



MODELING OF THERMOCHEMICAL CONVERSION PROCESSES | MTK

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

Team MTK



Prof. Andreas Richter
Professorship for Modeling of Thermochemical Conversion Processes

Fengbo An



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

Sophie Rodmacher



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

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



- Highly-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



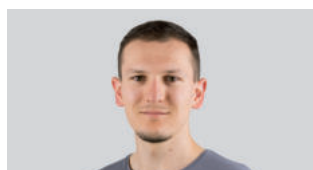
- Development of future technologies based on highly-resolved CFD
- Optimization of metallurgical processes

Johannes Scherer



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

Albrecht Voigt



- Modeling of reactive gas-liquid-systems
- Development of highly-resolved models for metallurgical processes

Lukas Etzold



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

Farideh Hoseinian Maleki



- Development of advanced machine learning techniques in thermochemical process modeling
- AI-based Modeling and Optimization of high-temperature Glass Melting Processes

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

Team MTK	2
Preface	3
Partial Oxidation of Gaseous and Liquid Feedstocks	4
High Temperature Conversion Processes in Chemistry	6
Fluidized-Bed Processes	8
Heat and Mass Transfer in Fixed Beds	9
Advanced Modeling in Metallurgy	10
Model-Based Laboratory	13
Flame Diagnostics	14
Equipment	15

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

References

Gonzalez-Ortiz et al., Experimental and numerical study of high pressure partial oxidation of natural gas with CO₂ recycling, 11th International Freiberg Conference on Circular Carbon Technologies, 2023

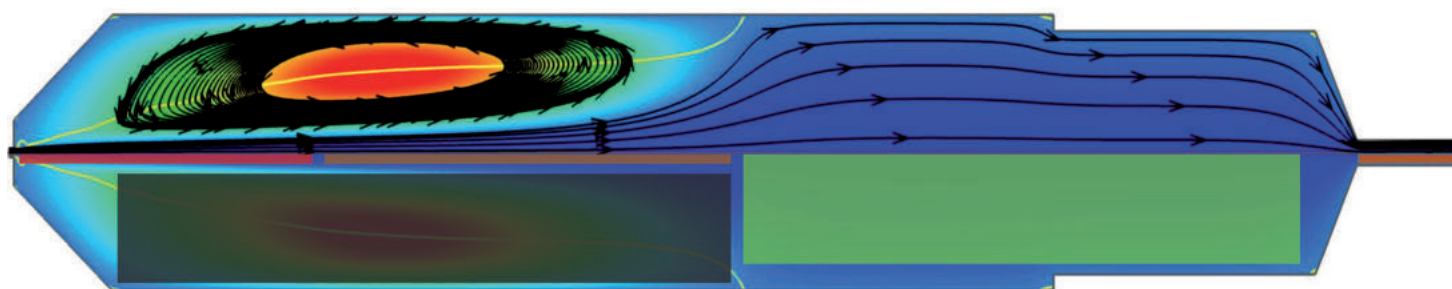
Rößger et al., Integrating biomass and waste into high-pressure partial oxidation processes: Thermochemical and economic multi-objective optimization, Journal of Cleaner Production 358, 2022

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



■ – Combustion Zone ■ – Bypass Zone ■ – Plug-Flow Zone
■ – Recirculation Zone ■ – Outlet Zone

Advanced CFD Modeling

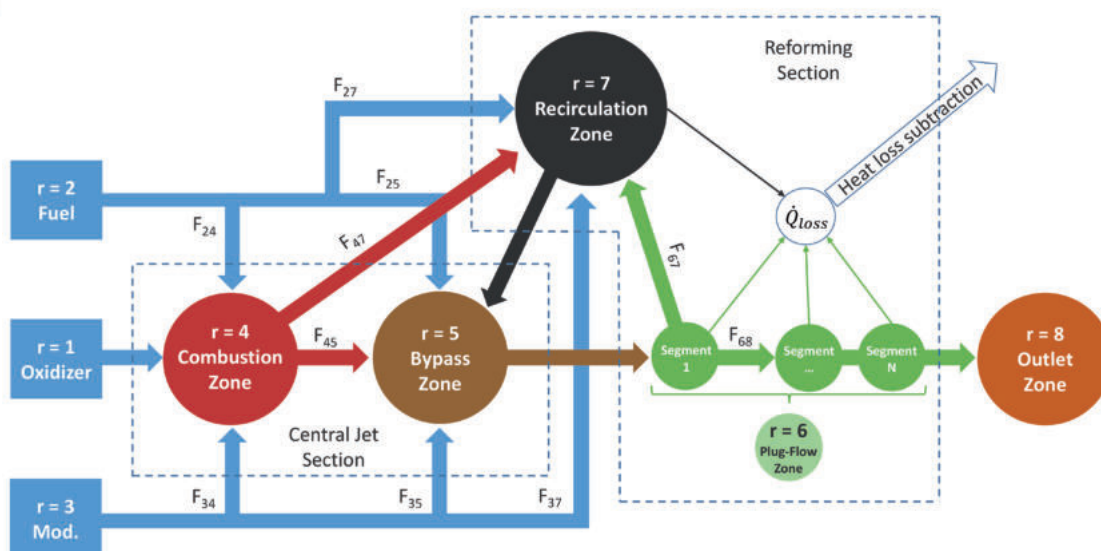
- Catalytic and non-catalytic reforming
- Conventional and alternative feedstocks (biogas, bio-oil, lean gases, process gases)
- Detailed process analysis
- Burner development and optimization

