9th International Conference on Modeling and Simulation of Metallurgical Processes in Steelmaking - STEELSIM2021

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Book of Abstracts

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Modelling of Fluid Flow and Heat Transfer at Tata Steel

Corresponding Author: dirk.van-der-plas@tatasteeleurope.com

For the steel industry, modelling is an indispensable tool in process and product development. This will be illustrated by some typical examples from across the production chain, showing model development across several length and time scales. Taking industrial scale CFD and FEM approaches as the starting point, further development is in two directions. The first direction is towards simplification, allowing vast parameter studies or bringing the modelling results to the shop floor. To date, we have been using traditional approaches here, but more advanced approaches towards reduced order modelling, and combining CFD and machine learning tools come into view. The second direction is towards the fundamental side, and involves a critical assessment of modelling assumptions and simplifications that are inherent to industrial size computational efforts. Partly this is done in house, using the opportunities from continuous software and hardware development, e.g. in replacing RANS with LES. Another strain of this work is in collaboration with academic partners, involving a combination of smaller size fundamental numerical models and experimental validation.

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Thermomechanical modelling of additive manufacturing at different scales

Corresponding Author: michel.bellet@mines-paristech.fr

Additive manufacturing by selective laser fusion of powder appears as a promising process to elaborate high performance parts. Numerical simulation is a valuable tool for understanding laser matter interaction as well as the main physical phenomena governing liquid flow and solidification. It allows determining the influence of the different process parameters, and defining appropriate process windows. The presentation will illustrate this point through multiphysics numerical simulations at different scales, essentially applied to the LBM process (laser beam melting) for metals. Another topic that will be addressed is the behavior of metals at very high temperature, which is critical in terms of predicting stresses in the neighborhood of the melting pool, and associated defects such as solidification cracking. On the basis of mechanical tests performed under resistive heating, and instrumented by non-contact measurement techniques, the use of inverse finite element methods allows identifying parameters of elastic-viscoplastic constitutive models.

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Modelling and simulation of ironmaking blast furnaces for low CO2 emission and high process efficiency

Corresponding Author: aibing.yu@monash.edu

The design and control of blast furnace (BF) ironmaking must be optimized in order to be competitive and sustainable, particularly under the more and more demanding and tough economic and environmental conditions. To achieve this, it is necessary to understand the complex multiphase flow, heat and mass transfer, and global performance of a BF under different conditions. Mathematical modelling, often coupled with physical modelling, plays an important role in this area. This talk will present an overview of modelling and simulation of industrial BFs in our laboratory, focused on two aspects: model development and model application. The model development will be discussed

in terms of model formulation, new features and model validation. Our recent efforts in modelling layered cohesive zone and particle size reduction and developing an integrated BF model will be highlighted. Then, the usefulness of the BF models will be demonstrated through various model applications in optimizing burden distribution, pulverised coal injection and BF profile, as well as exploring new ironmaking technologies such as oxygen BF and hydrogen injection. Finally, areas for future development will be briefly discussed.

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"Simulation and process modelling along the production route of high performance steels and high value added material"

Corresponding Author: harald.holzgruber@inteco.at

INTECO is a privately owned Austrian engineering and consultancy company founded in 1973 being specialized in metallurgical process technology and the related equipment for melting, refining, casting, atomization and solidification of high-performance steels, superalloys and titanium.
Over the past decades the product portfolio has been consistently grown ranging nowadays from primary melting in Electric Arc Furnaces, refining in secondary metallurgy and casting technologies up to remelting and atomization processes to produce high value added materials such as superalloys and titanium.
During product development the importance of simulation and process modelling combined with broad metallurgical process know-how has been recognized as essential tools to pursue our strategy of improving existing processes and developing new technologies and products.
Various projects and the cooperation with scientific institutes will be presented to illustrate our strategical approach and use modelling as a key tool to gain better insights into fundamental metallurgical processes which are currently impossible to be experimentally investigated. Results of modelling approaches to predict thermal and solidification characteristics will be highlighted. In addition examples in the field of Magneto-Hydrodynamics dedicated to the arcing in the electric arc furnace and the remelting behaviour in the VAR will be discussed. From a technology and equipment supplier´s perspective, simulation tools aiming for an optimized process control and providing valuable input to certain design issues such as structural mechanics and heat transfer simulations will be explained. In order to provide tools for INTECO's clients in the steel plant operation, process models have been developed such as temperature prediction modelling in the ladle furnace, degassing models in vacuum metallurgy or on-line solidification models to control the continuous casting process. Simulations related to steel plant logistics aiming for an optimization of the complex material flow within the steel mill and identification of potential bottlenecks will be revealed.

Finally possible ways of combining scientific modelling with validation in industrial operation to optimize operational parameters and to ensure a safe and repeatable production of high-quality material are demonstrated.

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The role of modelling and simulation in the development of refractory products used in the steel industry

Corresponding Author: gernot.hackl@rhimagnesita.com

Throughout the entire steelmaking production process, refractory materials play a key role. The functionalities of these materials are manifold, such as maintaining the integrity of furnace vessels and protecting the steel shells from high temperatures, therefore regulating temperature losses. The materials also guarantee a safe transfer of liquid steel from one operational unit to another and, with

respect to functional products, have a direct impact on the process and, ultimately, on the quality of the product. The materials are exposed to extreme conditions, including thermally induced mechanical loads and chemical attack. Due to the extreme conditions and the increasing demand on the durability and lifetime of the materials, constant research is required to improve and develop refractory products for the steelmaking industry.
In that respect, modelling and simulation has become an important discipline in the field of refractory materials engineering and development in recent years. We apply state-of-the-art methodologies, enabling us to effectively predict the behaviour of these products in use, meet specific customer requirements, produce innovative solutions to achieve production and cost efficiencies and improve safety. Developments in terms of material description in combination with advanced model approaches were realized to further increase the reliability of these methods. However, constant investment in fundamental research is still necessary to help us understand the complexity of the interdependencies involved.
In this presentation we discuss the application of numerical simulation tools as well as diverse experiments and complementary tools, which support activities relating to the development of refractory products for the steel industry. Several examples throughout the steelmaking process are provided to evaluate the impact on each individual process step. Furthermore, the latest activities connected with selected research topics are presented.

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Modeling of Steel Continuous Casting

Corresponding Author: bgthomas@mines.edu

Continuous casting of steel is an important commercial process that involves many complex, coupled physical phenomena, which have been the subject of significant computational modeling efforts over the past half-century. This paper summarizes the current state of the art in modeling and simulation of these phenomena. This includes models of heat transfer and solidification of the steel shell, interfacial heat transfer between the shell and the mold, flow and pressure distribution in the metal delivery system, fluid flow in the nozzle, nozzle clogging, multiphase turbulent flow in the mold region, electromagnetic effects, argon gas effects, particle entrapment, interfacial interaction with the surface slag layers, level fluctuations and slag entrainment, initial solidification at the meniscus during mold oscillation, thermal-mechanical behavior of the solidifying steel shell, mold distortion and taper design, stress, surface-depression and crack formation, segregation, and microstructure formation. These models are challenged by the wide range of length and time scales which govern the phenomena of interest. Attention will focus on the importance of model verification (with other calculations) and validation (with experimental measurements) at every step. Finally, examples will emphasize the application of advanced, computational models to gain practical insights into this widely-used, mature process, where even small improvements can have a big commercial impact, but where technology development by experimental trial and error alone is cost prohibitive. Lessons learned from the modeling of continuous casting can be applied to the modeling and simulation of other complex manufacturing systems, including other metallurgical processes in steelmaking.

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Numerical investigation of steelmaking by-products recycling using microwave radiation

Author: Luís Silva[1]

Co-authors: José Pereira [1]; Duarte Albuquerque [1]

[1] *Instituto Superior Técnico*

Corresponding Authors: duartealbuquerque@ist.utl.pt, jcfpereira@tecnico.ulisboa.pt, luismiguelnobresilva@gmail.com

The steelmaking industry plays an important role on the global anthropogenic CO_2 emissions, accounting to 7 % of all global emissions. In addition, this industry also produces many by-products whose direct disposal without a proper treatment represents an environmental hazardous. In recent years, the recycling of these by-products is gaining increased relevance, to achieve a more environmentally friendly and sustainable steel production. Several processes have been deployed in the industry, with most of them, being based in pyrometallurgical methods, whose energy consumption, operational costs, and CO_2 emissions, hinder the wider usage of these technologies. To decrease these factors, microwave heating is being suggested as an alternative technological since it is more efficient and cleaner than the conventional counterpart.
The aim of this work is to give an insight on the operational parameters of a continuous recycling process of steelmaking by-products using microwave radiation as the heating source. A mathematical model was implemented using COMSOL Multiphysics. Firstly, this model was compared with a previously validated simplified model from the literature, to access both COMSOL Multiphysics capabilities and the phenomena happening in the process. Afterwards, the numerical model is modified for the process under consideration and several parametric studies are performed to determine their influence on the operational conditions. The results showed that, that a scaled-up size and thermal insulation are essential to the process global efficiency. From an emissions standpoint, it was proven that using lower C/O ratio mixtures can reduced the emissions. As for the flow current orientation, it was concluded that the usage of co-current flow might provide better temperature conditions, without hindering the power requirements.

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Thermodynamic Performance Optimization of CaO-SiO2-MgO-Al2O3 Slag System Based on Response Surface Methodology and Multi-objective Optimization

Author: Zicheng Xin[1]

Co-authors: Jiangshan Zhang [1]; Junguo Zhang [2]; Yu Jin [2]; Jin Zheng [3]; Qing Liu [1]

[1] *State Key Laboratory of Advanced Metallurgy, University of Science and Technology Beijing*

[2] *Tangshan Branch, Hebei Iron and Steel Co., Ltd.*

[3] *Tangshan Branch, Hebei Iron and Steel Co. Ltd.*

Corresponding Authors: winnerzhengjin@163.com, sklxzc@163.com, zjsustb@163.com, qliu@ustb.edu.cn, jinyulnkd@163.com, zhangjunguo@hbisco.com

Ladle furnace (LF) refining is one of the most popular secondary refining processes to produce clean steel and largely takes the responsibility in the whole steelmaking process. The performance of slag dramatically determines the refining efficiency. In order to realize the precise control of the composition content for refining slag to ensure the optimal performance of CaO-SiO2-MgO-Al2O3 slag system, the optimization model of thermodynamic performance for refining slag was established and verified based on thermodynamic simulation and laboratory test. Firstly, the experimental scheme was designed according to the Box-Behnken principle. The melting point, sulphide capacity, and slag viscosity were selected as the response variables, and the temperature, basicity, w(MgO) and w(Al2O3) were selected as the process parameters. The value of response variables was obtained using the Factage© and KTH model based on the experimental scheme. Meanwhile, the effect of different process parameters on each response variable was analyzed. In addition, a continuous variable surface model of each response variable and different process parameters was established with the response surface methodology (RSM). Furthermore, the multi-response problem was transformed into a single response problem with the maximization of the weighted geometric mean of the composite desirability function by introducing the desirability function, and then the optimal experimental scheme was obtained. Finally, the laboratory test was conducted under the optimal scheme to verify the reliability and accuracy of the optimization model. This method can be used to calculate the precise composition content of slag system to ensure that refining slag meets the requirements of low melting point, high sulphide capacity and reasonable viscosity ranges.

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Prediction of mechanical properties of hot rolled steel plates using neural network and statistical method

Author: Xiaoan Yang[1]

Co-authors: Chenlei Leng [2]; Hongbiao Dong [1]; Jenny Shepherd [1]; Qin Tao [1]; Stefan Stein [2]

[1] *University of Leicester*

[2] *University of Warwick*

Corresponding Authors: xy149@le.ac.uk, js1005@leicester.ac.uk, qt15@leicester.ac.uk, c.leng@warwick.ac.uk, hd38@le.ac.uk, s.stein@warwick.ac.uk

Steel manufacturing is a long and complicated process involving iron-making, refining, casting, rolling, etc.; the result, hundreds of processing parameters all with a potential influence on the mechanical properties of final product. This complexity results in significant challenges in the correlation of input parameters with output mechanical properties.

In this work, we applied both a neural network based model and a statistic method in order to predict yield strength, ultimate tensile strength, elongation and impact toughness of hot rolled steel plates using chemical composition and process parameters (including finish rolling temperature and reduction ratio). The influential process parameters recognized by the neural network model were compared with the key features selected by the statistical method, initial Guided Analytics for parameter Testing and control band Extraction or iGATE . The differences between predicted results using iGATE and neural network were discussed and the effect of input parameter, including chemistry and process variables investigated.

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Effect of bottom tuyere blockage on the mixing efficiency of molten bath in a converter

Author: Jiankun sun[1]

Co-authors: Jiangshan Zhang [1]; Wenhui Lin [1]; Xiaoming Feng [2]; Qing Liu [1]

[1] *University of Science and Technology Beijing*

[2] *Xinyu Iron and Steel Group Co.Ltd*

Corresponding Authors: zjsustb@163.com, every18@163.com, fxm@xinsteel.com.cn, hblgsjk@163.com, qliu@ustb.edu.cn

The blockage of bottom blowing tuyere(s) has a significant impact on the refining efficiency in the converter steelmaking process. In this paper, the effect of different arrangements of tuyere(s) blockage on the mixing efficiency was investigated in a 100 t converter with six bottom tuyeres. Both hydraulic experiment and numerical simulation were employed and their results agree well in terms of mixing time. The flow characteristics were also discussed. The results show that partial blockage of tuyere(s) strengthens the flow circulation in the horizontal direction of the molten bath and breaks the barrier between the independent stirring sub-zones, which enhances the overall mixing of molten bath. Besides, there is a critical value of the bottom blowing flow rate to influence the mixing time, and too large bottom blowing flow rates will cause violent oscillation of the molten bath.

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Numerical Simulation of Solid Shell Distribution in a Funnel Shape Mold under Electromagnetic Braking and Strand Electromagnetic Stirring

Author: Changjun Wang[1]

Co-authors: Baokuan Li [1]; Zhongqiu Liu [1]

[1] *Northeastern University*

Corresponding Authors: liuzq@smm.neu.edu.cn, libk@smm.neu.edu.cn, wangchangjun_neu@126.com

Continuous casting of thin steel slabs is a cutting-edge technology in iron and steel industry. Electromagnetic Braking (EMBr) technique is widely implemented into thin slab casters to reduce defects caused by strong turbulence in the mold. A slab-casting Strand Electromagnetic Stirring (SEMS) system was developed to control heat transfer in the strand. Sophisticated phenomena, including turbulent flow, heat transfer, electromagnetic effects, and solidification in the mold were solved using numerical methods. Electromagnetic fields with the simultaneous work of EMBr and SEMS were calculated based on finite-element method. Large eddy simulation was used to predict the transient flow. An enthalpy-porosity method was selected to predict the solid shell distribution. Furthermore, special boundary conditions were considered in the present model as the special shape of the mold. It is demonstrated that SEMS has a great effect on the distribution of solid shell and undercooling in the melt. And the mushy zone thickness nearby the SEMS becomes thinner. In addition, the SEMS used in this work will affect the velocity of slag-melt interface which can be observed in situ. Further work is needed to do to predict the equiaxed crystal ratio in the slab with the effect of electromagnetic manipulation.

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Development of adaptive meshless solution procedure for phase field modelling of dendritic solidification in carbon steel.

