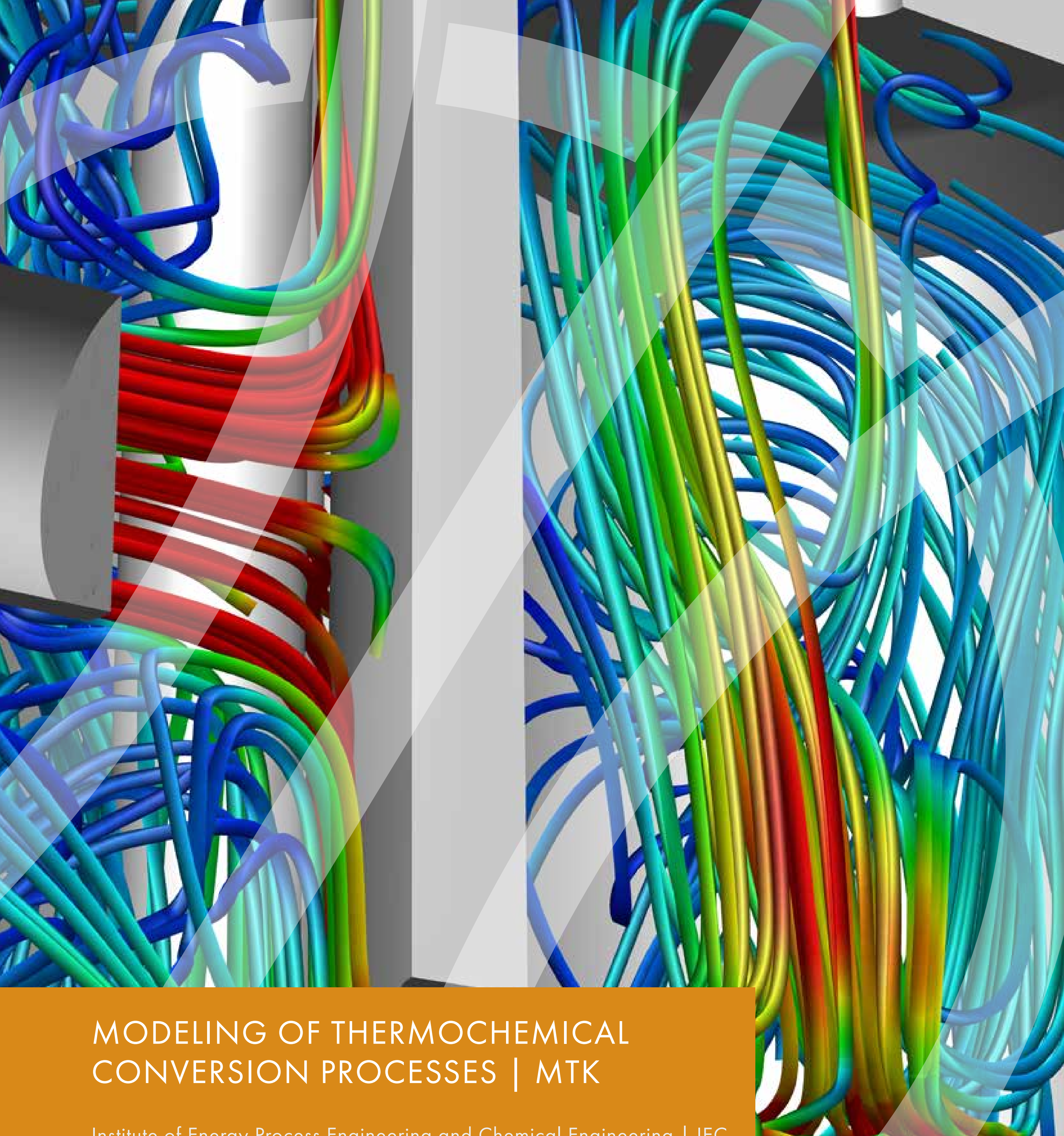


MODELING OF THERMOCHEMICAL CONVERSION PROCESSES | MTK

Institute of Energy Process Engineering and Chemical Engineering | IEC
TU Bergakademie Freiberg
Prof. Andreas Richter

TUBAF
The University of Resources.
Since 1765.

INSTITUTE OF
ENERGY PROCESS ENGINEERING AND
CHEMICAL ENGINEERING

PROFESSORSHIP FOR
MODELING OF THERMOCHEMICAL
CONVERSION PROCESSES

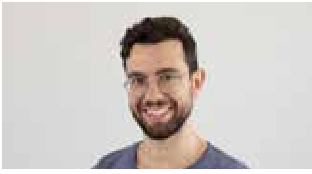
Team MTK

Prof. Andreas Richter
Professorship for Modeling of Thermocemical Conversion Processes

Fengbo An

- Modeling of reactive gas-solid systems
- Senior expert for reactor optimization

Johannes Scherer



- Modeling of thermo-chemical conversion of biogenic feedstocks
- Model driven process optimization and burner development

Lukas Porter

- Experimental and numerical study of fluidized-bed processes
- Expert in multivariate data analysis

Mohsen Gharib*

- Optical data analysis of high temperature and high-pressure processes and development of customized user tools
- Utilization of AI for automated flame analysis

Gabriel Gonzalez Ortiz

- Model development of HP-POX
- Model-driven design and optimization of high-temperature processes

Philip Rößger

- Expert for multi-criterial optimization of several high temperature conversion processes
- Model development for automated process optimization

Shreyas Rohit Srinivas

- High-resolved modeling of fixed-bed processes for chemistry and metallurgy
- Expert for experimental and numerical analysis of heat and mass transfer processes

Sesi Preetam Kota

- Development of future technologies based on high-resolved CFD
- Optimization of metallurgical processes

Sophie Rodmacher

- Electrification of high temperature processes with focus on plasma integration
- Development of reduced-order-models

Martin Hutter

- CFD-based modeling of glass melting processes for the integration of hydrogen
- Development of reduced-order-models for process control and optimization

Lukas Etzold

- High resolved modeling of flames
- Specialization on Large Eddy Simulations

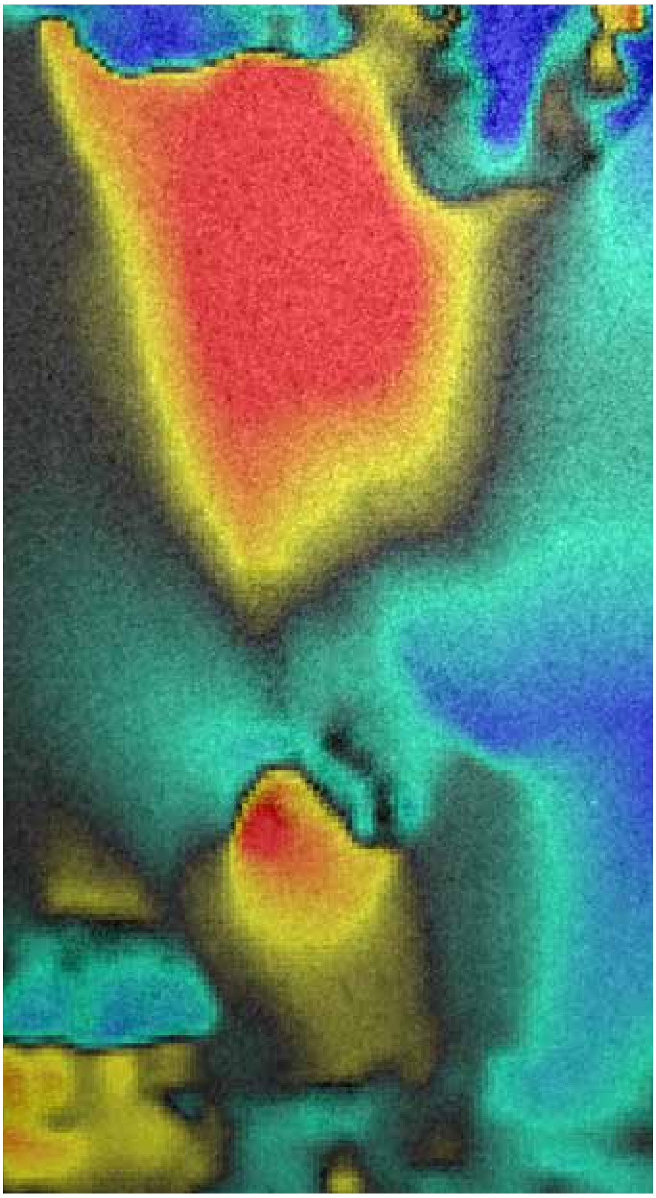
We would like to thank all our guest researchers, research partners and students for supporting our team with their scientific contributions.

