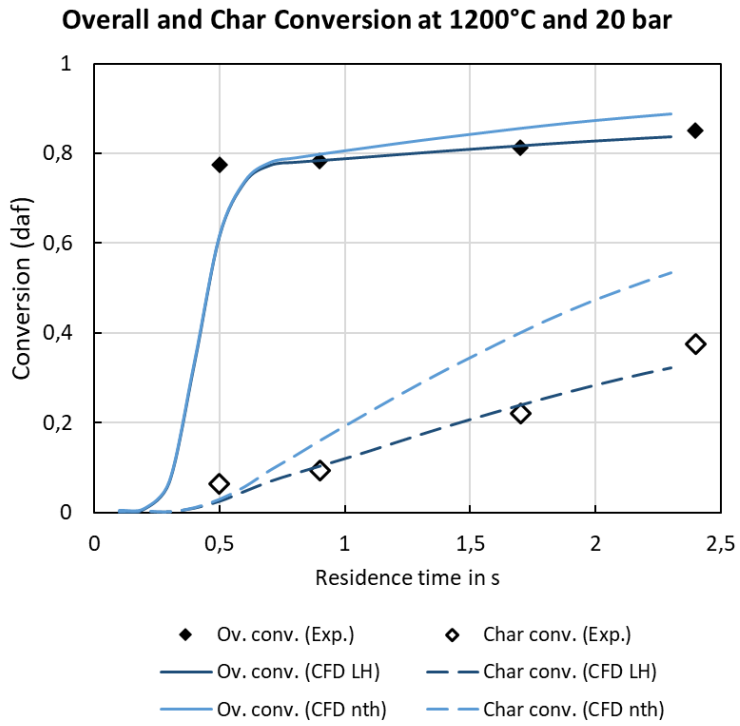


PiTER Simulation Results I

1200 °C with with pressure variation

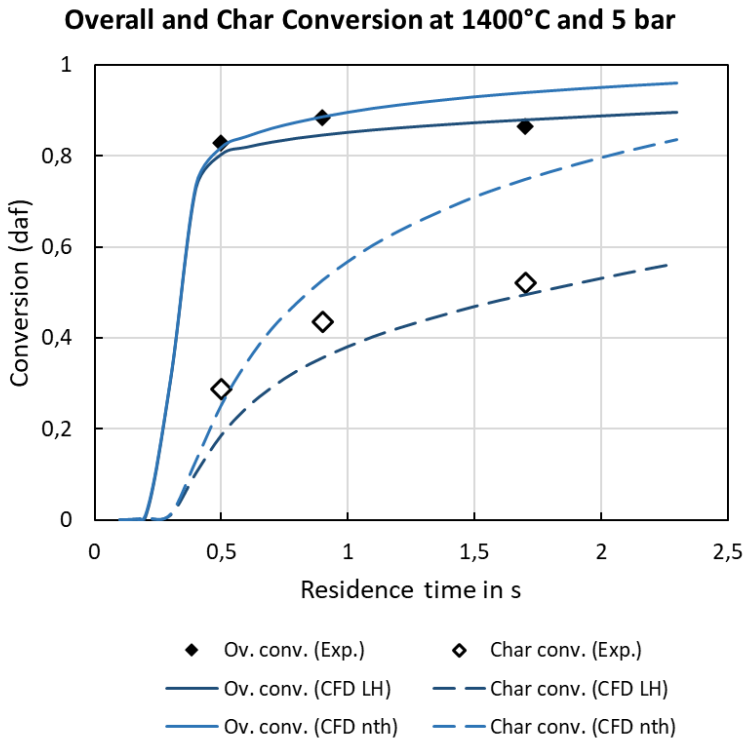


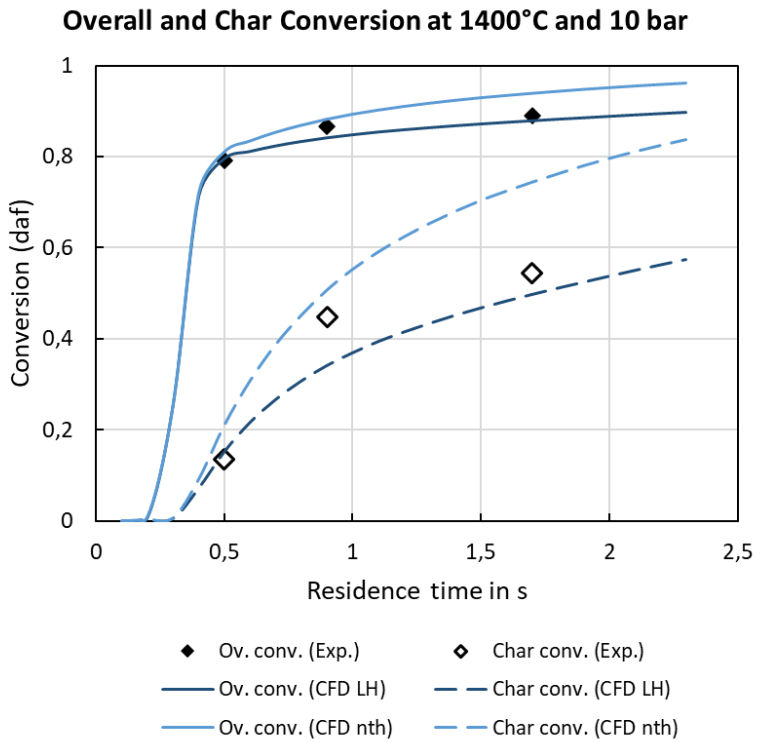




PiTER Simulation Results II

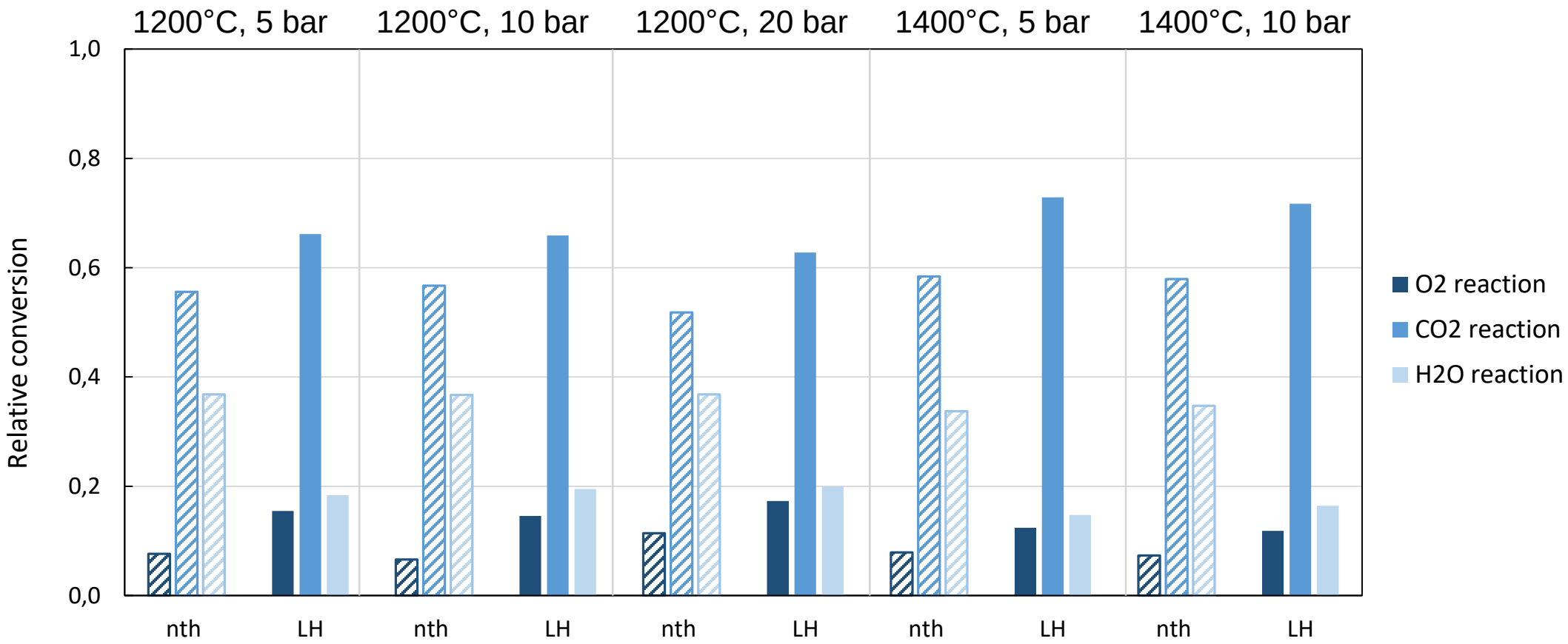
1400 °C with pressure variation





PiTER Simulation Results III

Relative char conversion with O_2, CO_2, H_2O



Summary and Outlook

- Successful implementation of Langmuir-Hinshelwood Kinectics to describe char reaction rates with CO_2 and H_2O in an CFD model for entrained flow gasification
- Kinetic studies and CFD-model results on a drop tube entrained flow reactor are showing a significant deviation of reaction kinetics over a wide range of partial pressures and temperatures
- Overall good prediction of measured char conversion and overall conversion
- Significant increase in relative char conversion of the CO_2 reaction

Next steps:

- Implementing a more accurate calculation of the partial pressure on the particle surface of the product gas
- CFD simulations on different reactor models from lab scale to industrial scale and different feedstocks
- Further model validation with experimental results of a lab-scale entrained flow reactor

Feel free to get in touch!

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