Author: Tadej Dobravec[1]

Co-authors: Boštjan Mavrič [2]; Božidar Šarler [2]

[1] *Faculty of Mechanical Engineering, University of Ljubljana, Slovenia*

[2] *Institute of Metals and Technology, Slovenia; Faculty of Mechanical Engineering, University of Ljubljana, Slovenia*

Corresponding Authors: tadej.dobravec@gmail.com, bozidar.sarler@fs.uni-lj.si, bostjan.mavric@imt.si

A novel solution procedure is developed for the phase field-based simulation of dendritic solidification in Fe-C alloys. The adaptive solution procedure is based on the dynamic quadtree domain decomposition which divides the computational domain into quadtree sub-domains of different size. Each quadtree sub-domain has its own distribution of computational nodes in which the meshless radial basis function-generated finite differences method and the forward Euler scheme are applied for the discretisation of the partial differential equations. The h-adaptivity is ensured by keeping a constant number of the nodes in each of the quadtree sub-domains. Different, mutually coordinated stable time steps are used in different quadtree sub-domains. The procedure dynamically ensures the highest density of the computational nodes at the solid-liquid interface and the lowest density in the bulk of the phases. The developed adaptive solution procedure is verified by solving the benchmark for isothermal solidification of binary alloys. The solution procedure is demonstrated on the constrained growth of a single equiaxed dendrite in a Fe-C alloy with imposed cooling rate. The impact of the distance between the two neighbouring equiaxed dendrites and the cooling rate to the dendrite morphology and micro-segregation is analysed. The developments represent a part of the micro-segregation module in multi-scale and multi-physics simulation system for continuous casting of steel.

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On the Role of Heat Transfer in the Thermo Chemical Conversion of Pulverized Coal

Author: Markus Bösenhofer[1]

Co-authors: Christoph Feilmayr [2]; Franz Hauzenberger [3]; Hugo Stocker [4]; Magdalena Schatzl [5]; Michael Harasek [6]

[1] *TU Wien / K1-MET GmbH*

[2] *voestalpine Stahl GmbH*

[3] *Primetals Technologies Austria GmbH*

[4] *voestalpine Stahl Donawitz GmbH*

[5] *K1-MET GmbH*

[6] *TU Wien*

Corresponding Authors: markus.boesenhofer@tuwien.ac.at, christoph.feilmayr@voestalpine.com, hugo.stocker@voestalpine.com, michael.harasek@tuwien.ac.at, magdalena.schatzl@k1-met.com, franz.hauzenberger@primetals.com

Injecting pulverized coal into the raceway zone of blast furnaces is a stat of the art process to optimize the operation of the furnace. Modeling the thermo chemical conversion of pulverized coal in the raceway zone is commonly used to investigate its effect on the blast furnace process or to optimize the coal injection process. The quality and accurateness of the employed models determine the reliability of the simulation results. In case of pulverized coal conversion, heat transfer rates control the initial drying and devolatilization stages and simulation results are sensitive to the employed heat transfer model. In particular, the high heat of evaporation of water and the endothermy of the thermal break down of volatiles cause the heat transfer control of the thermo-chemical conversion. Since coal conversion is a sequential process, changes in the drying and devolatilization will also affect the conversion rates and also the overall conversion duration. Overestimating the heat transfer rates would then result in coal particles being consumed within the raceway zone in simulations, while they could reach the bulk coke bed at low conversion.in reality.
To assess this effect, we evaluate the influence of the heat transfer model on the overall thermo-chemical conversion of pulverized coal. For this purpose, we first introduce common thermo chemical coal conversion models and heat transfer models, which is followed by a simplified test case to evaluate the heat transfer's impact on the thermo chemical coal conversion. Finally, we verify these results using experimental data for coal combustion from literature.

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Real Time Modelling of Burden Components Distribution during Hopper Outflow and Burdening via a rotating Chute

Author: Stephan Hojda[1]

Co-authors: Frank Rückert [2]; Heike Busch [1]; Katharina Amend [2]; Martin Pollet [1]; Rongshan Lin [1]

[1] *AG der Dillinger Hüttenwerke*

[2] *University of Applied Sciences Saarbrücken (htw Saar)*

Corresponding Authors: rongshan.lin@dillinger.biz, stephan.hojda@dillinger.biz, heike.busch@dillinger.biz, katherina.amend@t-online.de, frank.rueckert@htwsaar.de, martin.pollet@dillinger.biz

The burden distribution in the blast furnace has a major impact on the process and its stability. The iron bearing burden consists normally of several components, such as sinter, pellets, lump ore, silica addition and nut coke. Therefore, the exact composition at discrete positions and times in the blast furnace is of great interest. While the charging via a rotating chute is well investigated by computationally costly methods like Discrete Element Method, there is a lack of models with real time capabilities to track the burden materials. This holds especially if not only a single process is in the focus but the tracking incorporates blending operations on conveyer belts, in hoppers and finally on the chute and in the blast furnace. In the current work a concept to model the material flow along the process chain from stock house to blast furnace is presented. The focus of this paper is to simulate material discharging from the hopper and distributing of the material inside the blast furnace. The hopper is modelled with a cellular automaton, the material position after charging is calculated by a semi-empirical charging model. As additional information the material in the models can always be associated to information like the chemical analysis or the screen size. Both models are coupled and displayed via a web interface. The model enables for an offline optimization of the burden distribution from the hopper up to the blast furnace and also for online guidance and recommendations for the blast furnace operators.

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A new sinter plant model for flowsheet simulations

Author: Johannes Niel[1]

Co-authors: Bernd Weiß [2]; Walter Wukovits

[1] *Institute of Chemical, Environmental and Bioscience Engineering, TU Wien, Austria*

[2] *Primetals Technologies Austria GmbH,Linz,Austria*

Corresponding Authors: bernd.weiss@primetals.com, johannes.niel@tuwien.ac.at

Lowering emissions of pollutants and carbon consumption has become increasingly imperative in our society nowadays. The worldwide growing restrictions of waste gas emissions on integrated steelworks are the focal motivation of this work. The sintering process is a highly energy-intensive, and a vast material-consuming process unit in the hot metal production. Iron ore sintering depends on the raw mixture, sinter plant geometry, and operational conditions. The difficulties for an accurate description of the off-gas properties in the wind boxes lie in their varying temperatures, changing composition, and different mass flows. A detailed description of the off-gas properties will give a profound basis for decision for required raw mixture compositions, wind box geometries, and operational settings for a selective waste gas recirculation (SWGR).
A sinter model based on temperature profiles and mass distributions was developed and implemented in an existing model library for iron and steel production. This unique approach allows flowsheet simulations for different plant geometries, with and without SWGR, and various operational conditions. The model contains (i) a burner model describing the combustion conditions underneath the ignition hood, (ii) a black-box model including the main sintering reactions and a gas-solid separation, and (iii) a wind-box model that splits the off-gas into a stack-gas and a recycle-stream.
The simulation results were validated on plant data and literature. The influence of temperature profiles on wind box gas composition was investigated by focusing on coke consumption and trace element emissions of a sinter strand. Differences and short comings of the developed model compared to models in literature are discussed.

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Species Diffusion Modeling in Porous Particles for Metallurgical Applications

Author: Matthias Kiss[1]

Co-authors: Magdalena Schatzl [1]; Markus Bösenhofer [2]; Michael Harasek [3]

[1] *K1-MET GmbH*

[2] *Technische Universität Wien, K1-MET GmbH*

[3] *Technische Universität Wien*

Corresponding Authors: markus.boesenhofer@tuwien.ac.at, matthias.kiss@k1-met.com, magdalena.schatzl@k1-met.com, michael.harasek@tuwien.ac.at

The thermo-chemical conversion of coke and reduction of iron ore particles both depend on mass transport from the bulk fluid phase towards the reactive sites in the solid phase. Pore diffusion limits this mass transport in porous particles at intermediate temperatures, while chemistry is limiting co nversion rates at low temperatures. Besides temperature, pore diffusion rates also depend on physical particle properties, e.g. pore diameter, tortuosity, fluid properties, and species gradients. Modeling approaches of different complexity for pore diffusion can be found in literature. Their diffusion rates can vary by orders of magnitude. Thus, the right choice of diffusion model is highly important for reasonable predictions. The wrong choice can lead to large under/over estimations of conversion or reduction rates.

We conduct a numerical study of the effects of different diffusion models on the conversion of a single fuel particle to evaluate their suitability for metallurgical applications. The numerical model we employ is fully implemented in the open source CFD package OpenFoam®-7. The inside of the solid fuel particle is modeled using an Euler-Euler approach, which implies that the particle pores are not resolved. The particle and surrounding fluid are coupled using explicit Robin-Neumann-coupling for species concentrations, pressure, and temperature.

In this work, we will briefly introduce the different diffusion models and their characteristics, followed by an explanation of the setup of our numerical experiments. Finally, the different diffusion models will be evaluated in regard to their quality of prediction compared to experiments available in literature, and their computational cost.

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Development of a porous solid model for DRI applications

Author: Quentin Fradet[1]

Co-authors: Mohammed Liaket Ali [2]; Uwe Riedel [2]

[1] *German Aerospace Center (DLR), Institute of Low-Carbon Industrial Processes*

[2] *German Aerospace Center (DLR)*

Corresponding Authors: mohammed.ali@dlr.de, uwe.riedel@dlr.de, quentin.fradet@dlr.de

The Direct Reduction (DR) of iron ore pellets with syngas or hydrogen is a promising technology to reduce the emission of iron making. The conversion rate of singe pellets to iron has been extensively investigated. A shrinking core model is commonly employed to reproduce the experimental observations.
Though, this model presents an inherent bias by assuming a sharp separation between a fully converted region and a fully unreacted one. In the present study, a porous solid model is proposed. This model solves for the mass balances of the individual gas species and the solid ones assuming a spherical symmetry. The governing equations, the main algorithm and validation cases will be presented. The open-source suite Cantera was integrated in the model. This allows the use of heterogeneous reaction mechanism and facilitates chemical kinetics calculations. The present model also offers a wide flexibility to incorporate complex phenomena such as pellet morphological changes or carbon deposition. Another advantage of the approach is its smooth transition to multidimensional computations. In this way, the reliability of the kinetic and transport models is insured when used in multidimensional CFD-calculations.

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Recent modeling approaches to close-coupled atomization for powder production

Author: Hans-Jürgen Odenthal[1]

Co-authors: Cameron Tropea [2]; Ilia Roisman [2]; Niklas Apell [2]; Norbert Vogl [3]; Tobias Brune [3]

[1] *SMS group GmbH, R&D Division*

[2] *TU Darmstadt*

[3] *SMS group GmbH*

Corresponding Authors: roisman@sls.tu-darmstadt.de, tobias.brune@sms-group.com, norbert.vogl@sms-group.com, apell@sla.tu-darmstadt.de, hans-juergen.odenthal@sms-group.com, tropea@sla.tu-darmstadt.de

In additive manufacturing of metals, high quality powder with uniform size distribution and spherical, satellite-free particles of defined size is required. SMS group has built-up a metal powder production plant which operates using the close-coupled atomization principle. For reliable plant operation, it is important to understand the atomization mechanisms, i.e. the effect of plant parameters such as nozzle geometry or melt and gas flow rates on the particle size. Thus, the challenge lies in modeling the atomization process under extreme plant conditions.
A cooperative project with five partners from India and Germany is being funded by the Indo-German Science & Technology Center with support from the Federal Ministry of Education and Research. The project builds on a coupled approach of laboratory experiments, numerical simulations and plant operation to develop models and design guidelines for production plants.
The basis is the production plant, which produces austenitic, nickel based, and in the future maraging steel powder. The nozzle system has been replicated in a one-to-one scale laboratory test rig. Here, the plant conditions are reproduced using heated water and air as fluids, satisfying most dimensionless numbers of the production plant. The test rig allows investigation of the interaction between shock/expansion waves and water flow by focusing Schlieren optics, high-speed imaging and phase Doppler anemometry. On the Indian side, a shock-droplet-interaction test rig and a supersonic wind tunnel have been built-up. Using high-speed shadowgraphy and Schlieren optics, the mechanisms of droplet breakup are visualized.
Parallel to the experimental work, CFD models are being developed to predict the behavior of the ligaments beneath the nozzles, liquid-gas-interaction and droplet solidification. Promising results have been computed for the flow of water and air, matching the conditions of the laboratory test rig.

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Computational fluid modelling of plastics injections in EAF metallurgical operation through innovative nozzles and industrial testing

Authors: Michele De Santis[1]; Filippo Cirilli[1]; Loris Bianco[2]; Daniele Gaspardo[2]; Matteo Chini[2]; Jaroslav Brhel[3]

[1] *Rina Consulting - Centro Sviluppo Materiali SpA*

[2] *Ferriere Nord*

[3] *HTT*

Corresponding Authors: michele.desantis_csm@rina.org, matteo.chini@pittini.it, loris.bianco@pittini.it, filippo.cirilli@rina.org, daniele.gaspardo@pittini.it, jbrhel@htte.eu

The H2020 project POLYNSPIRE was launched to improve energy and resource efficiency of post-consumer and post-industrial plastic recycling processes, targeting 100% waste streams. Pillars to reach this ambitious goal are: (1) Chemical recycling to recover plastic monomers and valuable fillers, (2) Advanced additivation to enhance recycled plastics quality, (3) Valorization of plastic waste as carbon source in steel industry, to recover a large amount of mixed plastic discarded from the recycling processes. Plastic is a "new" material for steel sector and can be used to replace fossil coal, reducing virgin raw materials demand, putting steel production in a general frame of circular economy. Its use requires ad-hoc plant components development, in this specific case, new injectors.
Computational Fluid Modelling (CFD) was developed in ANSYS-Fluent frame aimed at simulating

new injectors flow behaviour for EAF metallurgical operations. They were designed specifically for plastic injection while maintaining the same metallurgical performance of the standard injectors.
Starting from industrial plant reference conditions, the basic new injectors design, and their performance evaluated in presence of separate injectors for particles and oxygen and operating with a blend of plastic and fossil coal. The possibility of multi-fold injectors for coal and plastic was investigated aimed at achieving the best foaming behaviour. The fluid-dynamic quantities involved at EAF bath level allowed to calculate, by semi-empirical correlations, the penetration of the gas jet and coal particle into slag and steel. Modelling also included simulation of different powder material flow, transport gas flow and secondary boosting air nozzle flow. Moreover, the new feeding systems were simulated both as injectors and burners as flexible in function of the EAF metallurgical operations requested.
The CFD simulations results were assessed with the EAF steelmaking partners, and the performance of new plastic injection systems compared with reference coal case.

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Search for Compositionally Complex Coating Materials for a Sustainable Steel Industry

Author: Zihui Dong[1]

Co-authors: Francesco Fanicchia [2]; Hongbiao Dong [1]; Jihad Zraibi [3]; Marzuk Kamal [3]; Shiladitya Paul [2]

[1] *University of Leicester*

[2] *TWI Ltd*

[3] *AeonX AI*

Corresponding Authors: shiladitya.paul@twi.co.uk, hd38@le.ac.uk, zd47@le.ac.uk, francesco.fanicchia@twi.co.uk

Iron and steel production is an energy-intensive process, often associated with high greenhouse gas (GHG) emissions. There is a drive to reduce GHG emissions in energy-intensive industries. However, the existing technologies used for reducing CO2 emission have reached a plateau. The emergence of novel technologies such as carbon capture, utilisation and storage systems are proposed as a new strategy for the steelmaking industry to adopt more proactive, sustainable improvements which aim to advance current equipment with progressive production efficiency, component lifetime and reduced environmental impact. In order to realise aforementioned targets, capability of materials to tolerate the corrosive, erosive, reactive and high temperature process gases is essential to develop new coating materials. The EU-funded FORGE project plans to develop novel and cost-effective coatings of compositionally complex alloys, combining machine learning models, thermodynamic calculations, and high-throughput experiments. FORGE will demonstrate these coatings on processes such as CO2-capture, waste heat recovery, components in kilns and undergoing wear, and show the efficacy in defying the acting degradation forces, and assuring coating effectiveness with smart monitoring of their deterioration. FORGE aims to minimise the overall capital and operative expenses in steelmaking industry.