Process Optimization

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

Reduced-Order Modeling

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



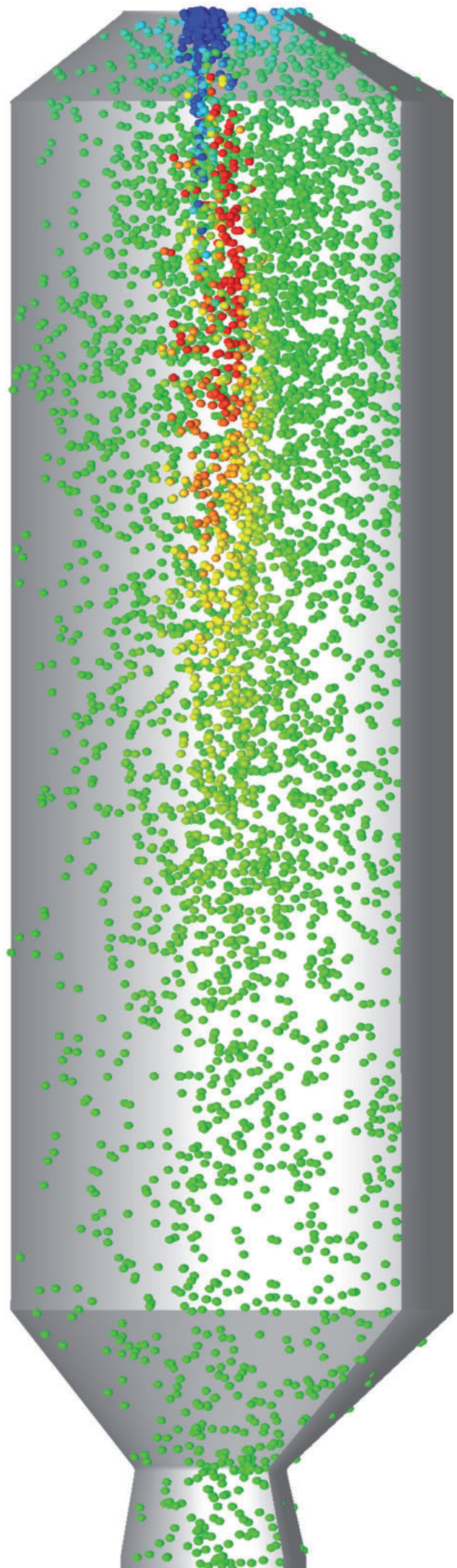
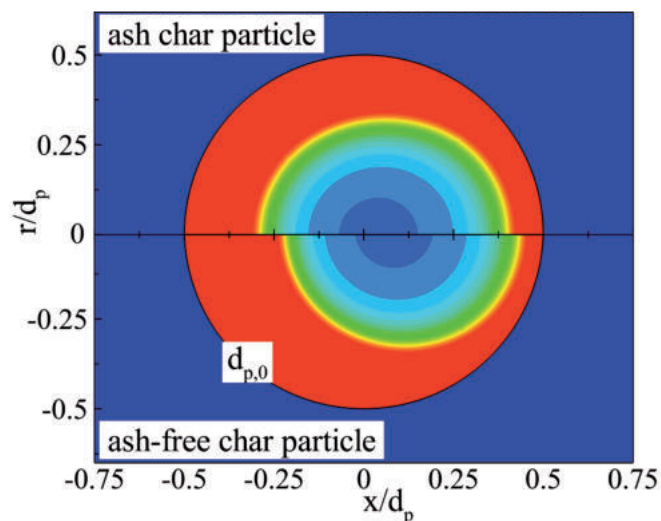
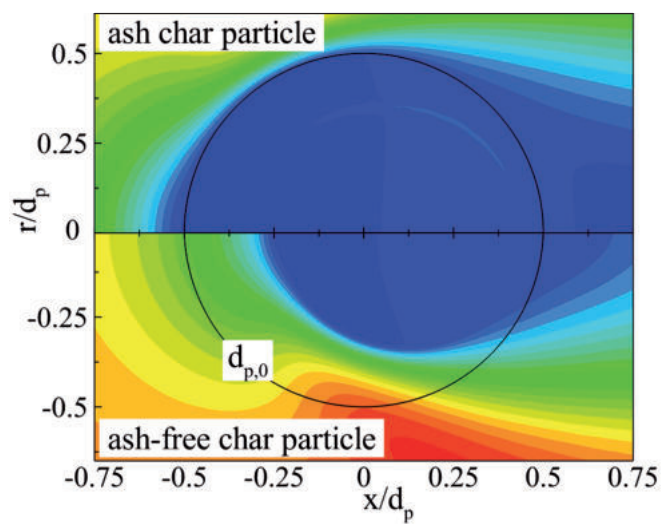
High Temperature Conversion Processes in Chemistry

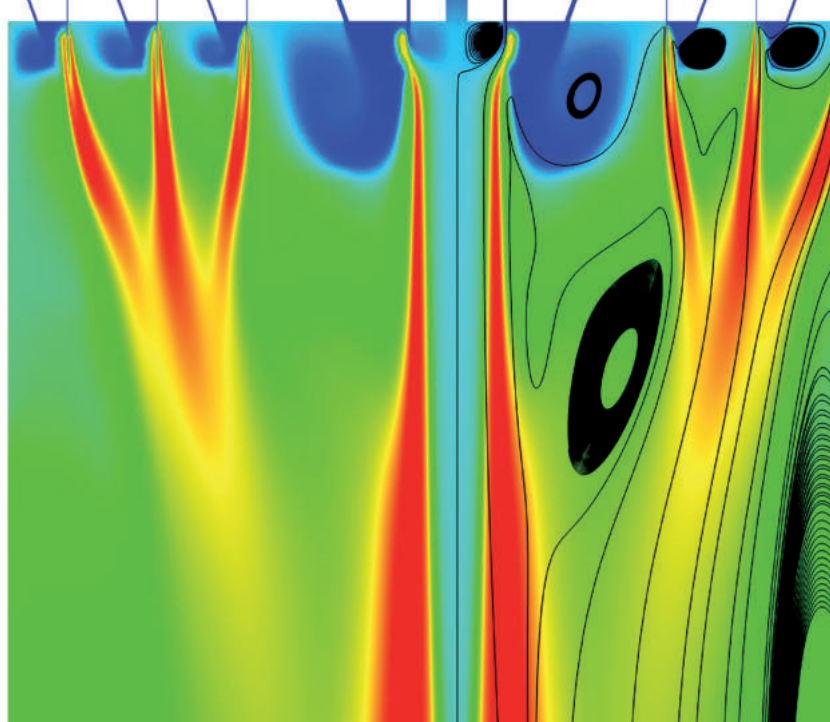
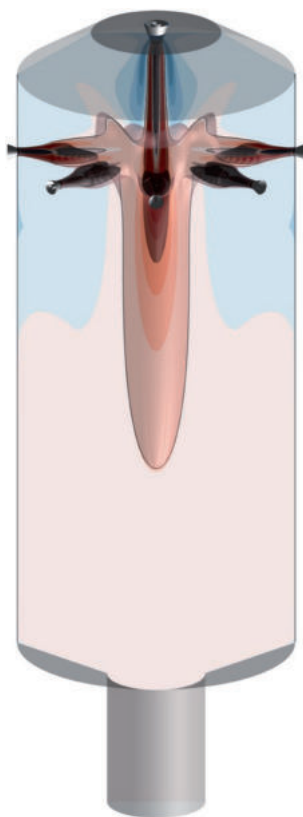
Process Modeling