** In cooperation with Professorship of Energy Process Engineering (EVT) and Fraunhofer Institute for Ceramic Technologies and Systems IKTS*

Preface

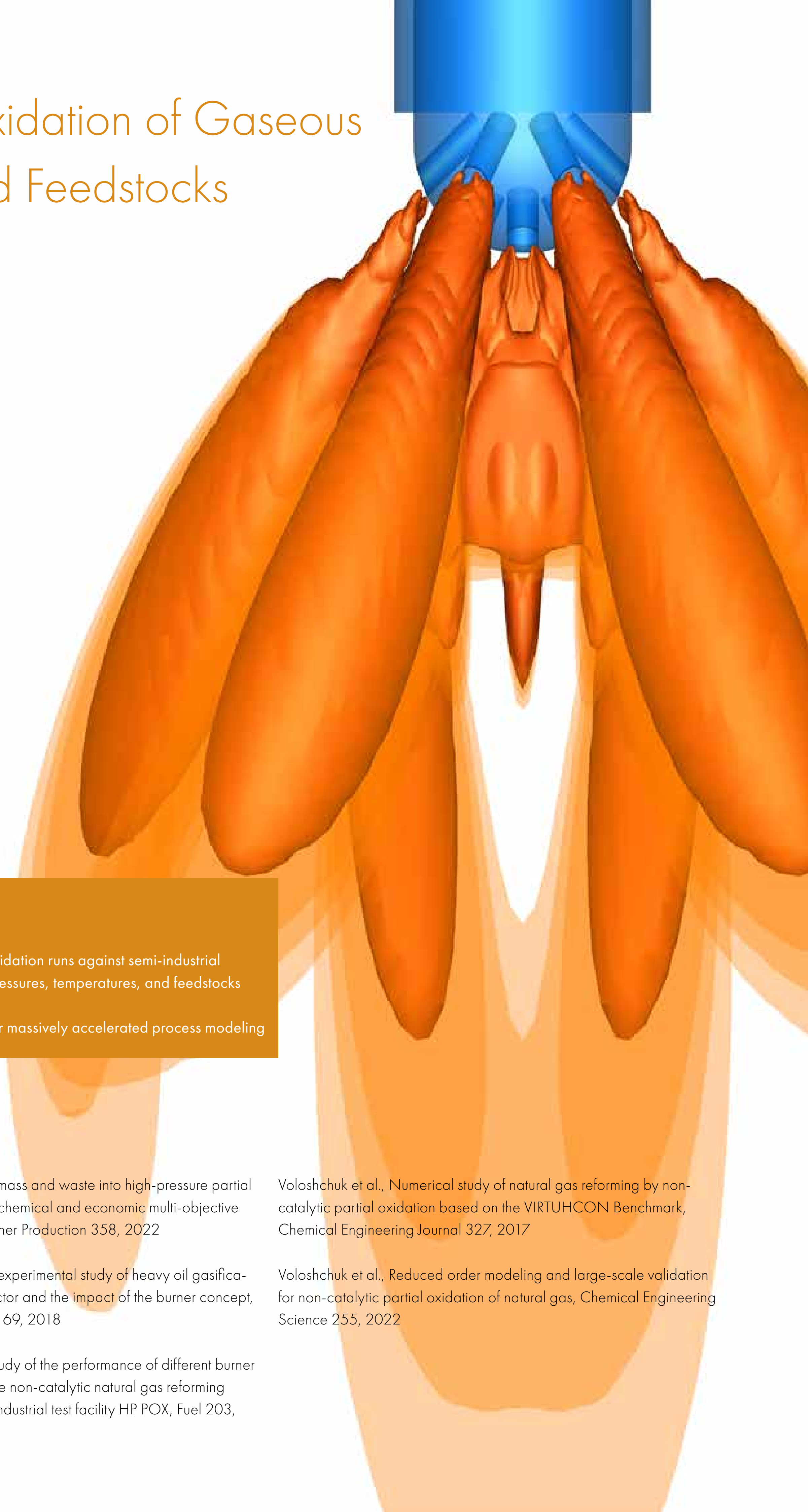
The development of new, sustainable technologies for the chemical or metallurgical industry, the computer-aided optimization of technical processes or the model-based evaluation of experiments – in each of these areas, modeling is an indispensable tool to accelerate development and work steps significantly and to test new concepts virtually on the computer.

The team of the Professorship Modeling of Thermochemical Conversion Processes (MTK) at the Institute of Energy Process Engineering and Chemical Engineering develops the necessary models and uses them to calculate, test and optimize a wide variety of reactors and syntheses. The R&D activities cover the entire range of scales from chemically reacting single particles to the whole reactor and extend from fundamental research to technology development together with our partners from industry and business.



Content

Partial Oxidation of Gaseous and Liquid Feedstocks



Highlights

More than 20 successful validation runs against semi-industrial process data for different pressures, temperatures, and feedstocks

Reduced-order modeling for massively accelerated process modeling

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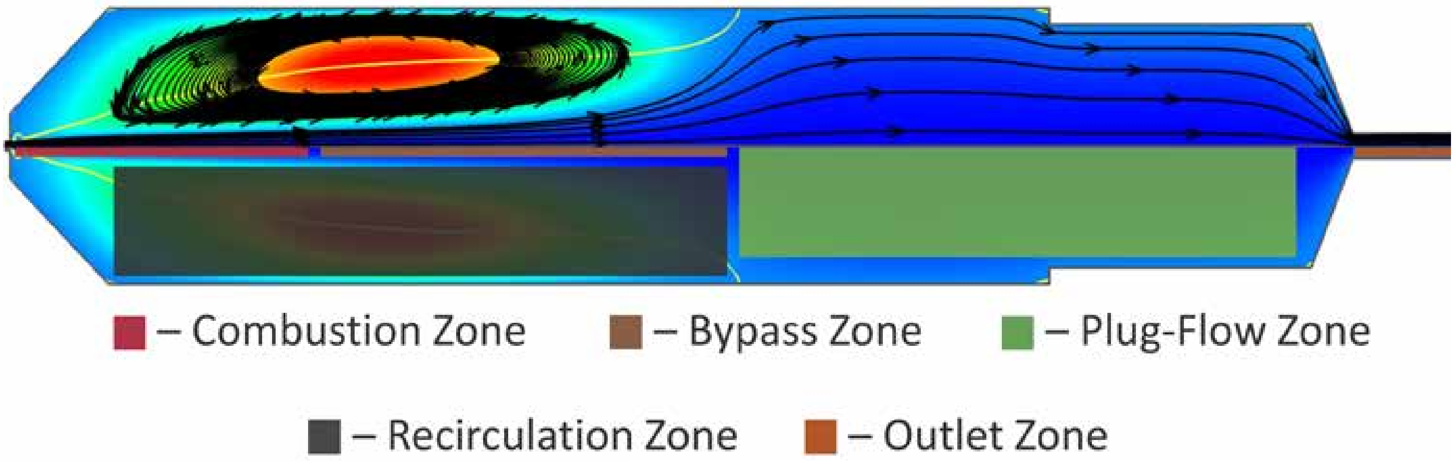
Rößger et al., Integrating biomass and waste into high-pressure partial oxidation processes: Thermochemical and economic multi-objective optimization, Journal of Cleaner Production 358, 2022

Bader et al., Numerical and experimental study of heavy oil gasification in an entrained-flow reactor and the impact of the burner concept, Fuel Processing Technology 169, 2018

Förster et al., 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, 2017

Voloshchuk et al., Numerical study of natural gas reforming by non-catalytic partial oxidation based on the VIRTUHCON Benchmark, Chemical Engineering Journal 327, 2017