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Hydrogen based direct iron ore reduction plant simulation

Author: Roland Eisl[1]

Co-authors: Clemens Oppeneiger [1]; Daniel Buchberger [1]; Marlen Hochwimmer [1]

[1] *ENRAG GmbH*

Corresponding Authors: marlen.hochwimmer@enrag.at, daniel.buchberger@enrag.at, roland.eisl@enrag.at, clemens.oppeneiger@enrag.at

The current work and paper bases on a new iron production route which uses iron ore fines direct reduction. This technology was invented by ENRAG and PRIMETALS and is in ongoing development by Primetals Technology. It is called HYFOR. This new direct reduction technology uses iron ore fines instead of pellets and is therefore more energy efficient and uses cheaper ore material compared to state-of-the-art technologies. Via a collaborative research project ENRAG developed the fundamentals of a fully transient simulation engine for the operation of a future HYFOR plant. The simulation engine consists of all process relevant parts including the reduction agent production (hydrogen), the ore preheater (or in case of magnetite pre-oxidation), the reduction section as well as all necessary bunkers and ducts.
The model can fully calculate all phenomena of transient behavior during start up, load change, and shut down of the reduction process. This also includes all partial transient energy- and mass storage processes in the plant. The current work consists of the model development and first findings on the first prototype plant currently being built. Based on the model different sub processes can be optimized and future industrial size plants can be designed and constructed based on the findings of this digital twin.

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Development of a kinetic mechanism for the direct reduction of hematite pellets in CO-H2 atmospheres using a porous solid pellet model

Author: Mohammed Liaket Ali[1]

Co-authors: Quentin Fradet [1]; Uwe Riedel [1]

[1] *German Aerospace Center (DLR)*

Corresponding Authors: mohammed.ali@dlr.de, uwe.riedel@dlr.de, quentin.fradet@dlr.de

Increasing interest in the direct reduction of Iron has revived investigations on the kinetics of gaseous reduction of iron oxides. Despite extensive investigations on the reduction of iron oxides with pure hydrogen or with syngas, the development of a generic reduction mechanism of iron oxides is still lacking. The conventional shrinking core model hardly distinguish between transport processes and reaction processes, leading to biases in the kinetic model. In the present study, a porous solid model, which solves mass balances of the individual gas species and solid ones assuming a spherical symmetry is used for developing a heterogeneous kinetic mechanism accounting for different iron oxides (Fe2O3, Fe3O4, FeO). It also accounts for carbon accumulation and iron carbide (Fe3C) formation at lower temperature to model phenomena like carbon-deposition and incomplete reduction of iron oxide using CO/-H2 mixtures. The present study will attempt to fit a single mechanism on multiple experimental data sets of single pellet reduction with syngas of varying content up to pure hydrogen from the literature. Finally, the effects of gas composition, flow rates, temperature and pellet characteristics such as porosity, tortuosity, diameter factor on the reduction of iron oxide will be investigated.

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Digital twin for continuous casters – Optimizing production with modeling and simulation methods

Author: Reinhold Leitner[1]

Co-authors: Brugger Christian [2]; Fuchshuber Daniel [2]; Pennerstorfer Paul [2]

[1] *Primetals Technologies Austria GmbH*

[2] .

Corresponding Authors: leitner.reinhold@primetals.com, daniel.fuchshuber@primetals.com, christian.brugger@primetals.com, paul.pennerstorfer@primetals.com

State-of-the-art automation technology enables digitalization of the continuous casting process that goes far beyond conventional automation of industrial production. Primetals Technologies provides a digital twin that combines an intelligent digital representation of a casting machine as well as the casting process and the slabs, blooms or billets that are produced. It allows metallurgists and process engineers to predict the behavior of the involved complex production process and optimize parameters before using them in real production. New steel grades or production processes can be evaluated off-line without any risks to process stability and product quality.
Primetals Technologies installs the digital twin with every new installation of a continuous caster optimization system. This paper describes how the setup and simulation possibilities of the digital twin provide numerous benefits by modelling and simulating the casting process. It allows for example the calculation of material properties according to the actual composition, strand surface temperature profiles and dynamic soft reduction before the final point of solidification. An outstanding feature of the digital twin is the replay functionality provided for various models to analyze and further optimize real production situations. The paper also gives examples how usage of the digital twin optimized production at various customers.

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Simulating the impact of complex rules' configuration on quality control in steel manufacturing

Author: Joachim Gnauk[1]

Co-authors: Alessandro Stenico [2]; Vladimir Berenzon [2]; Kai Huang [3]

[1] *PSI Metals*

[2] *PSI Metals GmbH*

[3] *PSI Information Technology Co., Ltd.*

Corresponding Author: astenico@psi.de

Configuring rules for automated quality evaluation within a quality management system is a complex task, especially when several processing lines along the production route are involved. In fact, the system user needs to transfer process and product knowledge of quality engineers and steel developers into the system in order to enable an automated quality decision that reflects the experts' knowhow. In this paper, a system that supports the definition of complex quality evaluation rules and validates them by simulating their impact on a large amount of historical, high-resolution production mass data, is presented. Examples are illustrated from a first successful installation in the integrated plant of a renowned Asian steel manufacturer.

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AI models for mechanical properties prediction and their application in product development

Author: Sonja Straßer[1]

Co-authors: Klaus Jax [2]; Du Ngyuen Duy [1]; Alfred Seyr [1]

[1] *Primetals Technologies*

[2] *Primetals Technologies Austria GmbH*

Corresponding Authors: alfred.seyr@primetals.com, du.ngyuen-duy@primetals.com, klaus.jax@primetals.com, sonja.strasser@primetals.com

Knowing the material properties seamlessly across the full product length is a prerequisite for enhanced product safety. Primetals Technology created a customizable IT solution based on artificial intelligence and machine learning algorithms which calculates the mechanical properties of a hot rolled or annealed or galvanized steel strip just in time and almost without additional equipment.
Chemical composition and measured process parameters, which are provided from a mill's data storage and processing systems, serve as input for purpose-built ML models which are able to calculate yield strength, tensile strength and fracture elongation over the whole strip length or at a certain position where normally test specimen are taken from.
Our solution, called Quality Guard, is designed to send back the predictions within a few seconds to the data storage and the results are available to react in time on deviations. For example, the estimated values of the models can be used to decide whether a material is well within a specified tolerance range or outside the tolerance and therefore it needs to be blocked and re-tested conventionally. The accurate predictions of this tool can also be used for automatic grading without physical testing.
In addition to this basic quality functionality we adapted our solution for product developers, process engineers and quality departments. This full featured solution, called Quality Lab, is a lab, where you can modify, like in a real lab, the relevant process parameter and the chemical analysis of your product by moving sliders or by direct numerical input. The built-in partial dependence plots provide structured visualization where graphs show how parameter variation is influencing the result. Analyzing various influences on actual product or optimizing or designing completely new grades becomes much more reliable and faster with this solution.

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Development of a Prediction Simulator Software for Blast Furnace Operation

Author: Tyamo Okosun[1]

Co-authors: Chenn Zhou [2]; Nick Rheinheimer [1]; Samuel Nielson [1]

[1] *CIVS, Purdue University Northwest*

[2] *Purdue University Northwest*

Corresponding Authors: tokosun@pnw.edu, czhou@pnw.edu, nrheinhe@pnw.edu, snielson@pnw.edu

In a blast furnace, hot pressurized air is forced into a packed coke bed where it combusts, generating hot reducing gases for liquid iron production. Stable operation of the furnace requires careful balancing of many operational conditions. Blast furnaces are very resource intensive, and any changes in operating conditions can take hours to produce results. Currently, operators generally rely on established rules of thumb to estimate the response of the furnace to changing conditions, but these rules can be limited in scope and often cannot account for the implementation of new process parameters such as novel injected fuels.
A software was developed to predict blast furnace performance based on pre-calculated simulations of furnace operation. This software uses datasets generated through the application of High-Performance Computing (HPC) to Computational Fluid Dynamics (CFD) of the blast furnace. While CFD allows researchers to determine the likely outcomes of operational changes with reasonable accuracy, the time required to complete a single simulation is typically on the order of days to a week. With this in mind, a large range of data sets were pre-simulated to determine key trends using CFD, comparable to rules of thumb for individual parameters.
The simulator software uses interpolation to create a set of equations relating all of the simulated operating conditions as input variables to specific output variables, such as coke rate, top gas temperature, gas utilization, and pressure drop. This tool can quickly and accurately predict the impacts of changing operating conditions within a given range, providing operators with a limited "what-if" scenario evaluation capability. A feature also exists to return the lowest possible coke rate based on a set of constraints. This allows operators to aim for reduced operating costs and lower carbon emissions from the blast furnace.

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Digital Twin of Steelmaking and -refining Process by On-Line Thermodynamic and Kinetic Model

Author: Anthony Nicholas Grundy[1]

Co-authors: Johan Jeppsson [2]; Lina Kjellqvist [2]; Ralf Rettig [2]

[1] *Thermo-Calc AB*

[2] *Thermo-Calc Software AB*

Corresponding Authors: nicholas@thermocalc.com, lina@thermocalc.se, johanj@thermocalc.se, ralf@thermocalc.se

Thermo-Calc Software is a well-known developer of large CALPHAD-type databases and software for property and phase diagram calculations based on Gibbs energy minimization. A database for oxides, TCOX, has been available since 1992 and development has been greatly accelerated in recenet years placing special emphasis on steel-slag interactions.
Parallel to the database, the Process Metallurgy Module (PMM) has been developed, that allows full kinetic simulations of steelmaking and -refining processes. The PMM graphical user interface enables simple and intuitive set-up of processes such as BOF, EAF, LF, VOD/AOD, etc… for the analysis and process optimization for different grades with different quality requirements. The model has been validated for several steelmaking processes including LF and VOD.
The PMM functionalities and models are currently being integrated into TC-Python, a software development kit, that allows openly coupling Thermo-Calc with other software. This enables directly accessing Level 2 systems and using actual stored steelplant process data and chemical analyses, to run process simulations off-line after the heat has been produced to understand the origin of quality issues and unexpected events that might have occurred during production or to investigate alternative processing routes that might have lower total production costs, have lower environmental impact, or might meet more stringent quality requirements.
We are also working on concepts to run the PMM on-line in parallel to the actual steelmaking and -refining process, thus effectively having a Digital Twin of the production process, enabling to track steel chemistry, inclusion amount and type, slag chemistry, viscosity and amount, steel and slag temperature, refractory wear, etc… in real time, allowing operators to perform corrective action for an optimal production process. To achieve the required calculation speeds and stability, it currently looks like this will require a metamodeling approach.

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Optimization of integrated steel plants operation using the m.simtop strategic planning platform

Author: Bernd Weiss[1]

Co-authors: Johannes Niel [2]; Stefan Tjaden [3]; Walter Wukovits [4]

[1] *Primetals Technologies GmbH*

[2] *TU Wien*

[3] *Process Engineer*

[4] *Assistant Professor*

Corresponding Authors: johannes.niel@tuwien.ac.at, walter.wukovits@tuwien.ac.at, bernd.weiss@primetals.com, stefan.tjaden.ext@primetals.com

Iron and steel making requires a wide range of different raw materials significantly influencing process performance which demands a continuous optimisation of process routes also with respect to energy efficiency as well as environmental emissions. Steadily changing raw material prices and qualities, market situations and product variations are challenging integrated steel plant operators in production planning and cost optimization. Primetals decided to develop a comprehensive metallurgical flow sheet model library for simulation and optimization of integrated steel plants. Intensive development efforts were taken in order to migrate existing well established calculation and engineering routines as well as integrate newly developed models. The generated model library enables the setup of mass and energy balances for integrated steel plants, development and evaluation of new process concepts as well as investigations on impacts of raw material changes and trace material distributions. By using this process integration platform, it is possible to compare different iron and steelmaking routes within one standardized environment. In this publication an insight will be given on the competence of mSIMTOP in depicting integrated steel plant operation, enhance raw material planning, show the effect of new raw materials and new internal recycles on realistic examples.

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Big data handling in process surveillance and quality control of secondary metallurgical processes

Author: Christine Gruber[1]

Co-authors: Birgit Bückner ; Magdalena Schatzl ; Maria Thumfart ; Ramona Eßbichl ; Roman Rössler

[1] *K1-MET*

Corresponding Author: christine.gruber@k1-met.com

The RH degassing plant is essential for producing ultra-clean steel, but its vacuum-based nature is hiding the process from close scrutiny. Despite recording the many inputs and outputs of process control and measurements surrounding the plant, the use of produced data is comparatively low, and data handling is a challenge, especially considering correlations of process control data with KPIs such as actual steel homogeneity and cleanliness after casting.
Within the scope of the EC-funded INEVITABLE project, the focus lies on improving sensor data quality and maximizing the utilization of the abundance of data obtained during the RH process. Visual surveillance offers the possibility of image analyses via conventional approaches such as surface flow observation inside the vacuum chamber and flow analysis with PIV or optical flow methods, but also machine learning can be applied, e.g., for blurriness detection or even flow pattern recognition. Time-series data from process control measurements like offgas composition or chamber pressure, even though highly connected to specific domain knowledge, can be tackled with machine learning methods as well, such as recognition of characteristic curve sections or categorization of curves. Ultimately, machine learning could be applied to correlate data on the quality of the cast steel with specific patterns occurring in the data during the cleaning and homogenizing steps of steel production.
In this talk we present examples for the application of machine learning techniques in the context of the RH treatment in steel plants and evaluate their success and relevance for improving the production of ultra-clean steels.

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Probabilistic EAF charge mix optimization using machine learning based scrap characterization

Author: Christoph Kirmse[1]

Co-authors: Maximilian Christ [1]; Sebastian Bangel

[1] *SMS digital GmbH*

Corresponding Authors: maximilian.christ@sms-digital.com, christoph.kirmse@sms-digital.com

The electric arc furnace (EAF) generates crude metal from virgin materials and recycled scrap.
Meeting the right concentrations of alloying elements in the crude metal (e.g., Cu, Ni) is crucial.
Scrap with higher uncertainty in the concentrations of such alloys is usually cheaper than virgin materials but might threaten product quality.
Using the cheapest input materials while complying with crude metal quality requirements are important goals of an EAF plant operator.

To support operators, we developed the Metallics Optimiser (MO) Application that calculates the cheapest commodity mix by integrating machine learning techniques into physical process models.
The physical models capture mass and energy balances of the EAF and consider weight and composition of the hot heel, slag weight and composition, dust losses and off-gas composition.
The machine learning models are estimating the concentrations of alloys in the scrap:
Based on historical charge mixes and chemical analysis of the crude steel, the MO backward calculates the most likely alloy composition of all used input materials over time.
This can be used in future heats to predict the chemical composition of different charge mixes.

The hot heel of the previous heat is, apart from the scrap, an incoming material stream for the EAF.
Thus, the hot heel properties have an influencing factor on the steel quality and must be considered in the prediction.
However, the exact weight of the hot heel cannot be determined for each heat, introducing an instability in the estimation.

Early results show that the MO is able to find scrap mixes that result in lower production costs than current systems while maintaining requested quality requirements and even decreasing process uncertainty.
Using a dynamic scrap element characterization allows to recycle more scrap, leading to higher savings compared to static element characterizations and static charge mix optimizations.

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Estimation of the bath temperature in an electric arc furnace using operational data and fuzzy modelling approach

Author: Aljaž Blažič[1]

Co-authors: Igor Škrjanc [1]; Vito Logar [1]

[1] *Faculty of Electrical Engineering, University of Ljubljana*

Corresponding Authors: aljaz.blazic@fe.uni-lj.si, igor.skrjanc@fe.uni-lj.si, vito.logar@fe.uni-lj.si

Steel recycling in electric arc furnaces (EAFs) is crucial to achieve environmental as well as economic sustainability of the steel industry. Although the EAFs impose a smaller environmental imprint in comparison to basic oxygen furnaces (BOFs), they still represent an energy-intensive process, with numerous possibilities for improvements. Digitalization and informatization of the steelmaking processes opened numerous possibilities in the field of production optimization using large amounts of data, where EAFs are no exception. In the following paper, a fuzzy-model-based approach for estimation of the bath temperature in an EAF is presented. As known, in most EAFs, disposable measuring probes are used to determine bath temperature prior to tapping. Since the EAF needs to be switched off during the measurement procedure, each measurement increases the losses and imposes a certain operational delay. Considering that several temperature samples are taken, i.e. 3 – 6 on average, the losses and delays are no longer neglectable. Furthermore, as the bath temperature between the measurements can only be roughly estimated by the operators, the control of the EAF cannot be as precise as it would be if the temperature was known. Therefore, the proposed methodology combines computational intelligence in soft sensor design and the operational measurements of all influential EAF inputs, to continuously estimate the bath temperature during the refining stage of the recycling process. The goals of the proposed approach are twofold, both leading to higher plant efficiency, i.e. first, to reduce the number of necessary temperature measurements, and thus decrease the losses and delays; second, to provide more information to the operators, and thus allow more precise EAF

control. The results have shown high prediction accuracy of the proposed approach; thus, the developed methodology will be implemented in an industrial environment, running in parallel with the actual EAF process.

