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K1-MET
metallurgical competence center

5th K1-MET Simulation Conference

3 April 2024, voestalpine Stahlwelt, First Floor,
voestalpine-Strasse 4, 4020 Linz, in the neighbouring building BG 44

09:30 – 10.00	Get-together with coffee
10:00 – 10:10	Welcome and introduction (Christine Gruber)

Morning session

10:10 – 11:00	Keynote 1: Thomas Lichtenegger (JKU-PFM) Towards fast long-term simulations of complex flows using hybrid models
11:00 – 11:20	Hadi Barati (K1-MET) Metallurgy driven modeling of multi-physics phenomena inside submerged entry nozzle in steel continuous casting
11:20 – 11:50	Coffee break with refreshments
11:50 – 12:10	Gerhard Holzinger (K1-MET) Data & Blast Furnace Simulations
12:10 – 12:30	Shengli Jin (MUL-CoC) Thermal and thermomechanical responses prediction with GPR and SVM

12:30 – 13:30 Lunch break

Afternoon session

13:30 – 14:20	Keynote 2: Valentina Colla (SSSA) Hybrid-AI for modelling purposes in the metallurgical field
14:20 – 14:40	Martin Barna (JKU-ISW) Modelling magnetohydrodynamics in continuous steel casting
14:40 – 15:10	Coffee break with refreshments
15:10 – 15:30	Golnaz Zarabian (TUW-ICEBE) Numerical Investigation of Alternative Reducing Agent Injection to the Raceway under Blast Furnace Conditions
15:30 – 15:50	Emerson Edilson Barros de Souza (K1-MET) Numerical development of a thermal pre-processing step for the recycling of Lithium-Ion batteries

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KEYNOTE 1: Towards fast long-term simulations of complex flows using hybrid models

Speaker: Thomas Lichtenegger (JKU-PFM)

Co-author(s): Stefan Pirker (JKU-PFM)

Many fluid-mechanical systems exhibit spatio-temporal multi-scale dynamics. Detailed methods that resolve the smallest and shortest scales cannot reach the larger and longer ones. Phenomenological models, on the other hand, are connected to a larger degree of uncertainty. To overcome these limitations, hybrid models combine knowledge of the laws of physics with observational data to include mesoscopic information. Since high-fidelity data for large-scale flows are expensive to obtain, we developed the hybrid simulation technique "recurrence CFD" that approximates the evolution of dynamic systems with relatively little data. For a given flow field, we determine the most similar reference state in a precomputed database and apply the corresponding evolution over a large time step. Upon iteration, long time series can be constructed and slow transport processes simulated with conventional models. Future research may focus on the generalizability to off-database conditions and emergent dynamics where no governing equations are available to guarantee physical plausibility.

Metallurgy driven modeling of multi-physics phenomena inside submerged entry nozzle in steel continuous casting

Speaker: Hadi Barati (K1-MET)

Co-author(s): Menghuai Wu (MUL-SMMP), Susanne Michelic (MUL-ESM), Sergiu Ilie (VAS)

In steel continuous casting, submerged entry nozzle (SEN) conveys the melt from the tundish to the mold. SEN protects the melt from oxidation and stabilizes the process. Various phases, like liquid metal, solid inclusions, and gas bubbles, along with different physics, like fluid flow and chemical reactions result in complex phenomena like clogging inside SEN. This contribution is to present a comprehensive numerical prediction of multi-physics phenomena in the SEN based on different experimental analyses and observations.

Data & Blast Furnace Simulations

Speaker: Gerhard Holzinger (K1-MET)

Over the course of the last years the blast furnace has been studied in terms of particle simulations using the discrete element method (DEM). Two projects will be discussed in terms of their link between particle simulations and available data from the blast furnace operations.

Blast furnace charging strategies were studied in terms of the potential influence of the hopper that the blast furnace is charged out of, and the changes between the available hoppers. Furthermore, the influence of the chute's start angle has been studied since the chute's motion determines the resulting burden pattern with the blast furnace. Noticeable influence on the burden distribution has been found for both the hopper change and the chute's start angle. This influence has then been corroborated by measurement data from the blast furnace for a period in which the regimes for hopper change and chute start angle has been altered. Blast furnace charging is also being studied currently in terms of the resulting surface of the charged burden within the blast furnace. The blast furnace operators in Linz have a radar installed which periodically measures the surface profile of the burden within the blast furnace.

Our current project is aiming to validate our simulations using the measured surface profiles from the blast furnace's burden radar. The DEM simulation is based on the surface profile from before a new batch of material has been charged into the blast furnace. After the simulation has concluded, the comparison between the resulting surface profile of the simulation and the measure surface profile is of great interest for us.

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Thermal and thermomechanical responses prediction with GPR and SVM

Speaker: Shengli Jin (MUL-CoC)

A steel ladle consists of refractories and a steel shell. From thermal and thermomechanical standpoints, an effectively engineered refractory lining system should minimize heat loss from the steel shell and reduce stress concentration within the linings. To refine the lining concept design approach, a comprehensive database of steel ladle lining parameters with thermal and thermomechanical responses was established, utilizing finite element modelling incorporating elastic material behaviour. The predictive capabilities of several machine learning techniques were evaluated, including back-propagation artificial neural networks (BP-ANN), Gaussian process regression (GPR), and support vector machines (SVM). Furthermore, a novel approach was introduced, which utilizes GPR for prediction while factoring prediction errors from SVM. This hybrid method demonstrates superior predictive accuracy, particularly when the relationships between variables and responses are intricate.