Voloshchuk et al., Reduced order modeling and large-scale validation for non-catalytic partial oxidation of natural gas, Chemical Engineering Science 255, 2022



Advanced CFD Modeling

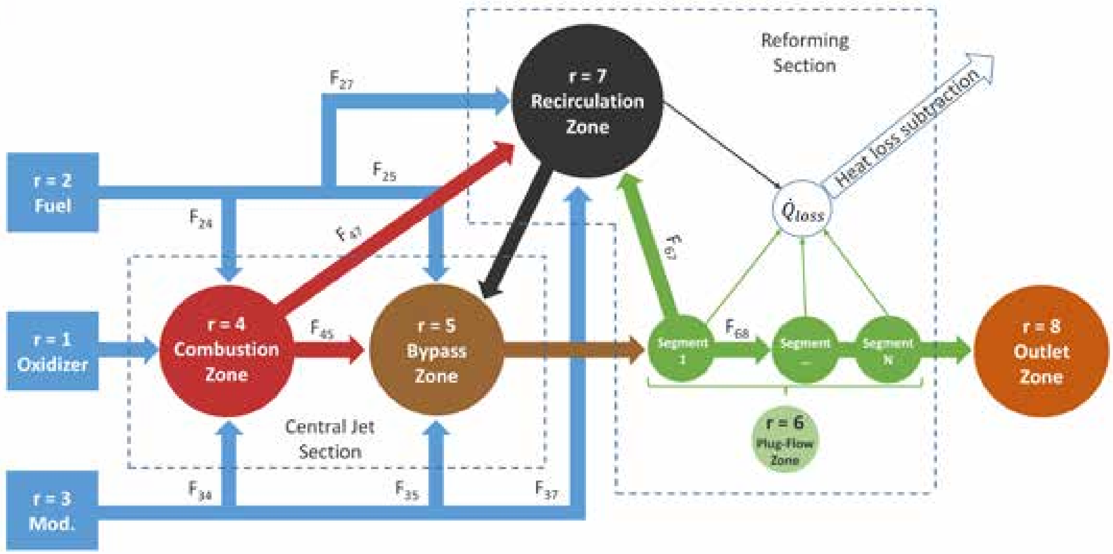
- Catalytic and non-catalytic reforming
- Conventional and alternative feedstocks (biogas, bio-oil, lean gases, process gases)
- Detailed process analysis
- Burner development and optimization

Process Optimization

- Automated process optimization
- Multi-objective multi-parameter optimization

Reduced-Order Modeling

- Rapid process modeling
- Excellent agreement with CFD results and industrial data



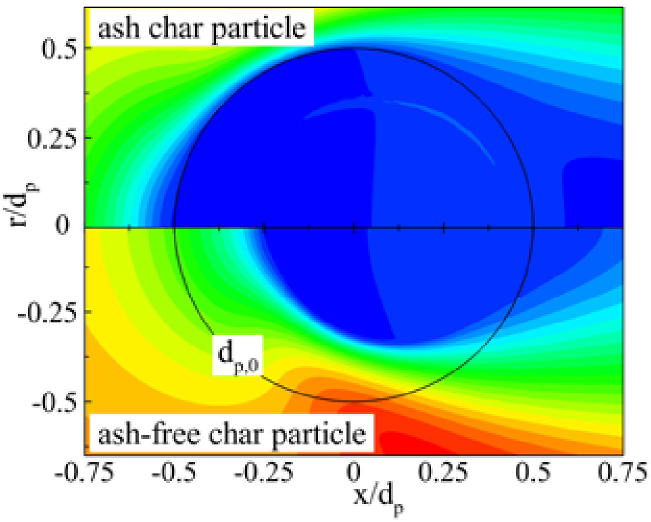
High Temperature Conversion Processes In Chemistry

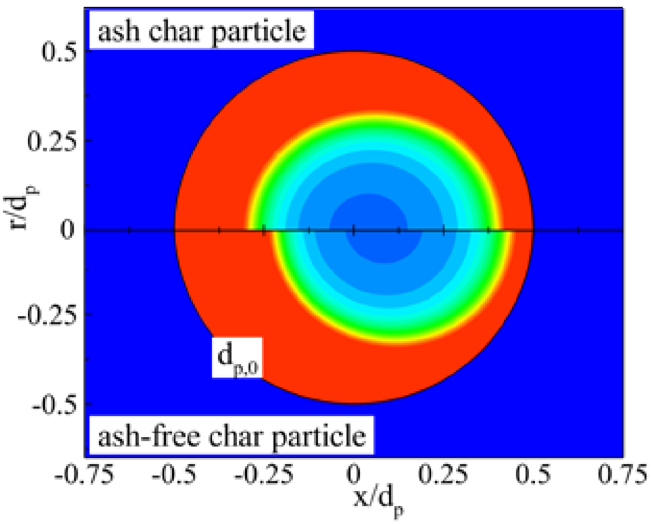
Process Modeling

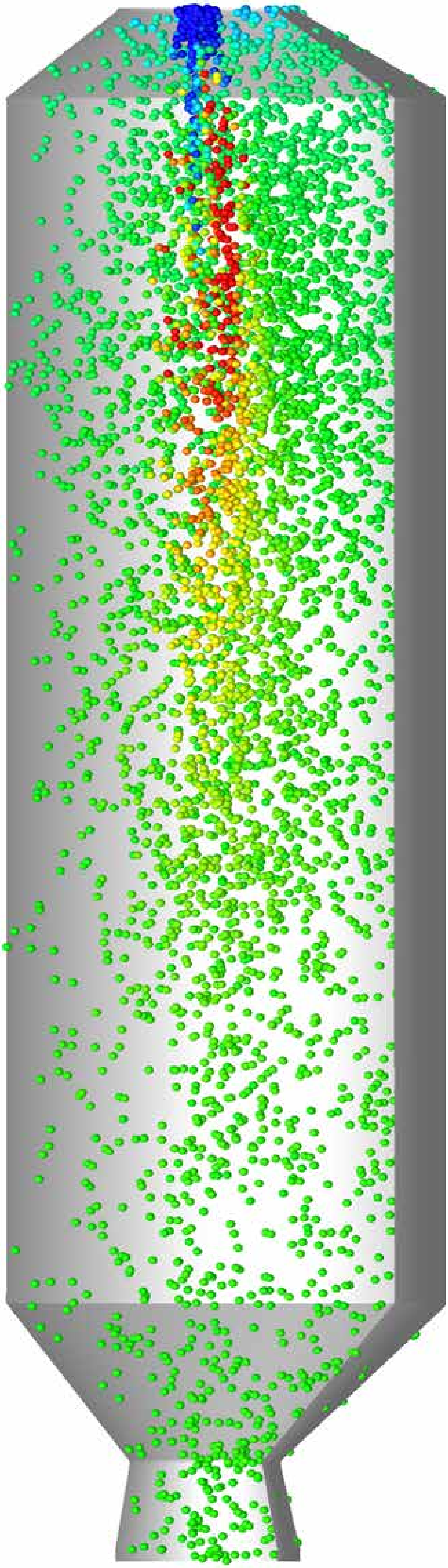
- Entrained-flow, fluidized-bed and fixed-bed processes for the conversion of biomasses, residues and other carbonaceous feedstocks
- Burner and process development