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Digitalization and Software Support of the Electric Arc Furnace Process

Author: Vito Logar[1]

Co-authors: Goran Andonovski [1]; Igor Škrjanc [1]; Simon Tomažič [1]

[1] *University of Ljubljana, Faculty of electrical engineering*

Corresponding Authors: simon.tomazic@fe.uni-lj.si, goran.andonovski@fe.uni-lj.si, vito.logar@fe.uni-lj.si, igor.skrjanc@fe.uni-lj.si

In the last decades, steelmaking processes have been a subject to substantial modernization in terms of digitalization and informatization of various plants. Whether in the past operational measurements acquired by SCADAs have been used solely for process monitoring and fault detection, a closer inspection of the gathered data reveals numerous possibilities also for process enhancement and optimization. As such, modern methods of modelling, simulation and data mining can be applied using vast amounts of historical data, aiming to improve different processes in different steelmaking areas. The following paper presents the means and the methods of digital transformation of the electric-arc-furnace (EAF) process in SIJ Acroni steelworks. The work as presented in this paper is performed in the scope of the ongoing EU Horizon 2020 project, SPIRE initiative, INEVITABLE ("Optimization and performance improving in metal industry by digital technologies", Grant No. 869815). In this manner, different aspects and approaches of digitalization, and more important, proper software tools, to support and enhance the EAF process, are presented. First, the overall concept of digitalization, including data acquisition, protocols and data transfers, is presented, representing the fundamentals for higher software levels. Second, the developed methods, which aim to increase the efficiency of the EAF, are discussed in greater detail, explaining the concepts of theoretical modelling and parallel simulation, fuzzy-model based solutions and data-driven process optimization, in terms of energy and resource use. Third, the planned implementation of the developed methodology is presented, including the envisioned application of edge computing and cloud-based user interfaces. Finally, some of the proposed goals and expectations from the developed solutions are explained and discussed.

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Implementation of a surface-to-surface model for implicitly solved multiple one-dimensional simulations

Author: Andreas Rath[1]

Co-authors: Christoph Spijker [1]; Harald Raupenstrauch [1]

[1] *Montanuniversität Leoben*

Corresponding Authors: christoph.spijker@unileoben.ac.at, harald.raupenstrauch@unileoben.ac.at, andreas.rath@unileoben.ac.at

The impact on process performance after changing parameters like burner mass fluxes, dwell time, or gas composition is vital knowledge. It can be obtained by various methods as for example experimental setups, or computational fluids dynamic (CFD) simulation. The disadvantage of those conventional methods is that they are time-consuming and expensive for full-size industrial applications. However, another way of retrieving some of the desired knowledge is to apply a simulation procedure that divides the computational domain into multiple one-dimensional zones that are coupled with each other and implicitly solved. This reduces the complexity of the computational domain and makes it possible to generate transient simulation results for hours of process time of full-size industrial furnaces within minutes of computational time. A crucial factor to fully describe furnaces is the radiative heat transfer, which is regarding industrial furnaces the dominant mode of heat transfer. The motivation of this paper is to present a practical procedure to model radiation using a surface-to-surface (S2S) approach and implement it in the implicit multiple one-dimensional structure. A major challenge described will be its modification to allow the computation of dynamic systems without losing time to compute the required view factor matrices each time the computation geometry changes. Subsequently, the results of the implemented algorithm are statistically evaluated and checked for their plausibility and runtime performance.

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Metallurgical Data Science for Steel Industry

Author: Bogdan Nenchev[1]

Co-authors: Andrew Dunsmore [1]; Biao Tao [2]; Chinnapat Panwisawas [1]; Fang Wang [3]; Fucun Li [4]; Hongbiao Dong [1]; Jean-Christophe Gebelin [1]; Jun Fu [1]; Ming Li [2]; Qing Tao [1]; Xiaoan Yang [1]; Zihui Dong [1]

[1] *University of Leicester*

[2] *NISCO Research Institute, Nanjing Iron and Steel United Company*

[3] *NISCO Data Institute, Nanjing Iron and Steel United Company*

[4] *Jiangsu Jinheng Information Technology*

Corresponding Authors: bn55@leicester.ac.uk, lifucun@njsteel.com.cn, chinnapat.panwisawas@leicester.ac.uk, zihui.dong@leicester.ac.uk, hd38@le.ac.uk, liming1@njsteel.com.cn, xy149@leicester.ac.uk, jf320@leicester.ac.uk, wangf@njsteel.com.cn, qt15@leicester.ac.uk, acd33@leicester.ac.uk, taobiao@njsteel.com.cn, jg499@leicester.ac.uk

As one of the largest production chains in the world, the steel industry faces an ever-increasing demand for higher level of functionality and quality of final products at reduced environmental impact and manufacturing cost. The steel industry has developed an extensive range of sensors to generate data, monitor, and control steelmaking processes. Despite these advances, issues remain in the areas of data collection, storage, migration, lack of through-process data links and erroneous datasets, all of which significantly increase the complexity of the quality process control. The development of data-driven approach through advanced artificial intelligence (AI) techniques offers the opportunity to practically implement machine learning techniques to such datasets aiming to provide processing-property optimisation and identify gaps and errors in the data.

Recently, computational capabilities and algorithmic developments have significantly grown in power and complexity, accelerating the progress of process optimisation and materials defect and property prediction. However, addressing large scale industrial data process-property optimisation strategies is challenging as it involves numerous influencing factors each possessing with insufficient data. Herein, an integrated data-driven steelmaking case study is attempted with the aim of predicting and optimising the performance of final products. The key variables have been identified across multiple process chains such as steelmaking, casting, hot rolling and heat treatment. Machine learning has been used collaboratively with metallurgical knowledge, first-principal calculation, and feedback into non-linear neural network models. The integration of data mining, and machine learning generate reasonable predictions and improve productivity of the steelmaking industry. Hence, this data-driven strategy is able to provide predictive capability of composition design, processing optimisation, emerging microstructure and property.

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A numerical study on the impact of a time-varying axial magnetic field on an industrial vacuum arc remelting (VAR) process

Authors: Ebrahim Karimi-Sibaki[1]; Abdellah Kharicha[None]; Andreas Ludwig[None]; J. Bohacek[2]

[1] *Christian-Doppler Laboratory for Metallurgical Applications of Magnetohydrodynamics*

[2] *Faculty of Mechanical Engineering, Brno*

Corresponding Author: ebrahim.karimi-sibaki@unileoben.ac.at

Nowadays, the Vacuum Arc Remelting (VAR) process is effectively utilized to manufacture Titanium-based alloys. Most often, an external axial magnetic field (AMF) is deliberately introduced to stabilize the arc. The AMF also impacts the magnetohydrodynamics (MHD) in the melt pool, and consequently the solidification (macrosegregation and grain structure) of the ingot. To study the aforementioned phenomena, we propose a 2D axisymmetric swirl model that includes calculation of electromagnetic and thermal fields in the entire system (electrode, vacuum plasma, ingot, and mold) as well as MHD in the melt pool. Both sinusoidal and rectangular variations of AMF are examined. Additionally, the effect of reversal time of the direction of AMF (5 to 30 sec) on MHD in the melt pool, and consequently solidification of the ingot is analysed. Eventually, the model is validated against an experiment.

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Numerical Modeling of Scrap Melting and Heat Transfer During Electrode Bore-In IN AC EAF

Author: Yuchao Chen[1]

Co-authors: Armin Silaen [1]; Chenn Zhou [2]; Steve Ryan [3]

[1] *CIVS, Purdue University Northwest*

[2] *Purdue University Northwest*

[3] *NLMK Indiana*

Corresponding Authors: chen2058@pnw.edu, czhou@pnw.edu, sryan@us.nlmk.com, asilaen@pnw.edu

The electric arc furnace (EAF), as one of the most critical equipment in the modern steelmaking process, has gained rapid prominence in the industry over the last decades due to its high efficiency and low emission. Generally, EAF utilizes electrical and chemical energy to achieve the purpose of scrap melting while the heat released by arc plasma is considered as the major input to melt scrap. In the present study, a computational fluid dynamics (CFD) model was developed to reveal the scrap melting behavior during the electrode bore-down phase, and the experimental data collected by NLMK were used to validate the model. The developed model includes the innovative algorithm to include both electrode movement and the dynamic prediction of arc radiation on scrap surface in the simulation, and the model was used to investigate the liquid steel permeability and the potential cause of the arc reflection, which can further improve the scrap melting efficiency during the furnace operation.

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Numerical Simulations of the Molten Metal Droplet Formation in the Electro-slag Remelting Process with a Rotating Electrode

Author: Christian Schubert[1]

Co-authors: Herbert Pfeifer [1]; Moritz Eickhoff [1]

[1] *RWTH Aachen University*

Corresponding Authors: eickhoff@iob.rwth-aachen.de, pfeifer@iob.rwth-aachen.de, schubert@iob.rwth-aachen.de

The electro-slag remelting (ESR) is a well-known process, which is widely used in the production chain of high-quality alloys. These alloys are used for many different applications ranging from tool steels to superalloys used in aero- or spacecraft applications. The process design is mainly unaltered since several decades. There only have been improvements regarding the process control and the input materials, as well as some developed derivatives of the process. Two ideas are currently discussed in the scientific community, of how to improve the ESR process, namely the use of a rotating or respectively a vibrating electrode. These approaches promise some significant process enhancements as well as some benefits regarding energy efficiency. There have been experimental and numerical studies made using these process modifications, potentially showing some of those beneficial effects regarding lab scale plants. The changing of the droplet size and trajectory as well as the metallic film thickness at the bottom of the electrode tip are significantly influencing these improvements. Numerical simulations can be used to predict certain influences caused by the scaling of the process. In this paper, we show different results for the simulated droplet formation in an ESR process with both a stationary and a rotating electrode using a coupled simulation between ANSYS Fluent and ANSYS EMAG. The results for low rotational speeds show a strong effect on the local shaping of the liquid metal film below the electrode and consequently a radial shift of the droplet incidence into the metal pool, but no significant effect on metal film thickness, droplet trajectory or droplet size. Furthermore, we are giving an overview of current bottlenecks, restrictions and possible strategies for improved process simulations.

T_2 Blast furnace / 26

Analysis of a blast furnace behaviour through a resolving Euler-Lagrange approach

Author: Bernhard Peters[1]

Co-authors: Alban Rousset [1]; Henrik Rusche [2]; Xavier Besseron [1]

[1] *University of Luxembourg*

[2] *Wikki GmbH*

Corresponding Authors: xavier.besseron@uni.lu, alban.rousset@uni.lu, bernhard.peters@uni.lu, henrik.rusche@wikki-gmbh.de

A blast furnace belongs to the most complex and biggest reactors for the treatment of raw materials. One of the most promising approaches to describe numerically the complex process of a blast furnace is a coupled Euler-Lagrange simulation. It combines an accurate representation of the solid phase with its reducing gas formed by oxidation of coke and iron reduction in conjunction with the melting of iron and slag for the particulate phase. These processes are coupled via heat, mass and momentum transfer with the continuous phases of a multiphase flow consisting of gas, liquid iron and slag that operate in a counter-current flow. The extended discrete element (XDEM) method represents a simulation platform that predicts the thermodynamic state of both the particulate and fluid phase. The numerical framework describes the spatio-temporal thermodynamic state of each particle e.g. oxidation of coke, reduction of iron oxides and melting of iron and slag. OpenFoam as a multiphase CFD solver describes the flow, composition and temperature distribution in the void space between the particles. Thus, the key areas of a raceway, tripping zone, cohesive zone and shaft are modelled with high accuracy. An analysis of the results unveils the underlying physics and therefore, allows assessing performance and design issues. The current approach is more than easily adaptable to green blast furnace technologies that apply hydrogen as a reducing agent.

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CFD-DEM simulation of dynamics of the upper part of the blast furnance

Author: Debanga Mondal[1]

Co-authors: Han Wei [1]; Henrik Saxén [1]; Yaowei Yu [2]

[1] *Åbo Akademi University*

[2] *Shanghai University*

Corresponding Authors: hsaxen@abo.fi, yaoweiyu@shu.edu.cn, dmondal@abo.fi, han.wei@abo.fi

The burden materials in the blast furnace are traditionally charged to build distinct layers of ore and coke, which makes it possible to control the conditions in the shaft. Since ore and coke have fundamentally different density, the mass flow rates of solids at different radial locations will vary, which affects the heating of the burden upon its descent. Further, as the materials show different gas permeability, the burden distribution affects the gas flow distribution in the shaft, which, in turn, affects the thermal state and chemical reactions in the lumpy zone. The conditions close to the burden surface are complex due to the intermittent charging. Even though traditional (probe) measurements of the gas temperature in or above the bed surface seldom consider the rapid changes caused by charging, new acoustic gas temperature measurements may be able to do so in the future. In order to gain a better understanding of the effect of charging on the thermal and flow conditions in the upper shaft, an analysis based on Computational Fluid Dynamics combined with the Discrete Element Method (CFD-DEM) was undertaken. The model, which studies the counter-current flow of gas and solids and the temperature evolution of the two phases in a simplified setup, simulates the intermittent charging and descent of burden, consisting of pellets and coke, and the simultaneous ascent of gas through the particle bed. The results demonstrate the complex interaction between the solid and gas flows, which affects the radial temperature distribution of the due to both heat transfer and gas redistribution. These dynamic changes are analysed and illustrated for different parts of the simple charging cycle, and implications of the observed behaviour are analysed and discussed in the paper.

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Interpretation of the state of the blast furnance hearth by wear-model analysis

Author: Mikko Helle[1]

Co-authors: Bart de Graaff [2]; Cornelis van der Bent [2]; Henrik Saxén [3]

[1] *Abo Akademi University*

[2] *Danieli Corus*

[3] *Åbo Akademi University*

Corresponding Authors: hsaxen@abo.fi, cornelis.van-der-bent@danieli-corus.com, mihelle@abo.fi, bart.de-graaff@danieli-corus.com

The lowest part, the hearth, of the blast furnace is the most non-transparent region of the process as no measurements of the internal state are available due to extremely hostile conditions. Since the life of the hearth lining limits the furnace campaign length and the state of the hearth is of significant importance for maintaining an un-disturbed and well-controlled drainage of hot metal and slag and for the final composition of the hot metal, many attempts have been made to estimate the internal conditions based on indirect measurement information. The present paper presents an analysis of the hearth of a large blast furnace using a model of the lining wear, which is based on the solutions of a set of inverse heat conduction problems. The changes in the lining state throughout the campaign are estimated, and the findings are compared with independent measurements and observations of disturbances experienced in the operation. The hearth is demonstrated to perform efficiently during certain periods, while other periods are characterized by erratic behaviour with excessive growth of buildup material ("skull") on the hearth wall and bottom. Furthermore, a recurring behaviour is noted, where periods showing skull melting are followed by strong skull formation. Such cyclic behavior has been reported by other investigators and it is hypothesized that a reason could be transition between a floating and sitting state of the hearth coke ("dead man"). An attempt is finally made to quantify the floating state of the dead man by a force-balance based analysis. The results

indicate that a vertical motion of the hearth coke may be an underlying reason, but the factors that trigger these changes still remain largely unknown. This calls for a deeper analysis of the role of other variables in future research.