- Entrained-flow, fluidized-bed and fixed-bed processes for the conversion of biomass, 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

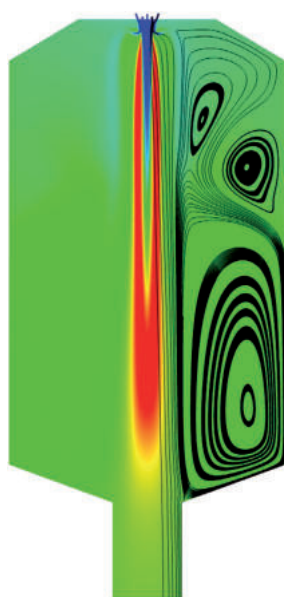




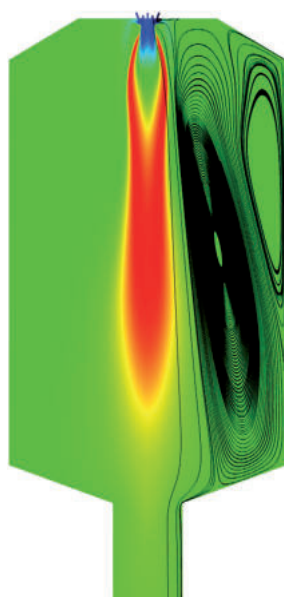
Highlights

Process development and optimization for several partners from industry

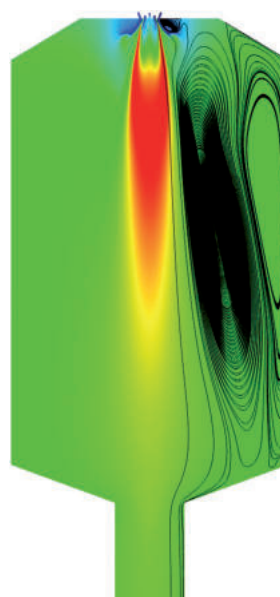
Validated large-scale models for a variety of conversion processes available



0°



45°



60°



75°

References

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

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

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

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

Rößger et al., Performance of different optimization concepts for reactive flow systems based on combined CFD and response surface methods, *Computers & Chemical Engineering* 108, 2018

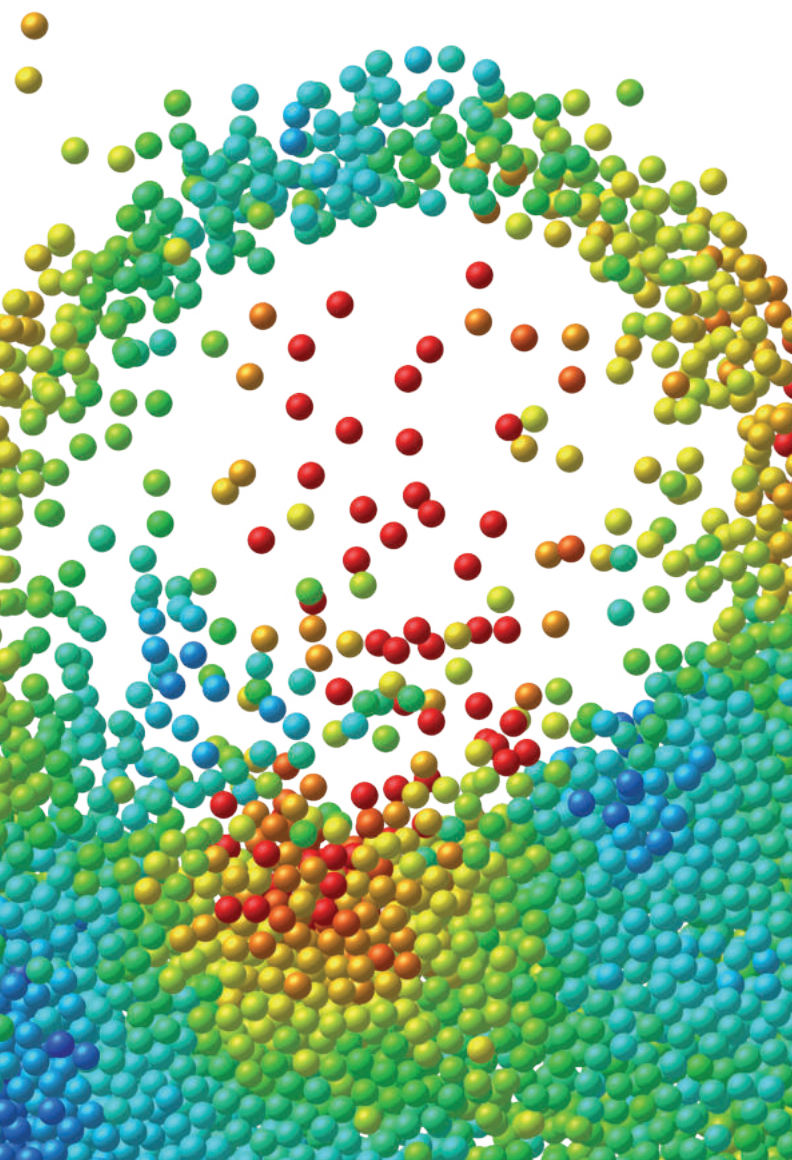
Fluidized-Bed Processes

Cold-Flow Experiments at IEC (EVT)