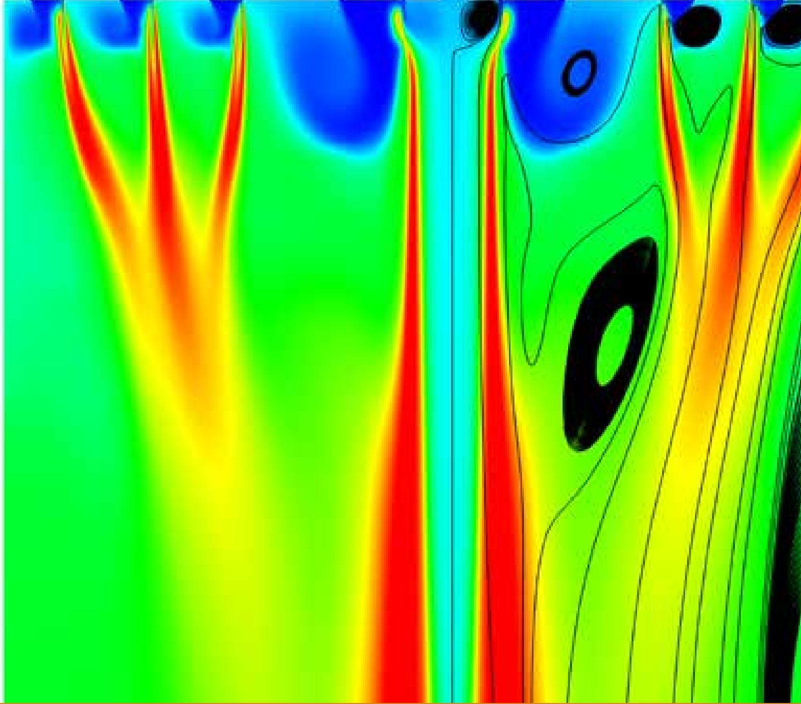
Process scale-up

- Automated multi-objective process optimization
- Advanced submodels for char conversion, slag formation and phosphor release
- Model validation against large-scale pilot plants at IEC for several reactor types
- Multi-step process validation from isolated particle to entire process





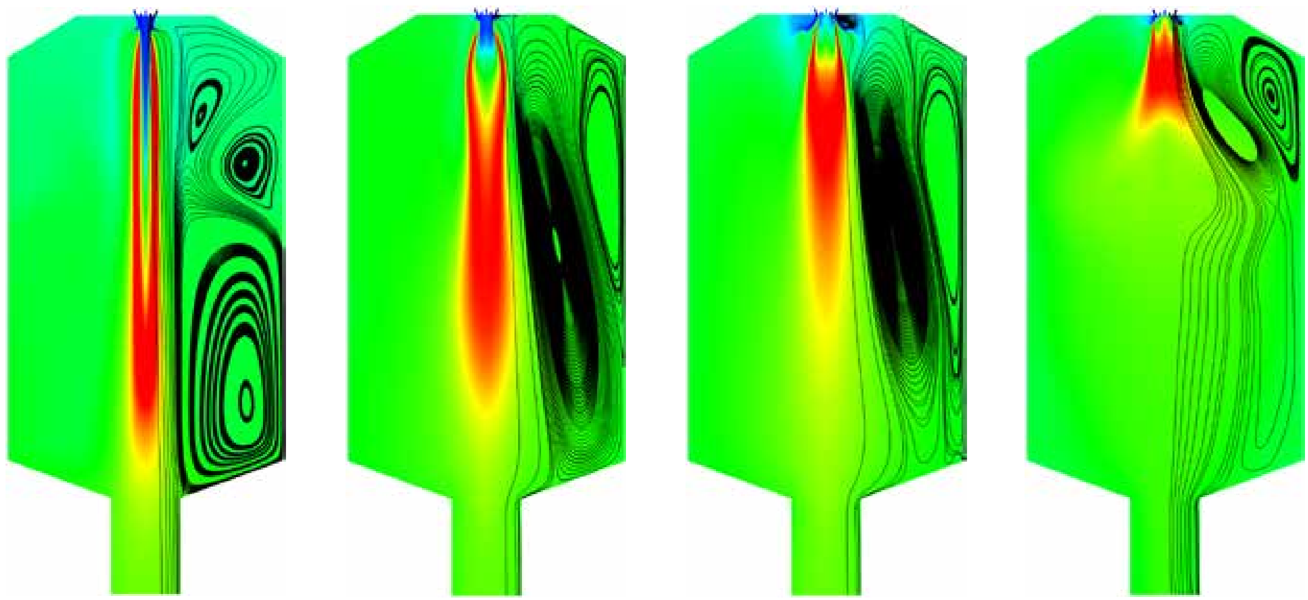




Highlights

Process development and optimization for several partners from industry

Validated large-scale models for a variety of conversion processes available



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Nguyen et al., The Morphology Evolution of Char Particles during Conversion Processes, Combustion and Flame 226, 2021

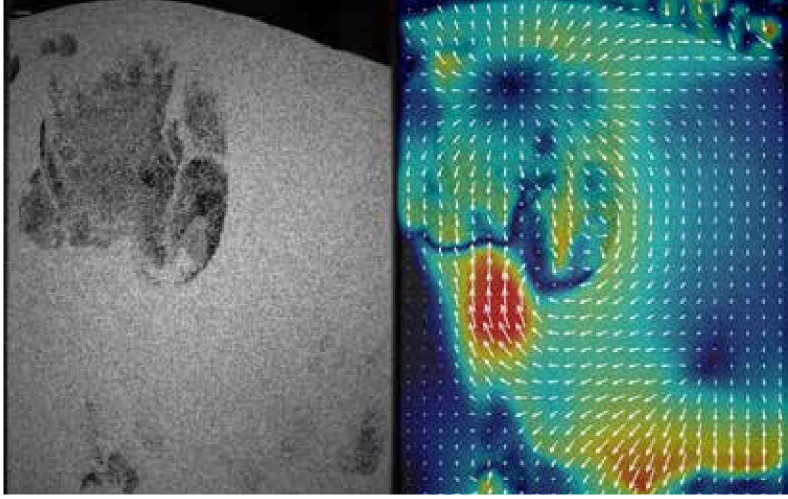
Safronov et al., Numerical study on entrained-flow gasification performance using combined slag model and experimental characterization of slag properties, Fuel Processing Technology 161, 2017

Nguyen et al., The shape development of spherical and non-spherical char particles in the flame zone of an entrained-flow gasifier –A numerical study, International Journal of Heat and Mass Transfer 149, 2020

Nguyen et al., A hybrid particle model with advanced conversion parameters and dynamic drag model applied for the CFD modeling of an entrained-flow gasifier, Combustion and Flame 240, 2022

Kriebitzsch et al., LES simulation of char particle gasification at Reynolds numbers up to 1000, Combustion and Flame 211, 2020