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How laser OES real time analysis enables the in-situ integration of slag analysis into simulation models

Author: Alexander Schlemminger[1]

[1] *QuantoLux GmbH*

Corresponding Author: alexander.schlemminger@gmx.de

Given the sheer volume of resources and energy used in smelters around the world, the optimization potential of simulation and modeling-based efficiency measures is huge.
However, simulations require representative input data in order to work properly. In other words: simulations can only be as good as the data they are built on. In addition to the detailed model the best possible measurement data from the up- and downstream material flows are essential. For this reason, new sensors and analysis techniques are constantly being established to improve the data basis. But despite all efforts, there are still a few blind spots.
As the expression "make the slag and the steel makes itself" suggests, the slag has a considerable influence on the quality of the steel produced. But the chemical composition of the slags could only be included post-mortem into the models since the analysis time was too long due to sample preparation times. Various quite limited workarounds have been established to include some kind of slag data into the model in real time. But e.g. the smell or the color appearance of the slag bath is quite unprecise.
The alternative is Laser OES technology which works analogously to Spark OES is capable of measuring the chemical composition on up to 1000 surface spots per second. That allows homogenization of data instead of physical samples. Thus, even hot slag can be chemically analyzed in 1-2 minutes and the precise values can be incorporated into the simulation.
With the precise slag analyses available in real time, the models and simulations can be optimized further and raised to a completely new level. The positive impact of simulations can also be increased even further. This not only makes economic sense, but is also smart in regards of Industry 4.0.

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Dynamic changes in slag properties during the reduction stage of the AOD process

Author: Ville-Valtteri Visuri[1]

Co-authors: Eetu-Pekka Heikkinen [2]; Timo Fabritius [2]

[1] *Outokumpu Stainless Oy; Process Metallurgy Research Unit, University of Oulu*

[2] *Process Metallurgy Research Unit, University of Oulu*

Corresponding Authors: ville-valtteri.visuri@outokumpu.com, eetu.heikkinen@oulu.fi, timo.fabritius@oulu.fi

AOD process consists of two main stages: decarburization and reduction of slag. In the decarburization stage, oxygen is injected through nozzles – and also through top lance in combined-blowing vessels – to remove dissolved carbon from the metal bath. The oxygen injection is diluted with nitrogen or argon to avoid excessive oxidation of alloying elements, such as chromium and manganese. After the decarburization stage, the slag contains large amounts of solid chromium-containing oxide phases, and it may also contain undissolved lime particles, so-called 'free lime'. Consequently, the slag has a high solid fraction and is highly viscous. During the reduction stage, the chromium oxide content of the slag is reduced by the addition of reductants. This, in combination with the addition of slag formers and fluxes, makes the slag almost completely liquid. However, there is a lack of information regarding the dynamic evolution of the slag composition and its physical properties during the reduction stage. To this end, a sampling campaign was conducted to measure the dynamic changes in metal and slag composition. To determine the phase structure and viscosity of the slag, comparative computational thermodynamics calculations were carried out using Thermo-Calc and FactSage software. The results provide new information on the dynamics of the reduction stage in the AOD process.

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Numerical Simulation on Refractory Wear and Inclusion Formation in Continuous Casting Tundish

Authors: Qiang Wang[1]; Chong Tan[1]; Ao Huang[1]; Wen Yan[1]; Huazhi Gu[1]; Zhu He[1]; Guangqiang Li[1]

[1] *Wuhan University of Science and Technology*

Corresponding Author: wangqiangwust@wust.edu.cn

The formation and removal of exogenous inclusions in a real-size two-strand tundish is simulated by the proposed unsteady 3D comprehensive numerical model of the respective fluid-structure interaction, which takes into account the impacting and washing effects on the refractory wear. A large eddy simulation is employed to describe the molten steel vortex flow. Thus, the thermal profiles of the molten steel and refractory lining are constructed. One-way coupled unsteady Euler-Lagrange approach is adopted to estimate the detachment and motion of the exogenous inclusion. The inclusion's Reynolds number is utilized for evaluating the inclusion separation at the refractory lining after formation and at the upper surface of the molten steel. At a 1.2 m/min casting speed, 49 and 38% of exogenous inclusions are created at the turbulent inhibitor inner bottom and long nozzle inner wall, respectively. In contrast, only 13% of new inclusions are produced at all other inner walls. About 80% of newly generated inclusions are then trapped by free surfaces, 78% of which are removed at the first free surface. The initial diameter of exogenous inclusions ranges from 13 to 48 μm. The removal ratio of exogenous inclusions in the tundish first grows from 61 to 80%, with the casting speed rising from 1.0 to 1.2 m/min and then drops to 63% after the further casting speed rise to 1.4 m/min.

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Improving the slag-metal separation of a Blast Furnance Trough with the use of numerical simulations

Author: Rodrigo Garcia Ribeiro[1]

Co-authors: Alexandre Dolabella Resende [1]; Aloisio Simões RIBEIRO [1]; Bruno Filipe Guimarães [1]; Gernot Hackl [1]

[1] *RHI Magnesita*

Corresponding Authors: gernot.hackl@rhimagnesita.com, alexandre.resende@rhimagnesita.com, aloisio.ribeiro@rhimagnesita.com, bruno.guimaraes@rhimagnesita.com, rodrigo.ribeiro@rhimagnesita.com

During slag granulation, after metal separation in the Blast Furnace Main Trough, the contact between water and slag can lead to explosions, due to presence of pig iron in the slag. Aiming to reduce the molten metal passage through the slag port of a main trough in a Brazilian steel mill, in order to avoid explosions during slag granulation, multiphase numerical simulations were performed for different geometric configurations of the main trough. It was used a VOF (Volume of Fluid) model to represent the interactions between the fluids (molten metal, slag and air), coupled with a DPM (Discrete Particle Model) to represent metal particles coming from the blast furnace. The metal separation was analyzed by measuring the amount of metal, both fluid and particle, which flows out through the slag port. The impacts of increasing the width, the depth and the slag thickness in the metal separation were analyzed. Simulation results show that the width increase reduces the metal passage through the slag port, while increase in depth can jeopardize the slag separation, due to higher wave velocities. Also, it was found that slag thickening impacts positively in the fluid separation, however, for the separation of metal particles in the bath, an improvement is observed only above a certain increase in thickness.

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A sub-particle model for inclusions at the gas/steel interface

Author: Zilong Qiu[1]

Co-authors: Annelies Malfliet [1]; Bart Blanpian [1]; Muxing Guo [1]

[1] *KU Leuven*

Corresponding Authors: zilong.qiu@kuleuven.be, bart.blanpain@kuleuven.be, annelies.malfliet@kuleuven.be, muxing.guo@kuleuven.be

The behavior of nonmetallic inclusions (NMs) on gas bubble surfaces has received increasing attention due to its importance in clean steel production. Agglomeration of NMs at the gas/steel interface is usually observed because of capillary attractions. The Kralchevsky–Paunov (K-P) model is often employed to calculate this capillary force quantitatively. In the K-P model calculation, nonspherical particles are simplified into spheres with an equivalent or effective radius. However, this simplification may introduce significant errors. In the present work, a numerical sub-particle model is developed to study gravity-induced capillary interaction between inclusions. This model is an extension of the K-P model from floating spheres to more complex shapes. In the model, the parent inclusions are reconstructed by close-packed smaller spheres (sub-particles) into a parcel resembling the inclusion closely. The capillary interaction between the parent inclusions is represented by the pairwise summation of direct interaction between constituent sub-particles. The capillary interaction between sub-particles is assumed to have a similar form between floating spheres in the K-P model. The net capillary 'charge' of a sub-particle parcel is considered to be identical to its parent particle. As a case study, capillary interactions between a pair of round discs and elliptical discs are investigated. For round discs varied with thickness, predictions from the sub-particle model are consistent with the analytical solutions with errors less than 5%, in contrast to the simplified K-P model that can be off by an order of magnitude. For elliptical discs, however, no exact analytical solution is available. Here also the difference between the force calculated with the simplified K-P model and the sub-particle model is substantial and is aggravated with increasing aspect ratio. Moreover, the sub-particle model captures the anisotropy of the interaction.

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Liquid-liquid mass transfer in steelmaking processes

Author: Nelson Joubert[1]

Co-authors: Jacob Maarek [1]; Pascal Gardin [2]; Stéphane Popinet [1]; Stéphane Zaleski [1]

[1] *Sorbonne Université*

[2] *ArcelorMittal Global R&D*

Corresponding Authors: nelson.joubert@gmx.fr, stephane.zaleski@sorbonne-universite.fr, popinet@basilisk.fr, jacob.maarek@sorbonne-universite.fr, pascal.gardin@arcelormittal.com

Mass transfer between liquid steel and slag is frequently encountered in the steelmaking processes: for composition adjustment such as desulfurization or dephosphorization, but also for lubrication of continuous casting mold, since the slag viscosity has a major effect and is mainly depending on the thermodynamic equilibrium between the phases. To predict the composition of both the slag and the steel, the local description of the flow at the interface between the two phases is needed. The paper describes some mechanisms to better understand the mass transfer. A water model with oil layer at the top and air stirring is used to visualize the interface behavior and make the link between the hydrodynamics and the global mass transfer. A CFD model is presented. It includes water, oil and air phases. It allows a very precise description of the boundary layers between the two fluids (water/oil), for both momentum and species concentration, and gives a unique insight into the local mass transfer. A key result concerns the prediction of the mass transfer and the very heterogeneous distribution of the mass transfer coefficient along the interface: the internal side of the open eye contributes mainly to the mass transfer. A methodology to cope with the industrial configuration is proposed.

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Study the effect of slag conductivity on liquid fe-c droplet decarburization kinetics

Author: Jayasree Biswas[1]

Co-author: Kenneth Coley [2]

[1] *McMaster University*

[2] *Western University*

Corresponding Authors: kcoley@uwo.ca, biswasj@mcmaster.ca

In basic oxygen steelmaking, the metal droplet decarburization plays a major role to determine the residence time and reaction (slag/metal interfacial) area of the droplets due to bloating while reacting in the emulsion zone. This 'residence time' and 'reaction area' controls the overall refining efficiency in BOF, more importantly dephosphorization efficiency. So, it is important to understand the mechanism of decarburization reaction to predict the bloating behavior accurately. In this study, an experimental study has been performed to understand the effect of slag conductivity on the decarburization reaction kinetics. A kinetic model based on Wagner's oxidation theory has been proposed and a kinetic analysis has been performed to explain the slag conductivity effect. It has been observed from study of decarburization on varying carbon content from 0.5% to 4.4% in oxidizing slag, that the droplet decarburization always shuts down in low conductivity slag much earlier than that predicted by the thermodynamics. It is proposed that during the decarburization process, due to the difference in diffusivities of ions and difference in the rate of cathodic and anodic reactions, there is a charge build up at the slag metal interface. This introduces an electric field which opposes the movement of oxygen ions towards slag-metal interface and this is attributed to the sudden shutdown of decarburization process for metal droplets on low conductivity slags whereas to continue decarburization until close to equilibrium in high conductivity slag due to fast charge dissipation.

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On the removal of a spherical Al2O3 inclusion at the steel-slag interface: A numerical study

Author: xiaomeng zhang[None]

Co-authors: Stefan Pirker [1]; Mahdi Saeedipour [1]

[1] *Department of Particulate Flow Modelling, Johannes Kepler University*

Corresponding Author: xiaomeng.zhang@k1-met.com

As an essential stage in inclusion removal processes, separation of inclusion at the steel-slag interface certainly affects the overall removal efficiency and is of great importance to molten steel cleanliness. In this study, the dynamics of a spherical Al2O3 inclusion (50 µm in diameter and with a typical contact angle of 45°) interacting with the steel-slag interface is investigated using computational fluid dynamics. We employed the volume of fluid (VOF) method in combination with the dynamic overset grid technique to account for particle motion near the steel-slag interface. This numerical approach is capable of capturing the meniscus in the course of particle motion and incorporating the Marangoni flow induced by particle dissolution. The results demonstrate that the capillary force arising from the formation and continuous evolution of a meniscus is mainly responsible for inclusion motion. In consequence, the spherical inclusion generally accelerates to a quite high velocity, then undergoes a deceleration stage, and finally settles in an equilibrium position at the interface in a very short time. Based on the case of rapidly trapped inclusion, the subsequent dissolution drives a flow along the interface. Eventually, this interfacial flow can further lift the inclusion up to a certain distance, which could facilitate the separation process. This study provides an understanding about the physics of inclusion removal which is essential for steel quality control.

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Melting Kinetics of Metallic Particles in a Bottom Stirred Ladle during the Tapping Operation of Liquid Steel from the Furnace to the Ladle

Author: Rodolfo Morales[1]

Co-authors: Alfonso Najer-Bastida [1]; Carlos Muniz [2]; Jafeth Rodriguez [3]; Kinnor Chattopadhyay [4]

[1] *Instituto Politecnico Nacional*

[2] *Universidad Autonoma de Coahuila*

[3] *Universidad Aut[onoma de Coahuila*

[4] *University of Toronto*

Corresponding Authors: kinnor.chattopadhyay@utoronto.ca, alfonso_najera@yahoo.com.mx, rodrigo.muniz@uadec.edu.mx, rmorales@ipn.mx, jafethrodriguez@uadec.edu.mx

Molten steel is alloyed during tapping from the melting furnace to the argon-bottom stirred ladle. The metallic additions thrown to the ladle during the ladle filling time are at room temperature. The melting rates or kinetics of sinking-metals, like nickel, are simulated through a multiphase Euler-Lagrangian mathematical model during this operation, carrying out a previous assessment of the most relevant correlations for the estimation of the heat transfer coefficient. The melting rate of a metallic particle depends on its trajectory within regions of the melt with high or low turbulence levels, delaying or speeding up their melting process. At low steel levels in the ladle, the melting rates are higher on the opposite side of the plume zone induced by the bottom gas stirring. This effect is due to its deviation after the impact of the impinging jet on the ladle bottom. The higher melting kinetics are located on both sides at high steel levels due to the more extensive recirculation flows formed in taller baths. Making the additions above the eye of the argon plume spout increases the melting rate of nickel particles. The increase of the superheat makes the heat flux more significant from the melt to the particle, increasing its melting rate. At higher superheats, the melting kinetics becomes less dependent on the fluid dynamics of the melt.

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Improving nitrogen control in AOD processes with the aid of computational fluid dynamics and thermodynamics databases.

Author: Björn Ahlin[1]

Co-authors: Mikael Ersson [1]; Anders Tilliander [1]

[1] *KTH- Royal Institute of Technology*

Corresponding Author: bjoahl@kth.se

Producers of stainless steels such as high alloyed duplex steels have shown an increasing interest in alloying with nitrogen. Alloying with nitrogen can replace some of the Nickel used since it affects mechanical strength, corrosion resistance and stabilizes the austenitic phase. Nitrogen is mainly used as a process gas instead of the more expensive argon gas. Depending on the ratio of nitrogen gas to argon gas, nitrogen content can be affected. However, controlling the level of nitrogen in liquid steel and predicting the final content is a difficult task often leading to a need of flushing with argon gas in order to reach desired levels of nitrogen content. Such an approach is both time and resource consuming.
Therefore, this study has developed a CFD model of an industrial AOD-converter that is coupled to the thermodynamic software Thermo-Calc. This type of model provides one possible route to establish nitrogen control in the AOD-process, combining both a kinematic understanding via the CFD calculations as well as an understanding of the thermodynamic situation. This combination applies non-ideal solution calculations for the thermodynamics and a more dynamic approach to the kinematic situation in comparison with existing prediction models that applies calculations using dilute solutions and kinematic expressions.

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A fundamental investigation of decarburization reactions in the AOD converter using coupled CFD and thermodynamics databases.