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

Model Development

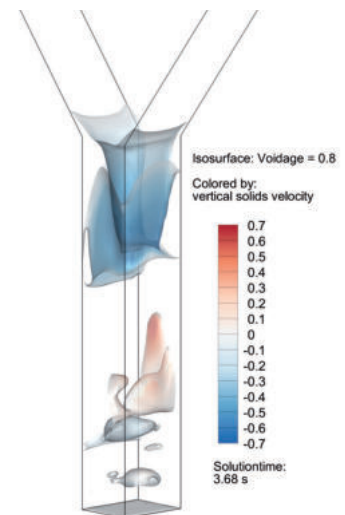
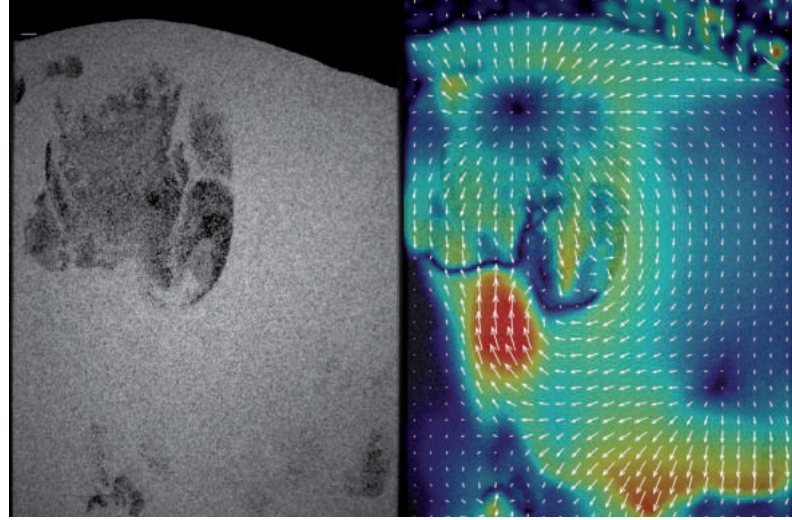
- Advanced conversion models integrated in reactor model
- Multi-scale approach from particle groups to industrial processes



Highlights

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

Multi-scale modeling for several processes



References

Khodabandehlou et al., Anticipating of ash agglomeration behavior in a fluidized bed by population balance equation, *Fuel* 358, 2024

Porter et al., PIV and Pressure Measurements for Fluidized Bed Model Validation: Building a Multi-Regime Reference Data Set, *Fluidization XVII Conference*, 2023

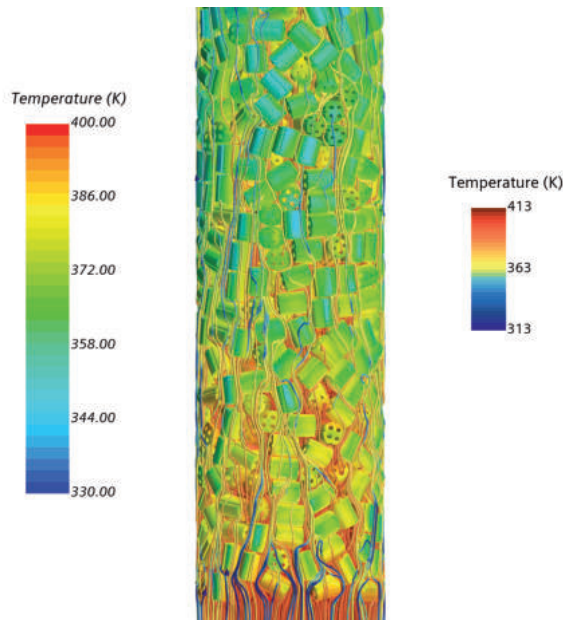
Alobaid et al., Progress in CFD Simulations of Fluidized Beds for Energy and Chemical Process Technology, *Progress in Energy and Combustion Science* 91, 2021

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

Rößger et al., Euler-Euler Simulation of a Bubbling Fluidized Bed Reactor: Development of a Shrinking Density Particle Conversion Model, *Fluidization XVI Conference*, 2019

Laugwitz et al., Towards a validated CFD setup for a range of fluidized beds, *Powder Technology* 318, 2017

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 measurements for model validation

Rapid process optimization based on reduced-order models

Heat Transfer in Fixed Beds

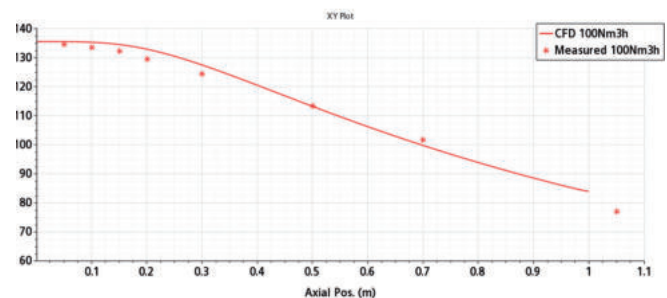
- Validated models for fixed beds of spherical and non-spherical particles
- State-of-the-art reference data for heat transfer in fixed beds based on in-house test rig (EVT)

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



References

Srinivas et al., Design of an Experimental Test Rig for Validation of Heat Transfer Models for Fixed Beds, 10th International Symposium on Turbulent Heat and Mass Transfer, 2023

Bassen et al., Numerical investigation of heat transfer in dense fixed beds of arbitrary shaped particles with immersed boundary methods, 4th Thermal and Fluids Engineering Conference, 2019