Fluidized-Bed Processes

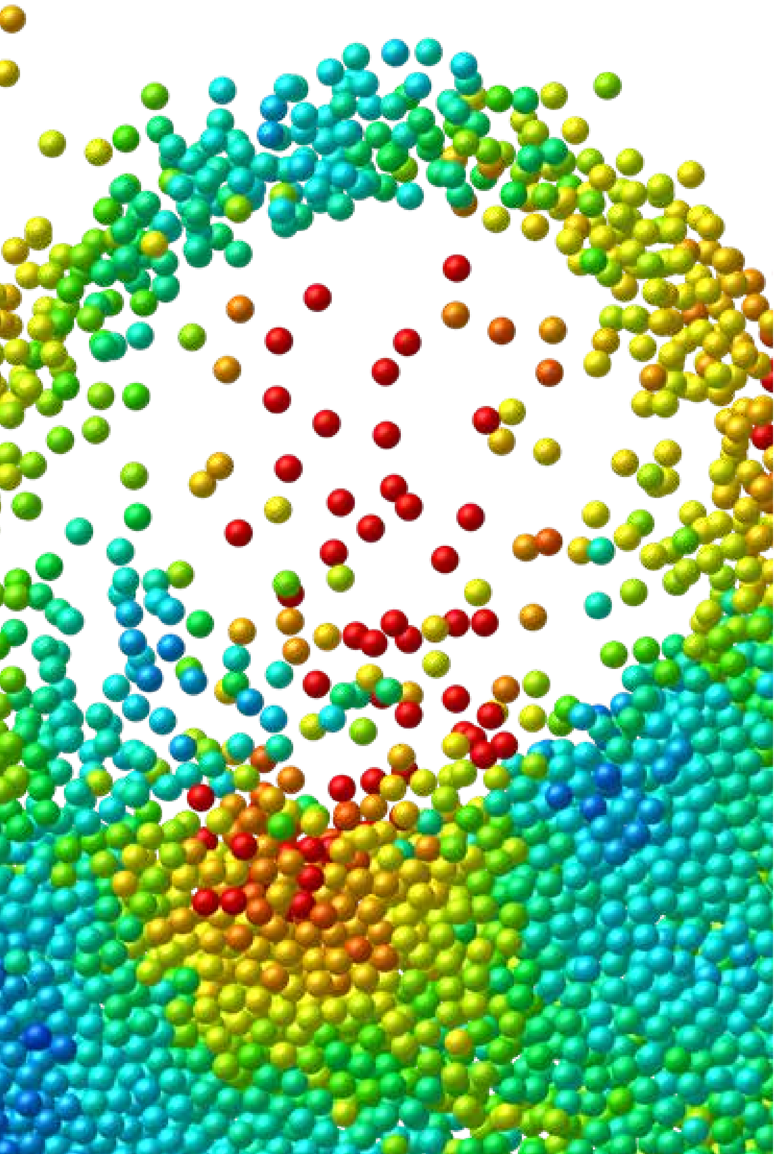


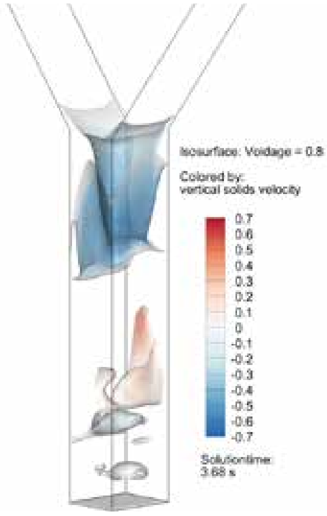
Cold-Flow Experiments at IEC (EVT)

- Validation for hydrodynamic models
- Multi-regime, variable geometries and particles
- High-Speed PIV flow analysis

Model Development

- Advanced conversion models integrated in reactor model
- Multi-scale approach from particle groups to industrial processes

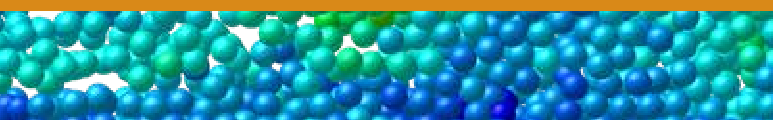




Highlights

Advanced model development supported by in-house experimental test rig and multiple measurement data

Multi-scale modeling for several processes



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Alobaid et al., Progress in CFD Simulations of Fluidized Beds for Energy and Chemical Process Technology, Progress in Energy and Combustion Science 91, 2021

Rößger et al., Numerical modeling of a batch fluidized-bed gasifier: Interaction of chemical reaction, particle morphology development and hydrodynamics, Powder Technology 384, 2021

Porter et al., Eulerian-Eulerian Modeling and Validation of Heat Transfer in Bubbling and Spouted Fluidized Beds, Fluidization XVI Conference, 2019

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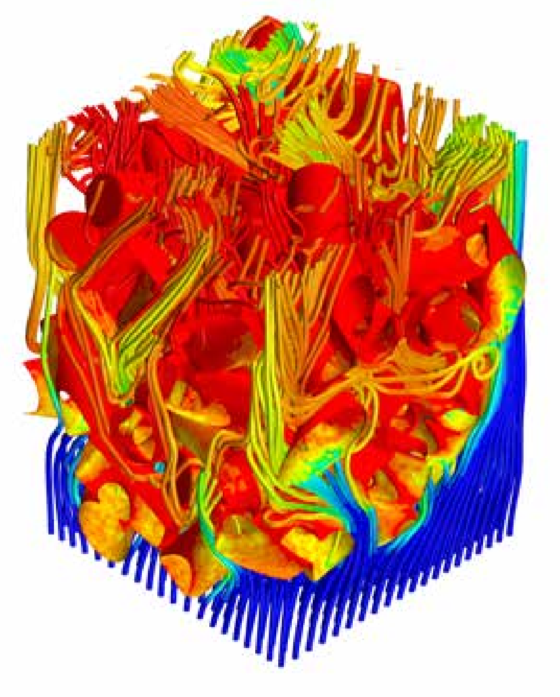
Rößger et al., Numerical investigations on the influence of heterogeneous reactions on the hydrodynamics of bubbling fluidized bed gasifiers, 23rd International Conference on Fluidized Bed Conversion, 2018

Heat and Mass Transfer in Fixed Beds



Highlights

Fixed-bed models from particle-resolved to continuum approach for each type of application

Variety of in-house reference measurement for model validation

Rapid process optimization based on reduced-order models

Heat Transfer in Fixed Beds

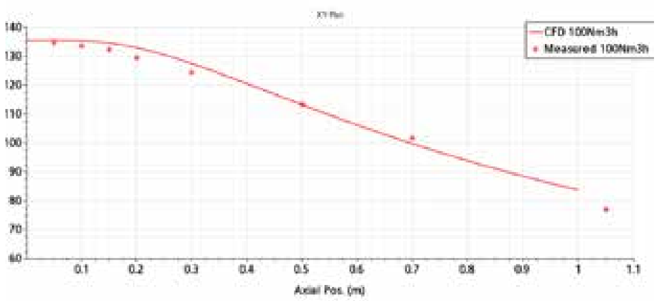
- Validated models for fixed beds of spherical and non-spherical particles
- State-of-the-art reference data for heat transfer in fixed beds based on in-house test rig (EVT)

Fixed-Bed Gasification

- Modeling of fixed-bed gasification lab-scale to industrial-scale
- Including advanced conversion models, validated against in-house experiments at EVT

Syntheses and Adsorption Processes

- From detailed, particle-resolved process analysis to rapid process modeling with reduced-order models



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Schulze et al., Particle-resolved numerical study of char conversion processes in packed beds, Fuel 207, 2017

Schulze et al., The porosity distribution in monodisperse and polydisperse fixed-beds and its impact on the fluid flow, Particulate Science and Technology 33, 2015

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Massoudi Farid et al., 3D lab scale fixed bed gasifier simulation using TFM–TRACER approach, 10th International Conference on Multiphase Flow, 2019

Massoudi Farid et al., 3D Eulerian–Lagrangian simulation of a lab scale fixed bed gasifier, 9th International Freiberg Conference on IGCC & XtL Technologies, 2018

Massoudi Farid et al., 3D TFM–TRACER approach to simulate a lab scale fixed bed gasifier, 35th Annual International Pittsburgh Coal Conference, 2018

Advanced Modeling in Metallurgy

Top-Submerged Lance Processes

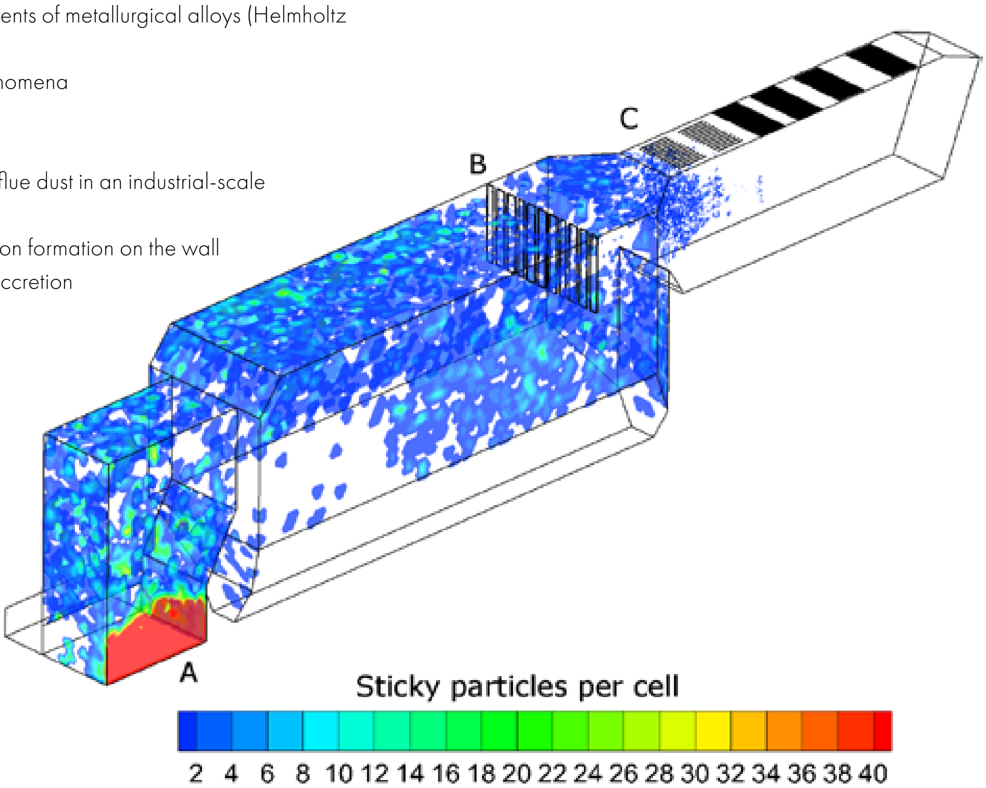
- Highly-resolved studies on multi-phase flow
- Validation against X-ray measurements of metallurgical alloys (Helmholtz Center Dresden Rossendorf)
- Detailed studies of interphase phenomena