Author: Serg Chanouian[1]

Co-authors: Mikael Ersson [2]; Anders Tilliander [1]

[1] *KTH Royal Institute of Technology*

[2] *KTH Royal institute of technology*

Corresponding Author: sergc@kth.se

Metallurgical processes such as the AOD converter generally utilize gas blowing for mixing and refinement of liquid steel. Due to the harsh environment of the complex and opaque system it is common to study the stirring of the process through physical and numerical models. Effective mixing in the bath has an important role for refinement such as decarburization and have been vividly studied before. However, high temperature chemical reactions also play a big part and is sparsely investigated. This project investigates the effect of altering the pressure around the nozzles on the decarburization in the AOD converter. The ferro-static pressure enforced by the liquid steel at the nozzles is practically lowered by lowering the bath height above the nozzles with the means of inclining the vessel or elevating the nozzles. With the help of physical and numerical modelling, a computational fluid dynamics (CFD) model coupled with a thermo dynamics model has been developed allowing the study of both the mixing and chemical reactions in the process. In the current work an investigation regarding the chemical reactions for a single gas bubble in the AOD has been performed. The results have been used as input to the understanding of industrial AOD decarburization mechanisms, especially focusing on where reactions take place, how fast and the role pressure plays during these reactions.

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From Bubble-Scale to Full-Scale: Optimization of Numerical Modeling of the Ladle Furnace

Author: Tim Haas[1]

Co-authors: Christian Schubert [2]; Herbert Pfeifer [3]; Moritz Eickhoff [2]

[1] *Department for Industrial Furnaces and Heat Engineering*

[2] *Department for Industrial Furnaces and Heat Engineering of the RWTH Aachen University*

[3] *RWTH Aachen University*

Corresponding Authors: schubert@iob.rwth-aachen.de, pfeifer@iob.rwth-aachen.de, eickhoff@iob.rwth-aachen.de, haas@iob.rwth-aachen.de

Numerical simulation plays a crucial role in the optimization of the ladle furnace. This work summarizes various works done to optimize flow modeling in the ladle furnace. This starts at the bubble scale with the development of a new measurement method based on machine learning. Then a comprehensive validation database was created on the physical modeling scale and the numerical model was optimized with it. Finally, this paper deals with the question of scaling the physical model scale to the industrial scale. For this purpose, different problems and their solutions are discussed and the flow of a full-scale 185 t ladle furnace calculated with the large eddy turbulence model is presented.

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Model predictive control of the AOD process for material and energy optimisation

Author: Ville-Valtteri Visuri[1]

Co-authors: Andreas Hammervold [2]; Martin Schlautmann [3]; Pentti Kupari [1]; Stein O. Wasbø [2]; Vera Peiss [3]

[1] *Outokumpu Stainless Oy*

[2] *Cybernetica AS*

[3] *VDEh-Betriebsforschungsinstitut GmbH*

Corresponding Authors: martin.schlautmann@bfi.de, pentti.kupari@outokumpu.com, andreas.hammervold@cybernetica.no, stein.wasbo@cybernetica.no, ville-valtteri.visuri@outokumpu.com, vera.peiss@bfi.de

The aim of the Horizon 2020 SPIRE project MORSE (Model-based Optimisation for efficient use of ResourceS and Energy) is to develop model-based, predictive raw material and energy optimisation software tools for a whole process route. This approach is demonstrated in several pilot cases within the steel industry, to improve resource and energy efficiency, as well as product quality. This paper presents a new software application for material and energy optimisation during the AOD process within the stainless steel production route at Outokumpu in Tornio, Finland. A dynamic model of the AOD process developed by BFI has been adapted to the converter and process characteristics at Outokumpu steel plant and integrated into a process monitoring, optimisation, and control application developed by Cybernetica. This model predictive control (MPC) application has been installed and tested within the online automation environment at Outokumpu's steel plant in Tornio. It continuously monitors the current heat state, predicts the end-point of the AOD treatment based on given target criteria, provides real-time predictions of expected heat trajectories using related recipe information, and dynamically adapts defined set-points of these recipes to achieve the target specification with minimum material, resources, and energy consumption. Preliminary results regarding achieved performances of the model application and related benefits for the steel plant are presented.

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Application of process simulation strategies in off line prediction models and on-line Decision Support Systems with through process approach on Feralpi sites

Author: Lorenzo Angelini[1]

Co-authors: Piero Frittella [1]; Massimiliano Bersani [2]; Maurizio Fusato [1]; Gianpaolo Foglio [1]; Francesco Guerra [2]; Christian Senes [2]; Cosmo Di Cecca [1]; Biagio Cinquegrana [1]; Alessandro Milan [1]; Ganna Tsymokh [1]; Francesco Fredi [1]; Giuseppe Miglietta [2]; Fabio Morandini [1]; Vincenzo Duro [2]; Mattia Tellaroli [1]; Alessio Ventua [3]; Davide Ressegotti [3]; Sofia Maurina [4]; Gabriele Galeazzi [4]; Carlo Mapelli [5]

[1] *Feralpi Siderurgica*

[2] *Acciaierie di Calvisano*

[3] *Rina Centro Sviluppo Materiali*

[4] *Visiorobotics*

[5] *Politecnico di Milano*

Corresponding Author: piero.frittella@it.feralpigroup.com

In modern steel productions, the necessity of a more precise knowledge and control of the process became more important in order to improve production performances, to maintain repeatability on the product quality, to support the necessary process flexibility due to frequent changes in production programs. This became more necessary in Feralpi Group for the case of special steel production. For this reason the capability to better understand the phenomena in the different process phases of the steelmaking process including scrap melting, steel treatments in ladle and solidification process in continuous casting is important to better setup the proper operating practices in a more precise manner. In this approach a through process view is necessary to respect the process and quality constrains aiming at the best performances of productivity and energy consumption.
To better summarize the knowledge and competences of steelmaking process and metallurgy gained in process management mathematical models have been created internally to Feralpi in order to be able to better setup the optimal operating practices for each process phases as EAF, Ladle Furnace, and continuous casting.
In this way with the contribution of the R&D department, process technology and production areas predictive mathematical models have been created for each production phase and also included in representation of whole steelmaking process.
Based on the off line approach also the on-line Dynamic Decision Support Systems have been created in order to gain in real time process management rules as guideline to support the production technicians in each process phase with a through process view of whole steelmaking area.
This realized for both production site of Feralpi Siderurgica and Acciaierie di Calvisano with the contribution of Rina Centro Sviluppo Materali, Politecnico di Milano and Visiorobotics collaborating as partners in European funded projects RFCS and at local level (Regione Lombardia).

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Simulation based Proof-of-Concept for Plant Transformation from Integrated BOF towards Hybrid BOF/EAF Production Route

Author: Stefan Mühlböck[1]

Co-authors: Bernhard Voraberger [2]; Gerhard Kurka [2]; Peter Oertelt [2]

[1] *Primetals Technologies GmbH*

[2] *Primetals Technologies Austria GmbH*

Corresponding Authors: gerhard.kurka@primetals.com, stefan.muehlboeck@primetals.com, bernhard.voraberger@primetals.com, peter.oertelt@primetals.com

The complexity of a steel plant's operations can be daunting, as all production steps are partially interdependent and impossible to isolate. Therefore, ever changing markets and product demands

make it a challenging endeavor to keep the production at highest efficiency, while staying competitive and complying with current environmental CO2 regulations.
Because of this demanding situation it is challenging to decide about investments, since every intervention into proven and established process routes by equipment modifications involves the risk of temporary production loss.
Hybrid steelmaking setups have recently become more and more attractive, as they enable the side-by-side operation of electric arc furnaces and basic oxygen furnaces. This approach allows for a gradual transition of the crude steel production from blast-furnace/BOF- to EAF-steelmaking with a lower CO2 footprint, while producing the same quantity of products.
Primetals Technologies uses dedicated simulation tools to model and simulate multiple customer plant-setups. By evaluating such digital plant-models that address the prospective plant-setup, ladle logistics, desired product mix and casting schedules, it becomes possible to make sound investment decisions based on digital plant-models instead of opinions. In general, the simulation models confirm expert opinions but often reveal additional issues across process boundaries, which are difficult to identify.
This paper summarizes the activities and outcomes of different customer studies, in which digital plant-models of the plant-setups have been used to figure out potential issues regarding logistics, layout and production scheduling for implementation of EAF steelmaking in an existing integrated BF/BOF steel plant or the general optimization of plant operations. The customer's focus in the most cases is keeping the production up over the whole period of this transformation process and enabling further extensibility of EAF production as well as to increase plant capacity.

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CFD modelling on impact of plug clogging in industrial scale steel ladles

Author: Kumar Subramanian[1]

Co-authors: Dirk van der Plas [1]; Erwin Harbers [1]; Marleen Wuestenenk [1]

[1] *Tata Steel*

Corresponding Authors: kumar.subramanian@tatasteeleurope.com, erwin.harbers@tatasteeleurope.com, dirk.van-der-plas@tatasteeleurope.com, marleen.wuestenenk@tatasteeleurope.com

A three dimensional Computational Fluid Dynamics (CFD) model using an Euler-Lagrangian approach is developed in order to understand the mixing of liquid steel in a ladle using Argon purging plugs in the bottom. The simulations consider liquid steel and slag as continuous liquid phases and Argon is considered as homogenous Lagrangian particles. The interfaces between the steel, slag, and top gas phases in the ladle are modelled using the volume of fluid (VOF) method.

The simulations were performed in the ladle geometry based on the 325 t industrial steel ladle from the IJmuiden steel plant. A detailed parameter study was performed, using either one of the plugs for purging, using higher flow rate through one of the plugs and comparing the results with the case of purging using two plugs. The results were summarized and compared in terms of slag open eye, wall shear and dead zone volume. Using one plug increased the mixing time and the choice of the plug did not play a role. The wall shear is seen clearly on the side of the plug which was used for the purging. The dead zone is predominantly present near the wall and in the area far away from the plug.
Tracer studies were performed to mimic the addition of alloys from a chute and through wire injection. The mixing times were quantified using tracer analysis to study the influence of different alloy addition areas.

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Modelling of steel-slag-inclusion reactions during refining of Si-

Mn killed steel

Authors: Angshuman Podder[1]; Kenneth Coley[2]; Andre Phillion[1]

[1] *McMaster Steel Research Center, Department of Materials Science and Engineering, McMaster University, Hamilton, Ontario, Canada, ON L8S 4L7*

[2] *McMaster Steel Research Center, Department of Materials Science and Engineering, McMaster University, Hamilton, Ontario, Canada, ON L8S 4L7; Department of Mechanical and Materials Engineering, Western University, London, Ontario, Canada, ON N6A 3K7*

Corresponding Authors: philliab@mcmaster.ca, poddea1@mcmaster.ca, kcoley@uwo.ca

Complex deoxidation by Si and Mn is beneficial for certain steel long products since it leads to the formation of low temperature melting manganese silicates. A better understanding of the mechanisms for inclusion formation in steels deoxidized by these elements need thorough investigation. In this regard, a kinetic model based on diffusion of steel species has been developed for deoxidation type inclusions to study the rate determining steps for steel-inclusion reactions. This model further incorporated the steel/slag coupled reaction model developed by previous researchers at McMaster University to understand the effect of slag-metal reactions on inclusions. The model calculations have been validated using experimental data. Additionally, the influence of process parameters on the composition of inclusions is examined through a parametric study. The results are useful for understanding inclusion dynamics during ladle refining of Si-Mn killed steel.

Keywords : inclusion; Mn/Si deoxidation; metal-slag-inclusion reaction; kinetic model.

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Euler-Euler Multiphase Simulation for Optimization of Bottom Tuyere Configuration in a Combined-Blowing Worn Out Converter

Author: Vinod Dhiman[1]

Co-author: Liesbeth Beunder [1]

[1] *Tata Steel Nederland B.V.*

Corresponding Authors: vinod.dhiman@tatasteeleurope.com, liesbeth.beunder@tatasteeleurope.com

Bottom blowing, combined with top-blowing, is a widely used approach in the BOS process to enhance the mixing across the phases and reduce the time to decarburize the hot metal. Damages due to scrap loading or blockages by solidified steel or slag could reduce the available number of bottom blowing tuyeres, particularly during the last heats of the campaign. This reduces the mixing efficiency and leads to issues like increased CO product. It is surmised that placing more tuyeres in the converter during the relining could lead to availability of more tuyeres near the end of the campaign. The objective of the current work is to use CFD to predict the effects of the bottom tuyere configurations and gas flow rates on the interfacial exchanges. Euler-Euler multiphase model has been used to predict the scalar transport across the metal-slag and metal-gas interfaces for various tuyere configurations and gas flow rates in a worn out converter. Passive tracers are used to study the transport and compared against the model representing the current configuration in use. It was observed that the total gas flow rate, the number of tuyeres, and the radial placements of tuyeres affect the performance significantly while the angular placements of the tuyeres and the flow rate per tuyere do not affect the performance in any significant manner.

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Application of Liquid-Liquid Mass Transfer for a Steel Ladle

Author: Marianne Doletschek[1]

Co-authors: Harald Harmuth [2]; Sandra Vollmann [3]

[1] *Montanuniversität Leoben*

[2] *Professorship at the Chair of Ceramics*

[3] *Montanuniversität of Leoben, Chair of Ceramics*

Corresponding Authors: marianne.doletschek@unileoben.ac.at, sandra.vollmann@unileoben.ac.at, harald.harmuth@unileoben.ac.at

A fluid/fluid mass transfer model implemented in computational fluid dynamics (CFD) is presented. This includes the model description, proving and application for a liquid steel/ slag mass transfer within a purged steel ladle. The model considers the prevailing flow as well as concentration and for the flow it distinguishes between laminar and turbulent flow. For the case of turbulent flow, the boundary layer at the liquid/liquid interface is modelled analogous to the wall treatment for species. Interface concentrations are determined by the diffusion equation. Contrary to other presently available mass transfer and reaction models the established model aims the calculation of the mass transfer coefficient depending on the local fluid flow- and concentration conditions. For a case without convection the model is tested by comparison with the solution of one-dimensional diffusion equation. In the ladle case the mass flux density is compared with data from literature. The model is applied for the steel/slag mass transfer in a gas purged steel ladle and it is found that the mass transfer increases with increasing purging rates within a certain range, slag bath heights as well as decreasing viscosities.

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Ensuring better inert gas shielding of ladle shroud-collector nozzle (LS-CN) assembly: A new gas delivery design and industrial scale assessment

Author: Suvam Mukherjee[1]

Co-author: Dipak Mazumdar [1]

[1] *IIT Kanpur, India*

Corresponding Authors: dipak@iitk.ac.in, suvamm@iitk.ac.in

Steel industry, even with best operating practices, has reported a minimum of 2 to 3 ppm nitrogen absorption, during transfer of molten steel from a ladle to tundish; up to 20 ppm of nitrogen absorption is not uncommon and have also been reported in literature. These imply that ladle shroud-collector plate nozzle (LS-CN) in practice is never perfectly secured and air ingression during ladle to tundish transfer, despite all precautions and improvements, takes place to varied degree in steel industry. Thus, to investigate the circumferential delivery and distribution of argon gas around LS-CN joint for various argon delivery arrangements, a non-isothermal, two component turbulent flow model has been developed and the resultant equations, in conjunction with appropriate boundary conditions, solved via ANSYS Fluent™. These indicate that at any given argon flow rate, gas delivery design influences distribution of argon and hence the effectiveness of the overall inert gas shrouding of LS-CN joint. Present work has clearly indicated that currently employed gas delivery designs function sub-optimally and do not ensure homogeneous, 360o shielding LS-CN joint. To improve argon distribution and attendant shielding of LS-CN joint further, a novel inert gas delivery design has been developed and is being tried in the industry. Preliminary industrial trials indicate that the new gas delivery design provides better shielding of the LS-CN assembly leading to reduced nitrogen pick-up from the atmosphere.