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

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

Advanced Modeling in Metallurgy

Top-Submerged Lance Processes

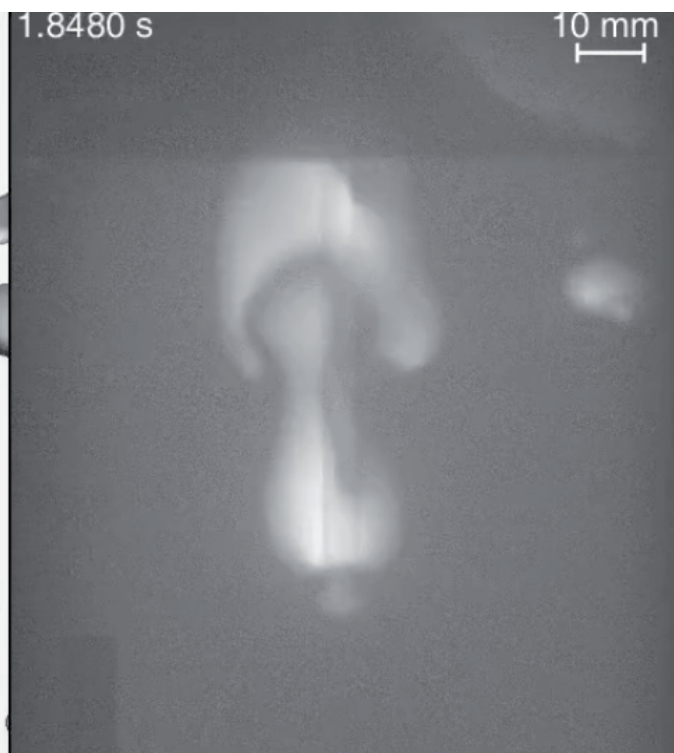
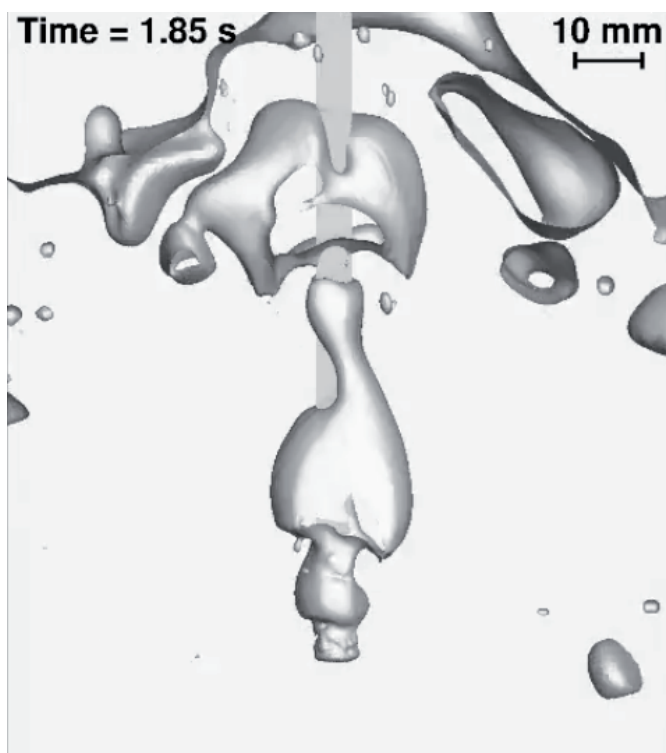
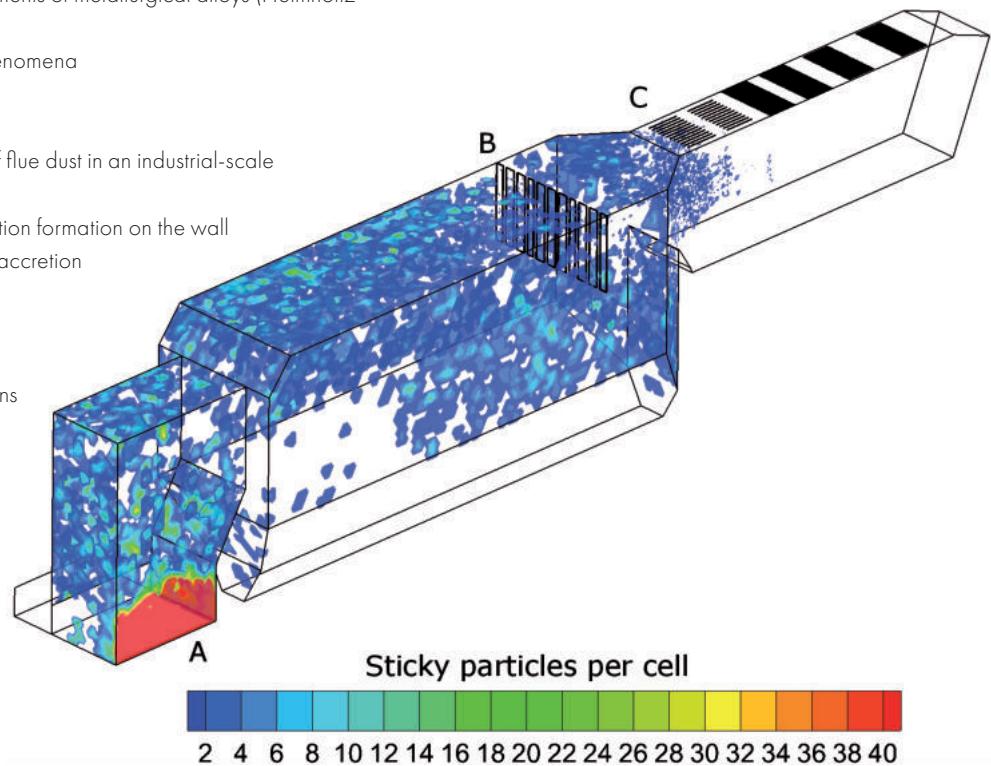
- Highly-resolved studies on multiphase flows
- Validation against X-ray measurements of metallurgical alloys (Helmholtz Center Dresden Rossendorf)
- Detailed studies of interphase phenomena