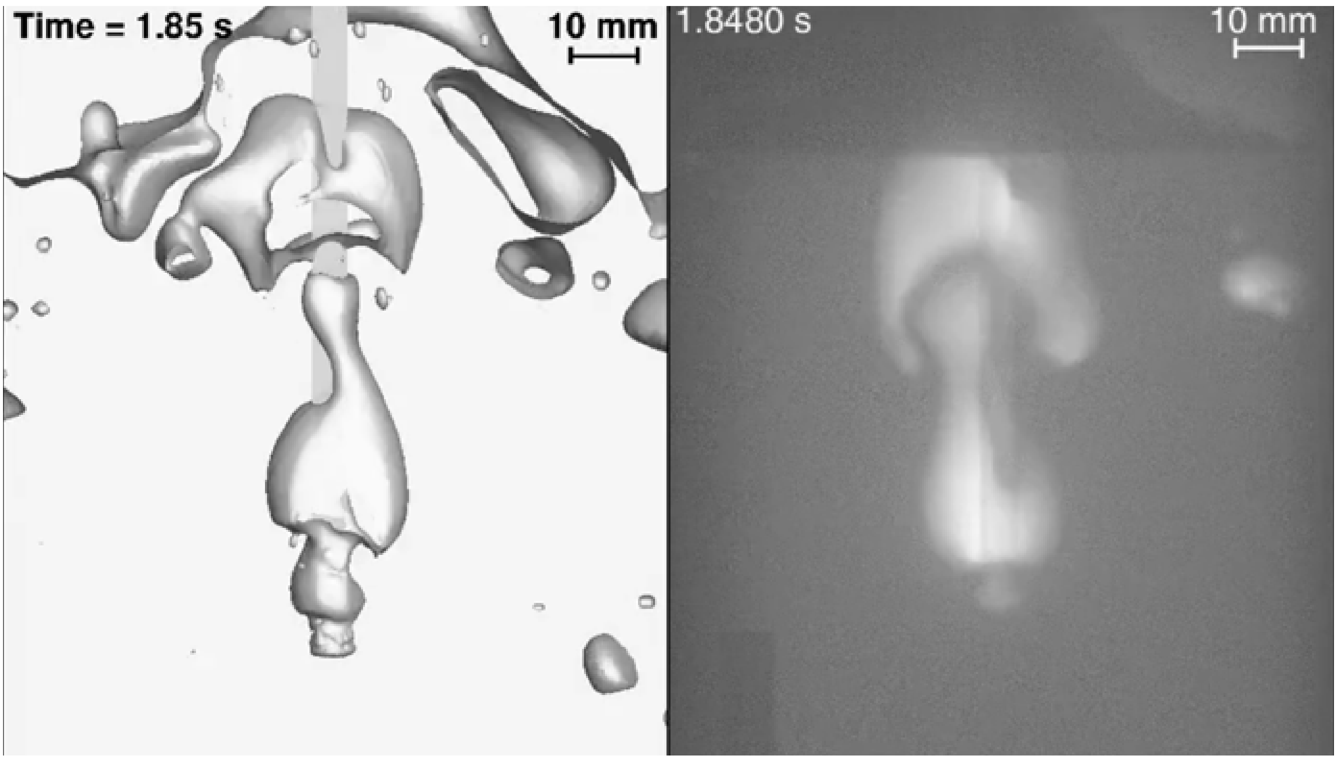
Copper Production

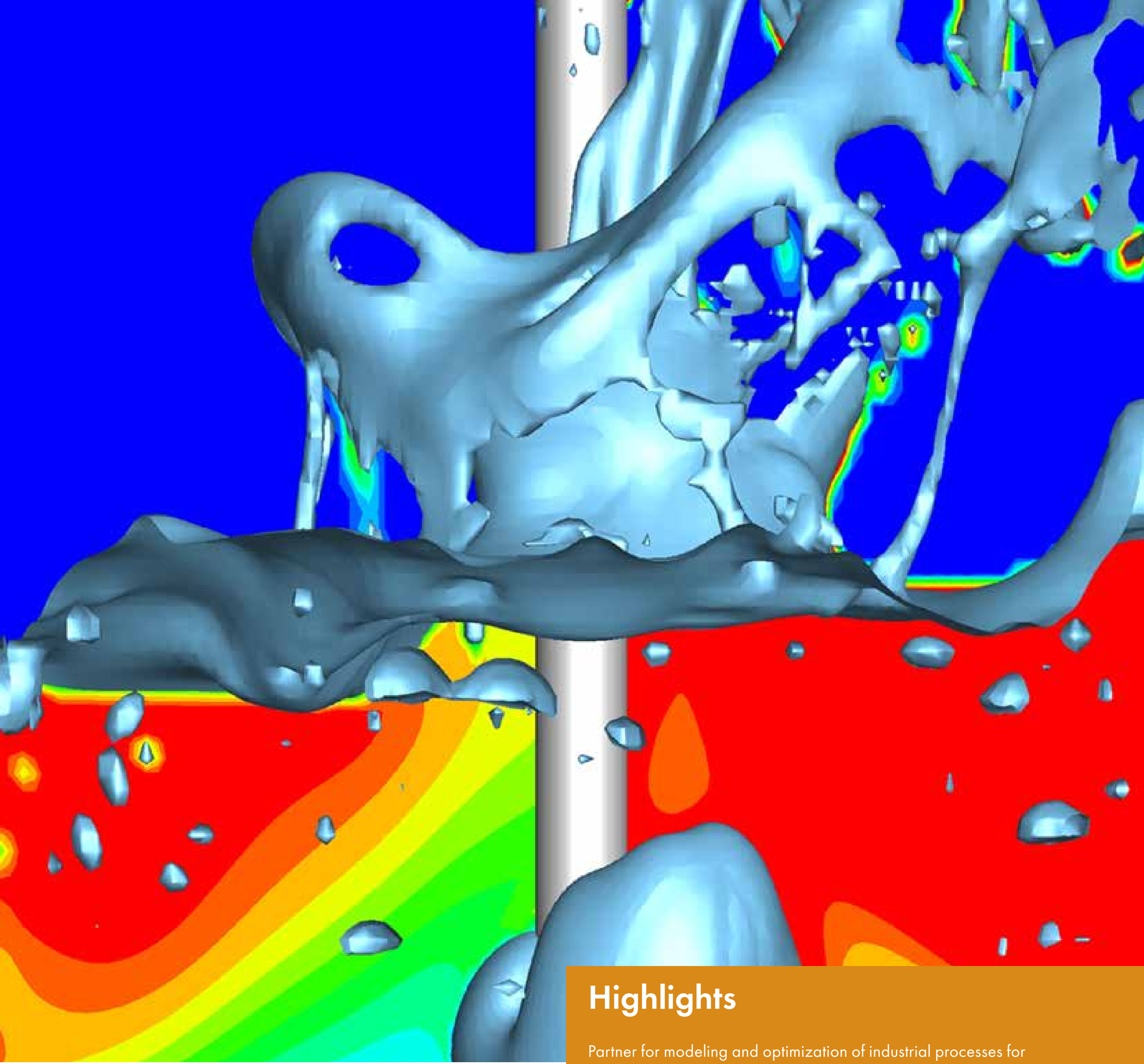
- CFD study of physical behavior of flue dust in an industrial-scale copper waste heat boiler
- Custom sticking function for accretion formation on the wall
- Recommendations for minimizing accretion

Blast Furnaces

- CFD-based process analysis
- Parameter and feedstock studies
- Process optimization