KEYNOTE 2: Hybrid-AI for modelling purposes in the metallurgical field

Speaker: Valentina Colla (SSSA)

Hybrid-AI is receiving increasing attention for modelling tasks as a viable way to improve not only the accuracy of ML-based models, but also their reliability, trustworthiness, and explainability. Hybrid-AI groups a quite broad variety of approaches aimed at somehow infusing physical knowledge in AI. This makes them particularly attractive for industrial applications. Different "hybridization" levels are possible, among which the most innovative ones, such as, for instance, Physics-Informed Neural Networks (PINN), embed first principles models and physics constraints directly in the learning procedure. An overview of Hybrid-AI approaches will be provided and some applications in the steel field will be presented and discussed.

Modelling magnetohydrodynamics in continuous steel casting

Speaker: Martin Barna (JKU-ISW)

Co-author(s): Bahareh Najafian Ashrafi (K1-MET), Bernd Willers (HZDR), Mirko Javurek (JKU-ISW), Klaus Timmel (HZDR), Sven Eckert (HZDR)

The continuous casting process is the prime production route for steel, with a share of over 96 percent or more than 1800 million tons worldwide. As in all industrial processes, there is a steady drive towards higher productivity while maintaining and/or further improving the quality of the final product. This demand gave rise to the employment of electromagnetic actuators, as a sophisticated, contactless method to control the liquid steel flow inside the strand and thereby also controlling the quality of the final product.

The complexity of the casting process requires a thorough investigation of the interaction between the electromagnetic actuators and the liquid steel flow, which cannot be solely achieved with plant trials. Therefore, a combination of measurements with numerical modelling – and plant trials as a finalizing step – is crucial. Only a well-founded knowledge of the magnetohydrodynamics makes it possible to further improve/optimize the continuous casting process.

In this presentation, an overview over magnetohydrodynamics in continuous casting - different electromagnetic actuators and their effects will be given. In addition, the numerical models and experimental setups developed and employed by ISW, K1-MET and HZDR will be discussed.

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Numerical Investigation of Alternative Reducing Agent Injection to the Raceway under Blast Furnace Conditions

Speaker: Golnaz Zarabian (TUW-ICEBE)

Co-author(s): Eva-Maria Wartha (TUW-ICEBE), Markus Bösenhofer (TUW-ICEBE, K1-MET), Michael Harasek (TUW-ICEBE)

This study investigates the injection of alternative reducing agents into the raceway of blast furnaces to reduce coke consumption. CFD models the raceway, focusing on the utilization of agents like pulverized coal. The aim is to understand heterogeneous reactions and thermochemical coke conversion. OpenFOAM 9 is utilized with second-order upwind discretization and the pimple method for pressure-based equations. The k-ε standard model handles turbulence, and the EDC model accounts for volumetric chemical reactions. Factors like coal type, injection conditions, and oxygen concentration are analyzed for their impact on blast furnace efficiency. Further research is needed to fully grasp the thermochemical processes.

Numerical development of a thermal pre-processing step for the recycling of Lithium-Ion batteries

Speaker: Emerson Edilson Barros de Souza (K1-MET)

Co-author(s): Christoph Spijker (MUL-TPT)

In the present study, a numerical model is being developed to simulate a step in the battery recycling chain, the thermal pre-treatment process. This process involves exposing battery cells to a high-temperature environment to induce thermal runaway, with the aim of maximizing the recovery of valuable metals in subsequent downstream recycling steps. The proposed numerical model utilizes the CFD-DEM framework, in which Computational Fluid Dynamics (CFD) is used to calculate gas phase variables, and the battery is considered a solid non-spherical phase, solved using the Discrete Element Method (DEM). In this context, an experiment was designed to reproduce the same conditions as those of a controlled battery thermal pre-treatment process. Finally, the results from the experiments will be compared to the numerical model, seeking further simulations using more realistic furnace designs.

Affiliations

HZDR	Helmholtz-Zentrum Dresden-Rossendorf
JKU-ISW	Johannes Kepler University Linz, Institute for Fluid Mechanics and Heat Transfer
JKU-PFM	Johannes Kepler University Linz, Department of Particulate Flow Modelling
K1-MET	K1-MET GmbH
MUL-COC	Montanuniversitaet Leoben, Chair of Ceramics
MUL-ESM	Montanuniversitaet Leoben, Chair of Ferrous Metallurgy
MUL-TPT	Montanuniversitaet Leoben, Chair of Thermal Processing Technology
SSSA	Scuola Superiore Sant'Anna, Pisa, Italy
TUW-ICEBE	Vienna University of Technology, Institute of Chemical, Environmental and Bioscience Engineering
VAS	voestalpine Stahl GmbH

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