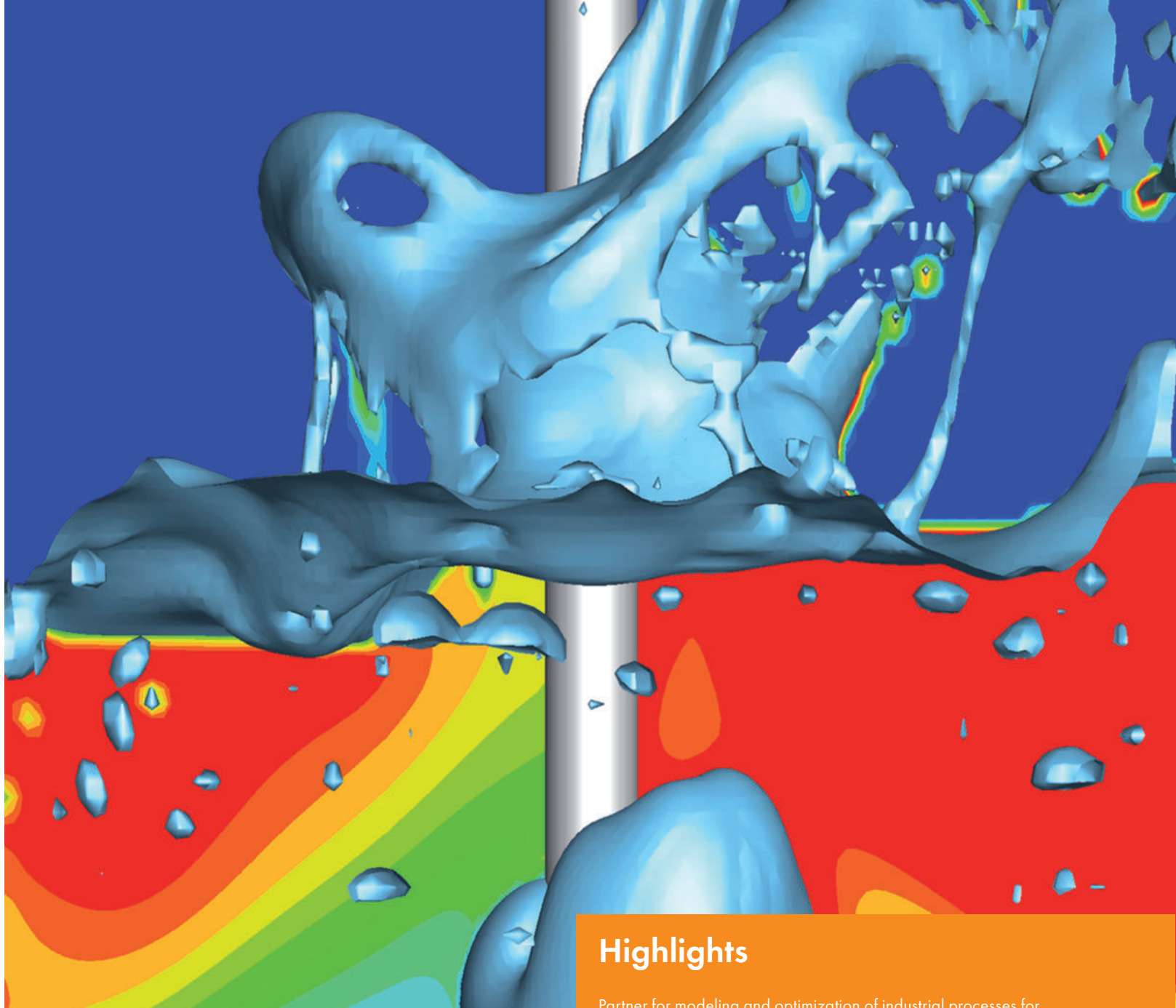
Copper Production

- 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

Glass Melting Processes

- CFD-based process analysis
- Detailed study of phase interactions
- 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

References

Kota et al., Experimental and numerical investigations regarding the thermochemical interaction between hydrogen and glass melts, 97th Glass-Technology Conference, 2024

Hutter et al., A Comprehensive modeling approach to analyze and optimize glass melting processes, 97th Glass-Technology Conference, 2024

Schmidt et al., CFD Study on the Physical Behavior of Flue Dust in an Industrial-Scale Copper Waste Heat Boiler, Metallurgical and Materials Transactions B 53, 2022

Obiso et al. (2021), CFD Investigation of Rotational Sloshing Waves in a Top-Submerged-Lance Metal Bath, Metallurgical and Materials Transactions B 52, 2021

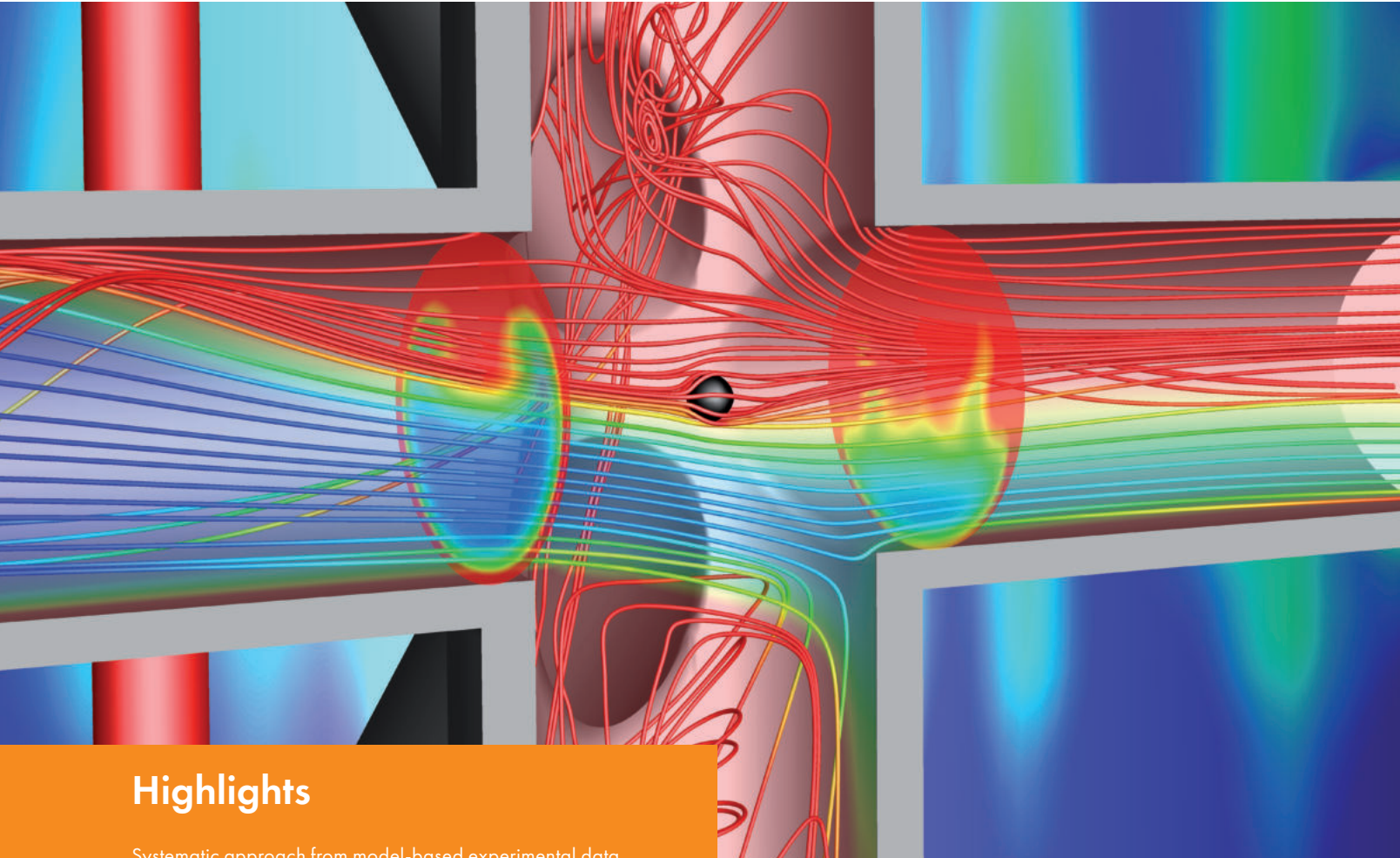
Obiso et al., CFD Investigations of Bath Dynamics in a Pilot-Scale TSL Furnace, Metallurgical and Materials Transactions B 52, 2021