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From real-time CFD simulations towards flow-based digital shadows of metallurgical processes

Author: Stefan Pirker[1]

Co-authors: Roman Rössler [2]; Stefan Puttinger [3]

[1] *Johannes Kepler University*

[2] *voestalpine Stahl GmbH*

[3] *Johannes Kepler University Linz*

Corresponding Authors: roman.roessler@voestalpine.com, stefan.puttinger@jku.at, stefan.pirker@jku.at

The recent development of data-assisted recurrence CFD (rCFD) has boosted the computational performance of CFD simulations by orders of magnitude. In a recent publication (Pirker et al, SRIN, 2020), we presented real-time simulations of multiphase fluid flow and alloy homogenization in a RH vacuum treatment plant on a computational grid of more than three million cells.

This computational efficiency opens the door towards incorporating high-resolution rCFD simulations in process monitoring and process control. In this paper, we discuss ways, limitations and perspectives of aligning real-time rCFD simulations to online process data, such that rCFD simulations act as a digital shadow of the real-world process.

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Model experiments in a liquid metal mockup focusing on the bubble dynamics in a steel ladle

Author: Thomas Wondrak[1]

Co-authors: Bernd Willers [1]; Christian Bruch [2]; Gernot Hackl [3]; Hans Bodo Lüngen [4]; Hans-Jürgen Odenthal [5]; Helmut Lachmund [6]; Klaus Timmel [1]; Pascal Gardin [7]; Sven Eckert [1]

[1] *Helmholtz-Zentrum Dresden-Rossendorf*

[2] *Saarstahl AG*

[3] *RHI Magnesita*

[4] *Director Technology VDEh*

[5] *SMS group GmbH, R&D Division*

[6] *AG der Dillinger Hüttenwerke*

[7] *ArcelorMittal Global R&D*

Corresponding Authors: christian.bruch@saarstahl.com, k.timmel@hzdr.de, b.willers@hzdr.de, gernot.hackl@rhimagnesita.com, helmut.lachmund@dillinger.biz, s.eckert@hzdr.de, hans-juergen.odenthal@sms-group.com, pascal.gardin@arcelormittal.com, hans-bodo.luengen@vdeh.de, t.wondrak@hzdr.de

In metallurgy, gas is often injected into melts for mixing, degassing or refining. The knowledge of the two-phase flow behaviour is of utmost relevance for optimisation and process control. However, the measurement of the flow structure, the gas distribution and the characteristics of the bubbles is very challenging, because of the opaqueness and the high temperature of industrial relevant melts. Although numerical models have significantly improved recently, it is indispensable to validate the simulation results with experimental data.

A new experimental facility has been designed and recently commissioned at Helmholtz-Zentrum Dresden - Rossendorf for systematic investigation of bubble plumes in liquid Sn-40wt%Bi at 200 ℃. The thermophysical properties of this alloy are very similar to those of steel. The experiment is a 1:5.25 model of an industrial ladle and consists of a cylindrical vessel with inner diameter of 600 mm, which is filled with 1.7 tons of SnBi. Gas can be injected at the bottom of the vessel at four different locations, which can be equipped with different plug types. Furthermore, low-pressure conditions

for modelling VOD (Vacuum Oxygen Decarburization) application can be achieved by the use of a vacuum pump.

The gas distribution was measured by an array of 64 resistive probes arranged in a rectangular grid with a spacing of 10 mm and a time resolution of 1 kHz. This technique allows also the determination of bubble properties like bubble speed and diameter. The velocity of the liquid was measured by Ultrasound Doppler Velocimetry. The paper provides a description of the new setup in detail and presents measurement results characterizing the bubbly flow for varying gas flow rates and different configurations for gas injection.

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Analysis of the hysteresis behavior in regime transition of co-current liquid-gas flow using computational fluid dynamics

Author: Mahdi Saeedipour[1]

Co-author: Stefan Pirker [1]

[1] *Johannes Kepler University*

Corresponding Authors: mahdi.saeedipour@jku.at, stefan.pirker@jku.at

The dynamics of co-current liquid-gas flow controls the flow patterns and phase distribution inside the submerged entry nozzle (SEN) in the continuous casting. According to the flow parameters during the argon gas injection, the unsteady two-phase flow in the SEN experiences different regimes from bubbly flow to annular flow. This regime transition is usually associated with a hysteresis effect that is not fully understood yet. In this study, we investigate the regime transition in an analogous downward water-air system using the volume of fluid (VOF) method. A vertical pipe with a liquid inlet is considered as the computational domain at the top of which the gas is injected at different flow rates. Initially, the gas is injected at lower rates to establish a bubbly flow. By a temporally-linear increase of the gas volume rate (ramp-up), the bubbles become larger and the flow approaches the transition point where a huge amount of gas forms an annular flow. Once the annular flow is established, the gas injection rate is reduced with the same slope (ramp-down) to its initial value. This results in a transition from annular flow to bubbly flow, but at a different operation point. This hysteresis phenomenon is pictured by the numerical simulation. We studied the turbulence-interface interactions during the regime transition and analyzed the production and dissipation mechanisms in the transport equations of turbulent kinetic energy and enstrophy in such inhomogeneous flow with density and viscosity contrasts. The analysis unveils the contribution of interfacial topological changes in the flow to the hysteresis occurrence. The findings provide physical insights into the formation of interfacial structures in turbulent multiphase flows and could have a direct implication in the quality control of the continuous casting process.

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Water model experiments on the influence of the phase distribution in the SEN considering varying operating conditions

Author: maria thumfart[1]

Co-authors: Gernot Hackl [2]; Wolfgang Fellner [2]

[1] *K1-MET*

[2] *RHI Magnesita*

Corresponding Authors: wolfgang.fellner@rhimagnesita.com, gernot.hackl@rhimagnesita.com, maria.thumfart@k1-met.com

In continuous casting of steel, argon injection into the SEN (submerged entry nozzle) via the stopper is common practice. Nonetheless, the resulting phase distribution in the SEN is still under discussion. The main available casting parameters at the steel plant to determine the flow situation in the SEN, are usually the stopper rod position, the argon feeding pressure, the mass flow rate of argon and the casting speed. To determine the potential influence of the phase distribution on the stopper characteristic and on the argon feeding pressure, water model experiments have been conducted using a 1:3 scale water model. The water flow rate was scaled using Froude similarity. The air flow rate was chosen to keep the ratio between liquid and gas volume flow constant. The casting parameters (liquid flow rate, gas flow rate, stopper position, gas feeding pressure) were measured. In addition, nine pressure sensors were attached at three different levels of the SEN. To relate this measurement data to the corresponding phase distribution, two cameras were installed to observe the phase distribution in the SEN. During these measurements four major phase distribution patterns were observed. It could be shown that a change between these phase distribution patterns leads to a significant change in the measured pressure levels and the dynamics of the stopper position.

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Analysis of inclusions removal during steel flow in multi-strand tundish using numerical modelling

Author: Markéta Tkadlečková[1]

Co-authors: Jiří Cupek [1]; Josef Walek [2]; Karel Michalek [1]; Tomáš Huczala [3]

[1] *VŠB - Technical University of Ostrava*

[2] *VŠB-Technical University of Ostrava*

[3] *TŘINECKÉ ŽELEZÁRNY a.s.*

Corresponding Authors: josef.walek@vsb.cz, jiri.cupek.st1@vsb.cz, tomas.huczala@trz.cz, karel.michalek@vsb.cz, marketa.tkadleckova@vsb.cz

Flow in the tundish region during the continuous casting of steel can influence many important phenomena, especially removal of the non-metallic inclusions. If they are not removed from the steel melt during its processing, it can reduce the quality of the finished steel product. Therefore, in this study, the complex numerical modelling in the CFD programme ANSYS Fluent was used for detection of non-metallic inclusions removal from the steel during the flowing in a five-strand asymmetric tundish with different configuration of the impact pad. The distribution of inclusions was ranging from 2 μm to 100 μm and density from 2500 to 3500 kg·m−3. Inclusion removal efficiency was used for evaluation of steady state steel flow character depending on internal configuration. Based on the results obtained from modelling, the main findings and recommendation for optimal conditions of steel flow in tundish were formulated.

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Experimental and numerical study of the open eye in the uphill teeming ingot casting process

Authors: Jun Yin[1]; Ersson Mikael[1]; Jönsson Pär[1]

[1] *KTH*

Corresponding Authors: bergsman@kth.se, jyin@kth.se, par@kth.se

Non-metallic inclusions generated by mold flux entrapment are detrimental to the final steel's quality. In this paper, a water model experiment was carried out to study the mold flux entrapment during the filling process. The side outlet was created at the mold to ensure the quasi-steady state of the filling process, which can help to visualize the formation of the open eye. Additionally, numerical

simulation was also implemented to study the mold flux entrapment. The simulation results are compared to the experimental results for model validation.

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Study of Bubble Breakup and Coalescence in Gas-Stirred Ladle Refining Process

Authors: Miaoyong Zhu[1]; Wentao Lou[2]; Xiaoyu Wang[2]

[1] *Northeastern University*

[2] *Northeastern University China*

Corresponding Authors: louwen.1984@163.com, louwt@smm.neu.edu.cn, myzhu@mail.neu.edu.cn

The bubble breakup and coalescence behavior and mechanisms in gas-stirred ladle were studied by establishing physical model and mathematical model. The mechanisms of bubble breakup and coalescence in the gas-stirred ladle and their influence on bubble size distribution were revealed. The results show that the bubble breaking behavior has little effect on bubble size and distribution. The bubble aggregation due to turbulent random collisions and buoyancy collision dominate the bubble size, while the bubble tail vortex capture mechanism has a weak effect. Compared with the slit-type ventilated brick, the bubble size of the diffused ventilated brick is significantly smaller, and based on this analysis, an empirical formula for the bubble diameter of the slit-type ventilated brick and the diffused ventilated brick under the current bottom blowing system is established.

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A temperature, concentration, stress and grain structure slice model for continuous casting of steel

Author: Božidar Šarler[1]

Co-authors: Boštjan Mavrič [2]; Robert Vertnik [3]; Tadej Dobravec [4]

[1] *University of Ljubljana & Institute of Metals and Technology*

[2] *University of Ljubljana & INstitute of Metals and Technology*

[3] *University of Ljubljana & Štore-Steel*

[4] *University of Ljubljana*

Corresponding Authors: robert.vertnik@fs.uni-lj.si, tadej.dobravec@fs.uni-lj.si, bozidar.sarler@fs.uni-lj.si, bostjan.mavric@fs.uni-lj.si

A simple Lagrangean traveling slice model has been successfully used in the past for prediction of the relations between the process parameters and the temperature field in steel continuous casters. Such models are used in basic process parameters optimization with respect to the casting format and steel-grade. It is the purpose of the present paper to include also the concentration, mechanical stress and deformation models as well as the grain structure model on top of the temperature model. The basis of all the mentioned additional models is the slice heat-conduction model that takes into account the complex heat extraction mechanisms in the mould, with the sprays, rolls and through the radiation. Its main advantage is very fast calculation time and disadvantage that there is no other interaction but the convection in the direction of the casting. The macroscopic model used in this study is based on the continuum mixture theory, calculating enthalpy and mixture composition as input parameters for microscopic calculations. The grain structure model is based on the cellular automata concept, replaced by a random node point automata concept. The macrosegregation model is based on the Scheil rule microsegregation model. The thermal conductivity and the species diffusivity of the liquid phase are artificially enhanced to consider the convection of the melt. The calculated

thermal field is used to estimate the thermal contraction of the solid shell, which, in combination with the metallostatic pressure, drives the elastic-viscoplastic model. The results of the model are used to estimate the areas susceptible to crack nucleation using several hot-tearing and damage models. A sensitivity study on the recently introduced standard continuous casting test geometry is performed as well as on the realistic conditions in a round and square billet caster. Possible additional refinements of the model are discussed.

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Simulation of SEN clogging during continuous casting of Ti-ULC steel using a combined model

Author: Hadi Barati[1]

Co-authors: Abdellah Kharicha [2]; Andreas Ludwig [2]; Menghuai Wu [2]; Sergiu Ilie [3]; Susanne Michelic [2]

[1] *K1-MET / Montanuniversität Leoben*

[2] *Montanuniversität Leoben*

[3] *voestalpine Stahl GmbH*

Corresponding Authors: susanne.michelic@unileoben.ac.at, menghuai.wu@unileoben.ac.at, sergiu.ilie@voestalpine.com, andreas.ludwig@unileoben.ac.at, abdellah.kharicha@unileoben.ac.at, hadi.barati@unileoben.ac.at

Ultra-Low Carbon (ULC) steel grade is used in automotive industry due to the good formability and a superior surface quality. Titanium is usually added to this grade in order to improve physical properties such as total elongation, normal anisotropy, and strain hardening. However, adding Ti increases clogging tendency comparing Ti-free ULC. For clogging in casting of Ti-ULC steel, two key mechanisms have been proposed: (1) formation of solid oxide due to the chemical reactions on the SEN refractory wall, called 'early stage' and (2) deposition of suspended solid non-metallic inclusions (NMIs) on the SEN refractory wall, called 'late stage'. In this paper a combined model is developed considering both stages. Modeling of early stage is based on the carbothermic reactions inside the SEN refractory and the further reaction of the generated CO gas with the steel melt [1]. Modeling of late stage of clogging is according to clog growth by deposition of the NMIs on the clog front [2]. The combined model is evaluated by comparison with analysis of an as-clogged SEN. The combined model can correlate several parameters, like velocity and pressure of the melt, composition of SEN refractory, size and number density of NMI in the melt, to the clogging tendency in the casting of Ti-ULC.

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Modelling the Effects of Different Degrees of NMI Adhesion on Particle Deposition Behaviour in a Nozzle

Author: Kaamil Ur Rahman Mohamed Shibly[1]

Co-authors: Andre Phillion [2]; Stephen Tullis [3]

[1] *Dept. of Materials Science and Engineering, McMaster University, Hamilton, ON*

[2] *McMaster Steel Research Center, Department of Materials Science and Engineering, McMaster University, Hamilton, Ontario, Canada, ON L8S 4L7*

[3] *Dept. of Mechanical Engineering, McMaster University, Hamilton, ON*

Corresponding Authors: philliab@mcmaster.ca, mohamk12@mcmaster.ca, stullis@mcmaster.ca

Clog formation within the submerged entry nozzle is highly detrimental to the fabrication of steel alloys during the continuous casting process. The growth of the clog is self-accelerating and leads to numerous issues in the manufacturing process, including reduced manufacturing speeds, changes to the steel solidification pattern and even the introduction of detached parts of the clog into the finished product. In this study we present a multi-scale approach to model the differing adhesion behaviour of various Non-Metallic-Inclusions (NMIs) and their influence on clog formation within the SEN. A macroscale transport model, developed in OpenFOAM is used to simulate the bulk transport of melt and particles, while a microscale model is used to simulate different adhesion behaviours of various NMI. This is combined with another microscale model to simulate the clog formation and growth, the presence of which, then effects the melt flow, in a positive feedback loop.

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Modelling Asymmetric Flow in the Thin Slab Casting Mould under Electromagnetic Brake

Author: Alexander Vakhrushev[1]

Co-authors: Abdellah Kharicha [1]; Andreas Ludwig [2]; Gerald Nitzl [3]; Gernot Hackl [3]; Josef Watzinger [4]; Menghuai Wu [2]; Yong Tang [3]

[1] *Christian Doppler Laboratory for "Metallurgical Applications of Magnetohydrodynamics"*

[2] *Montanuniversitaet Leoben*

[3] *RHI Magnesita*

[4] *Primetals Technologies*

Corresponding Authors: yong.tang@rhimagnesita.com, josef.watzinger@primetals.com, abdellah.kharicha@unileoben.ac.at, menghuai.wu@unileoben.ac.at, alexander.vakhrushev@unileoben.ac.at, gerald.nitzl@rhimagnesita.com, gernot.hackl@rhimagnesita.com, ludwig@unileoben.ac.at

Continuous casting is nowadays the world leading technology for the steel production. The thin slab casting (TSC) is featured by a slab shape close to the final products, which are casted at a high speed with the fast solidification rate. The quality of the thin slabs strongly depends on the uniformity of the turbulent flow, the super-heat distribution, and the growth of the solidified shell after the hot steel is fed into a funnel-shaped mold via a submerged entry nozzle (SEN). In most of the studies the focus is typically made on the calmness of the meniscus, the local remelting of the solidifying shell, the probability of slag and non-metallic inclusions entrapment, etc. It is commonly assumed that the SEN is properly arranged, and the melt inflow is symmetric. However, in reality due to misalignment or clogging of the nozzle, an asymmetric flow pattern can develop. In the present study the asymmetry of the melt flow is imposed with a partial SEN clogging: (a) an assumption of the local porous zone is employed to reflect the presence of the clog material; (b) the resistance of the clog is varied from the low to the high values. The solidification during TSC is modeled including the effects of the turbulent flow. The variation of the flow pattern and the solid shell thickness is studied for different permeability values of the SEN clogging. These effects are considered with and without the applied electromagnetic brake (EMBr), which is simulated using an magnetohydrodynamics (MHD) model, developed within the open-source CFD package OpenFOAM®.