Highlights

Partner for modeling and optimization of industrial processes for production of ferrous and non-ferrous materials

X-ray assisted model validation for process-relevant materials

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Obiso et al., Dynamics of Rising Bubbles in a Quiescent Slag Bath with Varying Thermo-Physical Properties, Metallurgical and Materials Transactions B 51, 2020

Obiso et al., CFD Modeling and Experimental Validation of Top-Submerged-Lance Gas Injection in Liquid Metal, Metallurgical and Materials Transactions B 51, 2020

Obiso et al., CFD Investigations of Bath Dynamics in a Pilot-Scale TSL Furnace, Metallurgical and Materials Transactions B 52, 2021

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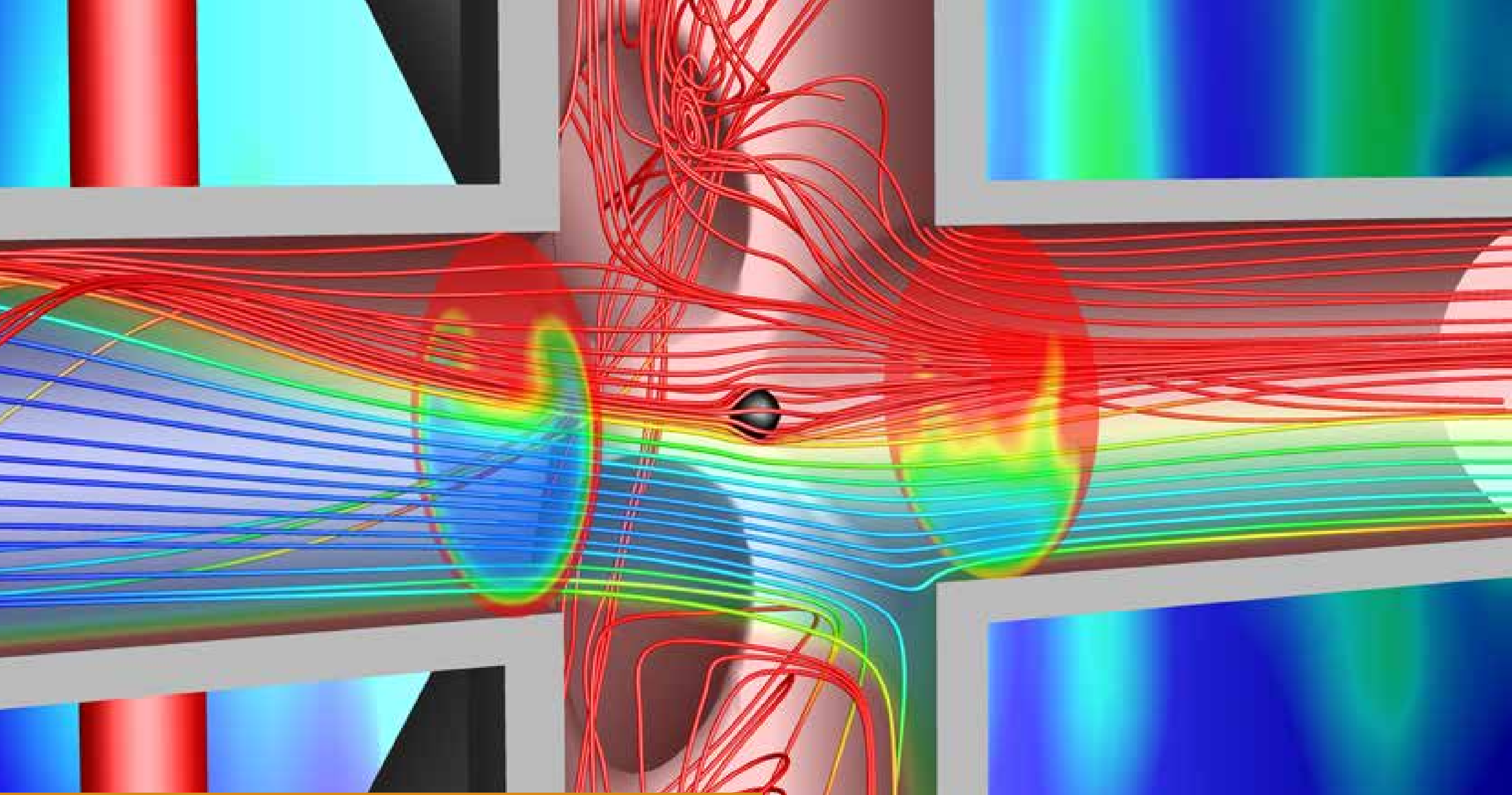
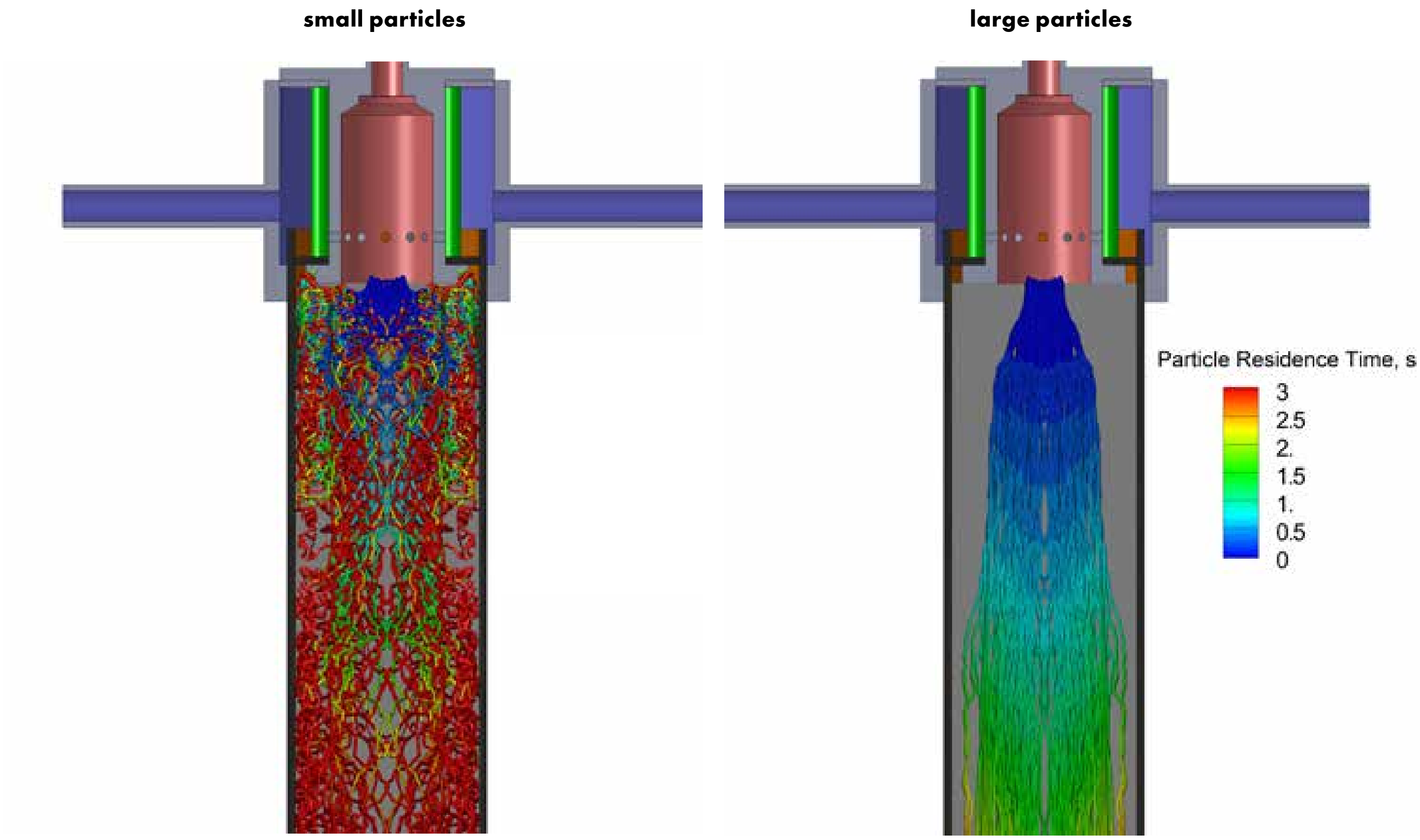
Schmidt et al., Transient CFD Modeling of Matte Settling Behavior and Coalescence in an Industrial Copper Flash Smelting Furnace Settler, Metallurgical and Materials Transactions B 52, 2020