Schmidt et al., Development of a Three-dimensional CFD Model for the Estimation of Accretion Formation in an Industrial-Scale Copper Waste Heat Boiler, World of Metallurgy - ERZMETALL 74, 2021

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

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

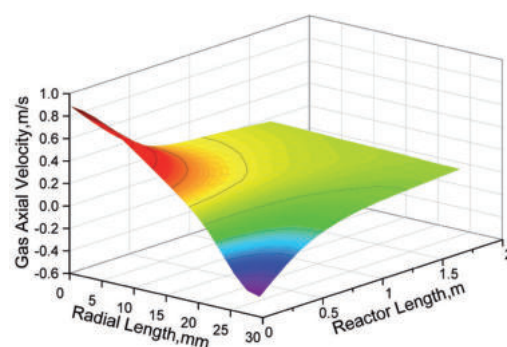
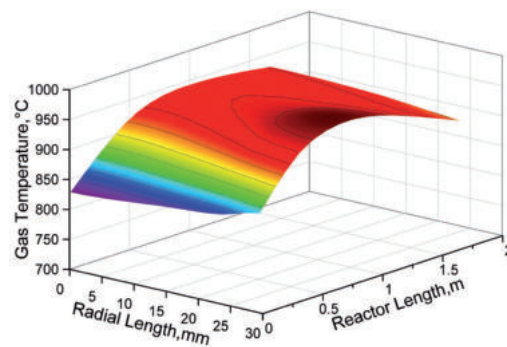
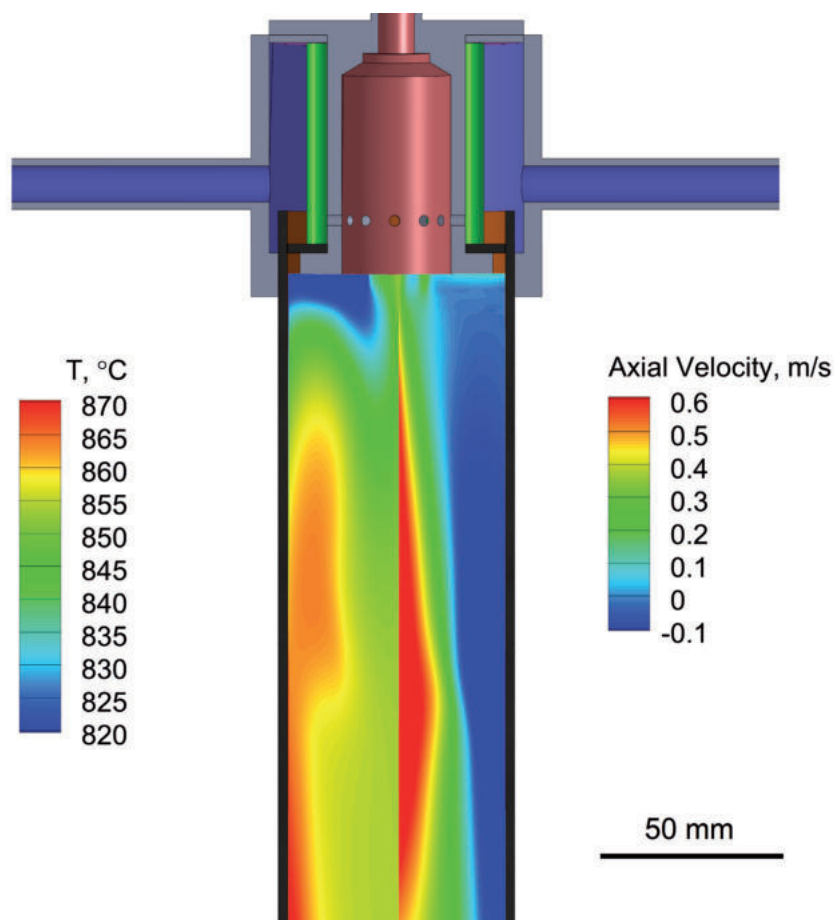
Obiso et al., CFD Modeling and Experimental Validation of Top-Submerged-Lance Gas Injection in Liquid Metal, Metallurgical and Materials Transactions B 51, 2020