Highlights

Systematic approach from model-based experimental data evaluation to industrial process

Design of new experimental test rigs



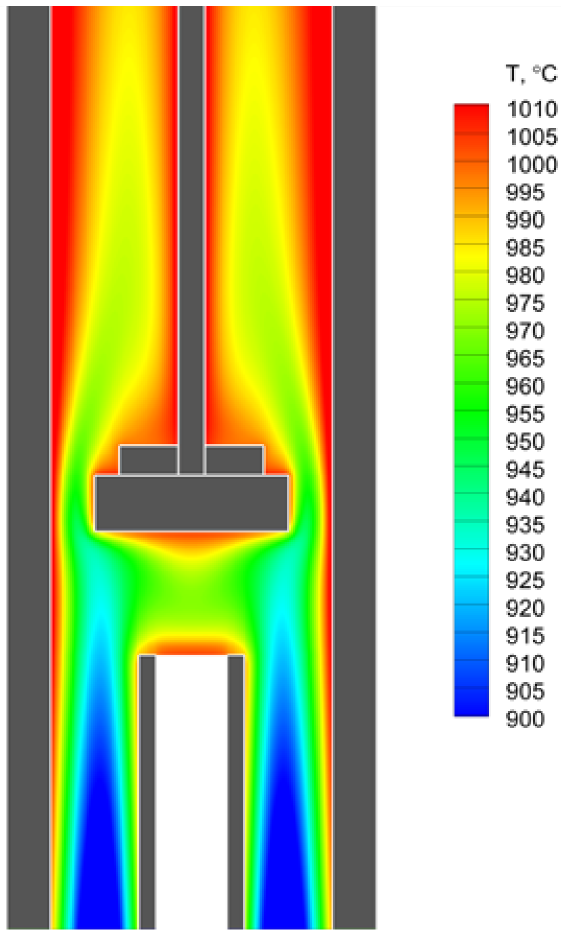
Model-Based Laboratory

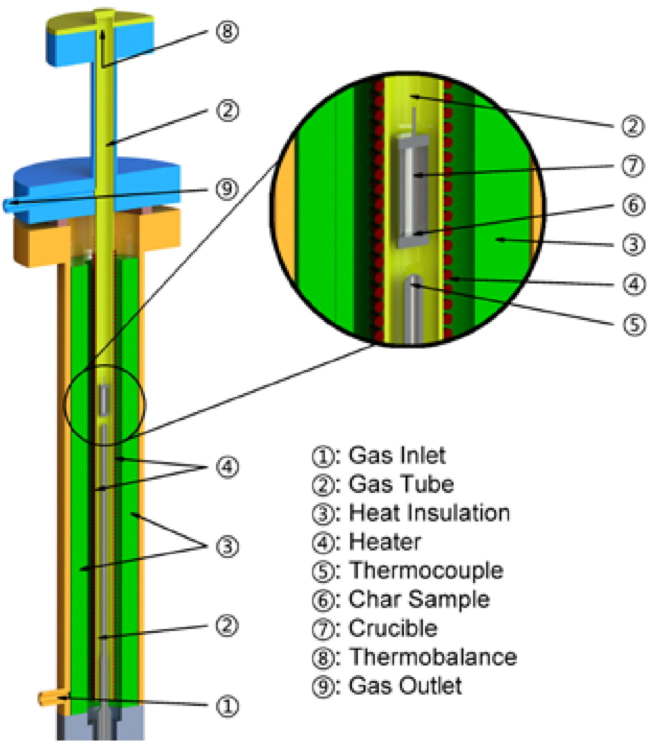
Design and Development of New Test Rigs and Optical Measurement Systems

- Model-based design of new high-temperature test rigs
- Optimization of existing test facilities

Model-Based Data Analysis

- Systematic model-based data analysis, evaluation and utilization in reactor models





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An et al., Numerical study on the effect of particle residence time on kinetics evaluation of gasification reaction in a drop-tube furnace, International Pittsburgh Coal Conference, 2020

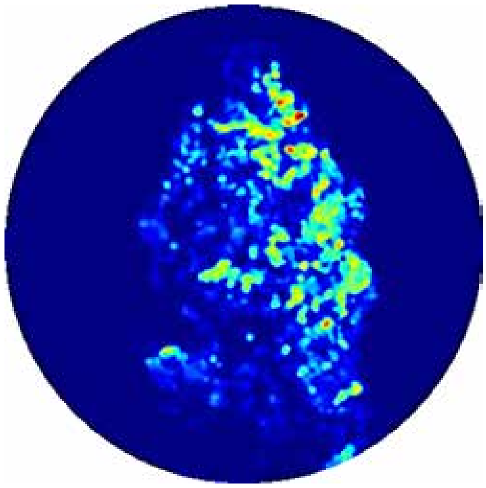
An et al., CFD investigation of an improved TGA design for heterogeneous reaction kinetic, International Conference on Coal Science & Technology, 2019

Schulze et al., Heat and mass transfer within thermogravimetric analyser: From simulation to improved estimation of kinetic data for char gasification, Fuel 187, 2017

Flame Diagnostics

Automated Flame Diagnostics

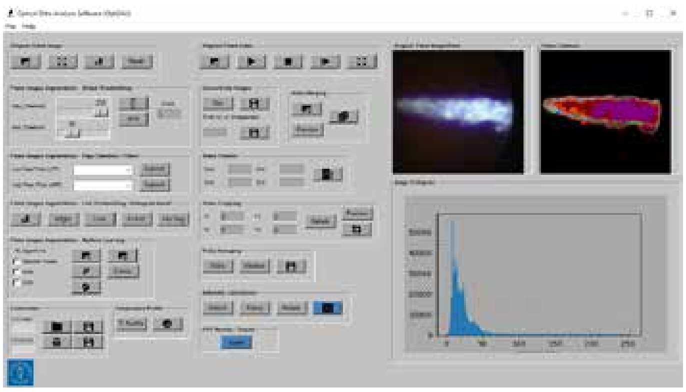
- Software development for real-time optical flame analysis
- In-situ flame analysis
- Automated estimation of flame characteristics (length, shape)
- Velocity and temperature distributions
- AI-assisted data evaluation
- Integrated in OptiDAS



Highlights

Model-driven, automated flame analysis integrated in graphical user interface

Comprehensive flame lift-off detector based on deep learning algorithms



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Gharib et al., Comprehensive Optical Investigation of Different Flame Types in a Multi-Feed Test Facility, 38th Annual International Pittsburgh Coal Conference, 2021

Gharib et al., New Approach for Flame Image Segmentation based on Machine Learning Algorithms, 37th Annual International Pittsburgh Coal Conference, 2020

Equipment

CAD
- Solidworks
- Autodesk AutoCAD

Meshing
- ANSYS ICEM CFD
- ANSA

CFD
- ANSYS Fluent
- StarCCM+
- Sub models for particle accretion, slag formation, char conversion
- In-house solver for accelerated fixed-bed modeling

Chemical Solver
- Cantera
- Chemkin Pro

Reduced-Order Modeling
- In-house tools coupled with Cantera and Chemkin

Data Visualization
- Tecplot 360 & Chorus
- CFD-Post

Analysis & Optimization
- MATLAB
- modeFRONTIER

Virtual Studio
- Green Screen
- Professional Studio Software (Cinector)
- Development of new presentation concepts for digital teaching

Flame Diagnostics, High-Speed Imaging and PIV
- OptiDAS
- Lavision Phantom v1840 (EVT)
- DaVis (EVT)

High Performance Computing Resources
- In-house HPC cluster for industrial projects: 360 cores (EVT)
- TU Bergakademie Freiberg Compute Cluster 2019: 4328 cores
- TU Dresden High Performance Computing and Storage Complex (HRSK-II): 40,000 cores

CONTACT

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