Highlights

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

Design of new experimental test rigs



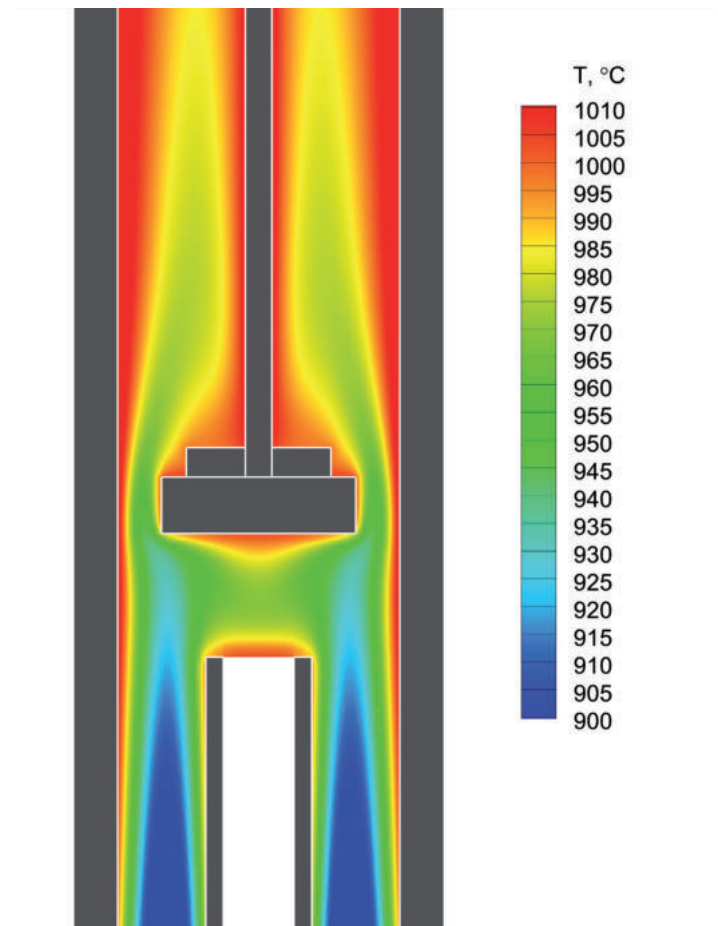
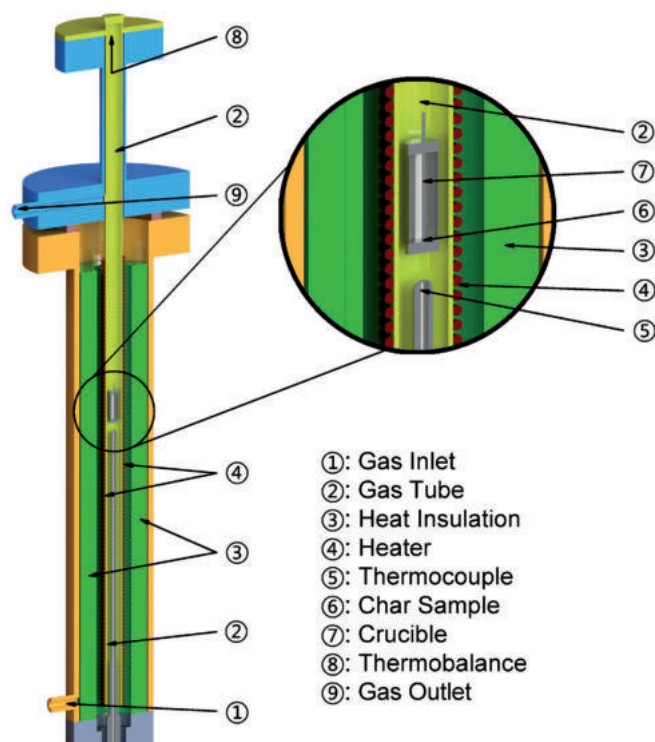
Model-Based Laboratory

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
- Model-based optimization of heterogeneous kinetic evaluations



References

An et al., Optimizing kinetic evaluation through CFD-based analysis of heat and mass transfer in a high-pressure TGA, *AIChE Journal* 70, 2024

An et al., Detailed analysis of the particle residence time distribution in a pressurized drop-tube reactor, *AIChE Journal* 69, 2023

An et al., Heat and mass transfer analysis of a high-pressure TGA with defined gas flow for single-particle studies, *Chemical Engineering Journal* 411, 2021

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

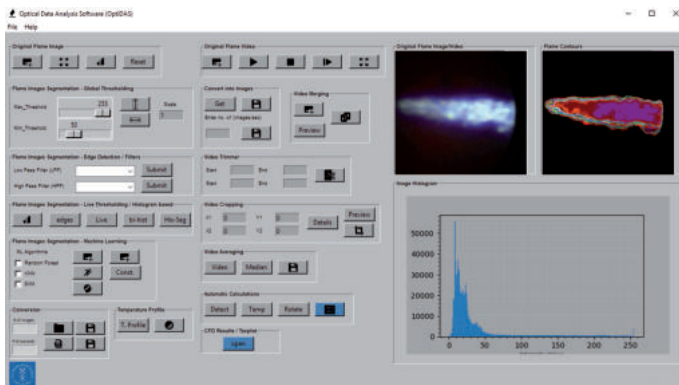
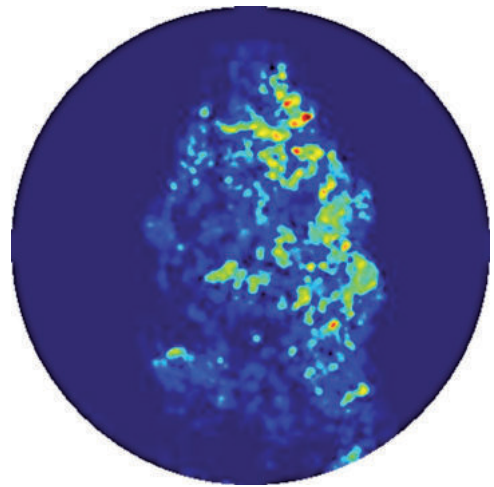
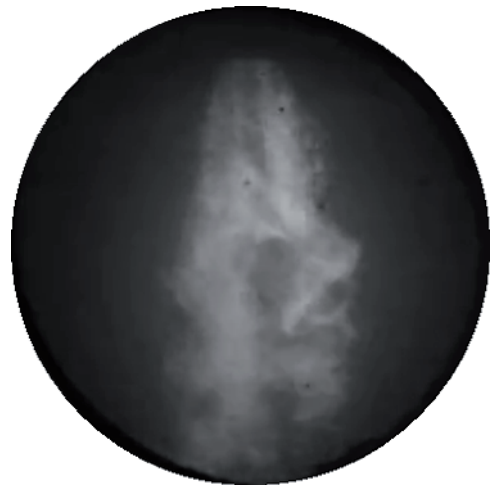
Automated Flame Diagnostics

- 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



References

Gharib et al., Flame lift-off detector based on deep learning neural networks. Combustion and Flame, 260, 2024

Gharib et al., Real-time flame monitoring system: a machine learning approach for flame detection and characterization, International Freiberg Conference on Circular Carbon Technologies (IFC), 2023

Gharib et al., Comparison between different flames in a multi-feed test facility and developing a flame lift-off detector using artificial neural networks, 13th European Conference on Industrial Furnaces and Boilers (INFUB-13), 2022

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
- National High Performance Computing centre at TU Dresden (NHR): 90,000 cores



CONTACT

TU Bergakademie Freiberg
Institute of Energy Process Engineering and Chemical Engineering
Professorship for Modeling of Thermochemical Conversion Processes
Fuchsmuehlenweg 9 D, 09599 Freiberg/Germany



PHONE +49 3731 39 4511
E-MAIL info-mtk@iec.tu-freiberg.de
WEB tu-freiberg.de/en/iec/mtcp