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Thin slab casting nozzle geomery design study with the aid of numerical and water modelling

Authors: Alexander Vakhrushev[1]; Yong Tang[2]

[1] *CD-Lab for Metallurgical Applications of MHD, University of Leoben, A-8700, Austria*

[2] *RHI Magnesita*

Corresponding Author: yong.tang@rhimagnesita.com

The internal geometric profile nozzle plays an important role in the obtaining proper flow patterns in the thin slab continues casting funnel mould. After some geometry design concepts are derived, numerical and physical modelling like water modelling is applied to elaborate and verify if the design can meet the expected target. For the numerical simulation, some attentions should be taken to avoid some numerical modelling uncertainty caused by the mesh quality, different turbulence models, multi-phase phenomena in the reality, etc. In this paper a so called "S-port" with patent protected thin slab casting nozzle from RHI Magnesita was introduced. The special featured nozzle structure working like traditional concepted flow divider elaboration with the improved numerical method to customize the flow to required casting conditions and throughout was discussed. Finally, the nozzle design and the numerical modelling method was verified and tested in the RHI Magnesita's water modelling laboratory in Leoben.

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Flow control in continuous slab casting by local electromagnetic braking

Author: Bahareh Najafian Ashrafi[1]

Co-authors: Martin Barna [2]; Peter Wimmer

[1] *K1-MET GmbH*

[2] *Institute of Fluid Mechanics and Heat Transfer Johannes Kepler University Linz*

Corresponding Authors: martin.barna@jku.at, bahareh.najafian_ashrafi@jku.at

Various quality problems emerging in the final product of the continuous casting of steel can be related to an insufficient control of the steel flow in the mold. To meet the requirements of high-quality products, electromagnetic forces are utilized to control the steel flow, and hence to improve the product quality. The usage of electromagnetic fields gained momentum in recent years due to their contact less way of flow control. In principle,the local electromagnetic brake can be placed above or beneath the jet in the mold region. In the current work, the local electromagnetic brake is applied beneath the jet to deflect the jets upward. The resulting braking forces will decrease the jet momentum, reduce the surface velocity, and lower the free surface elevation. The results were also compared with casting speed of 1.4 m/min (no brake), which poses as the reference case with an optimal flow. The numerical investigations are performed using Ansys Fluent with the SAS (Scale Adaptive Simulation) turbulence model. The first results show that the application of EMBr reduces the velocities in the entire mold region and bends the jets more upward. Consequently, the upward-deflected jets impinge at higher positions on the narrow faces and dampen the lower vortices.

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An integrated approach for near process modelling of the continuous casting of steel

Author: Gabriel Santos[1]

Co-authors: Christian Bernhard [2]; Julian Laschinger ; Lukas Preuler [3]; Matthias Taferner [4]; Michael Bernhard [5]; Sergiu Ilie [6]

[1] *K1-MET GmbH*

[2] *Montanuniversitaet Leoben*

[3] *Primetals Technologies Austria GmbH*

[4] *Chair of Ferrous Metallurgy, Montanuniversität Leoben*

[5] *Chair of Ferrous Metallurgy*

[6] *Research and Development voestalpine Stahl GmbH*

Corresponding Authors: lukas.preuler@primetals.com, michael.bernhard@unileoben.ac.at, g.trindadedossantos@voestalpine.com, matthias.taferner@unileoben.ac.at, sergiu.ilie@voestalpine.com, christian.bernhard@unileoben.ac.at

The market requirements on the production of high surface and internal quality steel products stimulate a deep understanding and systematic control of the steel solidification behaviour during the continuous casting process. Mathematical modelling is a crucial tool for this matter and therefore has been increasingly used for calculation of surface temperatures and shell growth during the continuous casting process. These decisive models play a crucial role for understanding and optimization of casting practices, cooling strategies and soft reduction calibration in order to prevent the formation of defects and enhance product quality. M2CAST is an off-line 2.5D mathematical heat transfer model, developed at the Montanuniversität Leoben in cooperation with industrial partners. The program uses accurate experimental set-ups, local boundary conditions and an in-house developed microsegregation model to simulate the solidification of a continuous slab casting and deliver helpful results for prediction of surface and internal quality issues. This paper will shortly present m2CAST in form of industrial applied case studies, with some validation, calibrations and adjustments in order to approach the model to real caster conditions. The simulation results were verified with slab temperature measurements and showed reasonable agreement in comparison to measured real data.

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Online 3D Heat Transfer and Solidification/Microstructure Models and their Capabilities for Simulation of Continuous Casting of Steel and Quality Prediction

Author: Seppo Louhenkilpi[1]

Co-authors: Aleksi Laukka [2]; Eveliina Piipponen [3]; Julius Norrena [2]; Jyrki Miettinen [4]; Timo Fabritius [2]; Tuomas Alatarvas [5]; Ville-Valtteri Visuri [6]

[1] *Casim Consulting Oy; Process Metallurgy Research Unit, University of Oulu*

[2] *Process Metallurgy Research Unit, University of Oulu*

[3] *SSAB Europe Oy, Raahe*

[4] *Process Metallurgy Research Unit, University of Oulu; Casim Consulting Oy*

[5] *Process Metallurgy Research Unit, University of Oulu, Finland*

[6] *Process Metallurgy Research Unit, University of Oulu; Outokumpu Stainless Oy*

Corresponding Authors: jyrki.miettinen@oulu.fi, tuomas.alatarvas@oulu.fi, julius.norrena@oulu.fi, seppo.louhenkilpi@casimconsulting.com, ville-valtteri.visuri@oulu.fi, aleksi.laukka@oulu.fi, timo.fabritius@oulu.fi, eveliina.piipponen@ssab.com

An existing and in-use online transient three-dimensional heat transfer model (3DHTM), combined with a solidification and microstructure model (SMM) for the continuous casting of steel are presented. The 3DHTM and SMM are integrated into a single online software entity and this has been installed in the automation systems of four slab casters in Finland. The development of this integrated concept is an on-going combined effort of several universities, one SME, and industrial partners in Finland. The principal objective for this integrated entity is to provide phenomena-based predictions for solidification microstructural changes during continuous casting in online plant use, including quality indices as well as accurate calculation of liquid pool shapes and end locations. The microstructural phenomena and the related quality indices developed will be used for quality prediction. The heat transfer model is validated with slab temperature measurements using pyrometers and some comparison with another heat transfer model is also carried out. Additionally, the is was to compare the quality indices between those calculated by the SMM and a steel mill's database to

validate the quality prediction capabilities of the SMM. The tools, the results and some industrial case examples from the online system are presented.

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Modeling of the as-cast structure and macrosegregation in the continuous casting of a steel billet: Effect of M-EMS

Author: Menghuai Wu[1]

Co-authors: Abdellah Kharicha [1]; Andreas Ludwig [1]; Haijie Zhang [1]; Zhao Zhang [1]

[1] *Department of Metallurgy, Montanuniversitaet Leoben*

Corresponding Authors: menghuai.wu@unileoben.ac.at, zhao.zhang@unileoben.ac.at, haijie.zhang@unileoben.ac.at, andreas.ludwig@unileoben.ac.at, abdellah.kharicha@unileoben.ac.at

A three phase mixed columnar-equiaxed solidification model coupling mold electromagnetic stirring (M-EMS) was used to investigate the initial solidification in the mold region of billet continuous casting (195 mm × 195 mm). This study focuses on the effect of M-EMS on the dissipation of superheat and its further impact on the formation of equiaxed zone. The equiaxed crystals originate from two mechanisms: heterogeneous nucleation and fragmentation of columnar dendrites. Additionally, parameter studies were also performed by varying the superheat (10˜30 K). Main findings are as follow.
1) The role of M-EMS is to speed up the superheat dissipation in the mold region, leaving the liquid core out of the mold region largely undercooled. This is beneficial for the heterogeneous nucleation of equiaxed crystals and survival of crystal fragments which are created by M-EMS-induced fragmentation of columnar dendrites. The equiaxed crystals or fragments will continue to grow and form an equiaxed zone in the strand center. The global heat transfer rate from the strand surface to the water-cooled copper mold is unlikely affected by the M-EMS.
2) The influence of M-EMS on the evolution of solid shell, which is defined by the volume fraction of solid (fs = 0.7), is not obvious, or not direct. The shell growth depends strongly on the degree of superheat. Before the superheat is fully dissipated in the liquid core region, the shell growth is relatively slow. Finally, the superheat needs to be specially controlled when M-EMS is implemented, as it tends to result in a sub-surface negative segregation (white band).

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Impact of radiative heat transfer on cooling of steel ingots during transport – a numerical analysis

Authors: Didier LAWRJANIEC[1]; Frederic Costes[2]; Victor Trejo[2]

Co-authors: Olivier Jaouen [2]; Stephane Andrietti [2]

[1] *Ascometal*

[2] *Transvalor SA*

Corresponding Authors: didier.lawrjaniec@ascometal.com, frederic.costes@transvalor.com, stephane.andrietti@transvalor.com, victor.trejo@transvalor.com, olivier.jaouen@transvalor.com

Regardless of the process (continuous casting, ingot or investment casting), the resolution of the thermal equations in FEM software remains a key point in order to have an accurate prediction. This aspect can be relatively complex when heat transfers are dealing with radiative phenomena. The aim of this paper is to describe these major phenomena which take place during the transport of large dimensions ingots coming from metal casting. In this context, the ingots are transported in wagons during several hours and it is crucial to study the relative position of each ingot to control the temperature variations due to radiative phenomena. The radiative heat transfers in a transparent medium is based on a method that uses purely geometrical factors called form factors (or view factors). Calculating these factors is preponderant and requires the use of high-performance digital tools (management of hidden surfaces, symmetries, etc.). In this paper, we will present the analytical solutions for simple geometries used to validate this radiation model and the benefits of these new tools for more elaborated industrial applications.

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Applicability of heat transfer and solidification simulations in investigating microstructural banding in continuously cast steel

Authors: Tuomas Alatarvas[1]; Matias Jaskari[1]; Antti Kaijalainen[1]; Sami Koskenniska[2]; Jari Asikainen[2]; Johanna Haapasalmi[2]; Kari Välimaa[2]

[1] *University of Oulu, Finland*

[2] *Ovako Imatra Oy, Finland*

Corresponding Authors: johanna.haapasalmi@ovako.com, jari.asikainen@ovako.com, kari.valimaa@ovako.com, matias.jaskari@oulu.fi, sami.koskenniska@ovako.com, tuomas.alatarvas@oulu.fi

Microstructural banding is observed as alternating microstructures in cast steel products, parallel to cast/rolling direction. Banding, causing hardenability issues and anisotropy of mechanical properties, is considered to originate from the interdenritic segregation during the solidification of steel. In this study, a three-dimensional heat transfer model (3DHTM) was used to simulate the steady-state local temperatures in a casting strand of 0.3C low alloy carbon steel, taking into account both primary and secondary cooling as well as other casting parameters. The calculated temperature profiles for a set of selected locations along the strand were used as input data for a solidification and microstructure model (SMM) for the continuous casting of steel. To assess the microstructure of the cast bloom, the prior austenite grain size, dendrite arm spacing, and the magnitude of elemental microsegregation between the dendrites were calculated with the selected temperature profiles for the steel grade. For validation purposes, bloom and bar samples were prepared from industrial trials. The calculated results are compared to the microstructural characterization of austenite grain size, and local elemental concentrations obtained with electron probe microanalyzer (EPMA). Based on the results, the effect of casting parameters and the total composition of steel to elemental microsegregation and microstructural banding is assessed. Additionally, a brief discussion of the segregation and microstructure between the bloom and bar samples is presented.

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Continuous Casting Secondary Cooling: Realtime Simulation of Local Strand Temperatures

Author: Mirko Javurek[1]

[1] *Johannes Kepler Universität Linz, Institut für Strömungslehre und Wärmeüübertragung*

Corresponding Author: mirko.javurek@jku.at

Real time simulation of strand temperatures is a common practice to adopt the cooling nozzle flow rates according to the desired strand surface temperatures. Usually only a smooth strand temperature is simulated by distributing the cooling heat fluxes smoothly over the strand surface. This simplification saves calculation time and is easier to use for control algorithms. In reality, the strand surface temperature rises in areas without cooling and drops in the impingement area of the spray cooling nozzle and during the roll contact. These temperature fluctuations can amount a few hundred degrees (peek to peek). Sometimes it is important to know the real, locally varying temperatures resulting from the inhomogeneous cooling heat flux distribution. One reason is that especially for higher cooling rates, the heat flux depends on the surface temperature and therefore, the local temperatures are needed to correctly consider the cooling heat flux. An algorithm is presented that allows a real time calculation of the local temperatures based on smooth temperature simulation results. These results can be used in enhanced cooling heat flux calculations, considerung the surface temperature influence gained from measurements.

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Defect monitoring tool for CC strands

Author: Susanne Hahn[1]

Co-authors: Christian Bernhard [2]; Georg Stechauner [3]; Jakob Six [3]; Peter Presoly [2]; Rainer Kaltseis [1]; Roman Krobath [4]; Sergiu Ilie [3]

[1] *Primetals Technologies*

[2] *Montanuniversitaet Leoben*

[3] *voestalpine Stahl GmbH*

[4] *Montanuniversität Leoben*

Corresponding Authors: jakob.six@voestalpine.com, georg.stechauner@voestalpine.com, peter.presoly@unileoben.ac.at, sergiu.ilie@voestalpine.com, susanne.hahn@primetals.com, rainer.kaltseis@primetals.com, roman.krobath@unileoben.ac.at, christian.bernhard@unileoben.ac.at

Primetals Technologies develops a new monitoring tool to evaluate the defect rate of a strand after casting based on its chemical analysis and its casting history. The defect monitor calculates different types of defect indices, for internal defects and for surface defects. All these indices are mathematical models mainly based on thermodynamical properties, like phase fraction, liquidus and solidus temperature, etc., that can be calculated by a modified version of the Primetals Technologies software DynaPhase and process parameters like temperature history, casting speed and external strain rates due to bending and unbending. The initial mathematical formulation of the indices has been developed in a joint research project of Primetals Technologies, voestalpine Stahl Linz, Montanuniversitaet Leoben and Aalto University in Helsinki. In an ongoing research cooperation with voestalpine Stahl Linz and Montanuniversitaet Leoben a trial version of the defect monitor is now installed on a continuous casting machine (CCM) of voestalpine Stahl Linz.
The defect indices are calculated for predefined segment lengths of the casted products for different points over the cross section of the segment, like corner, center, narrow side and wide side of a slab. The indices will then be used for quality rating of the casted products and help to decide which post-processing steps are necessary for different casting products (e.g. scarfing, down-grading….).
Unlike other quality rating tools, the defect monitor combines thermodynamical properties with process parameters and distils all this information with the help of physical considerations into simple defect indices with values between 0 and 1.
In this paper the defect monitor will be described in some detail. Moreover, some preliminary results of the validation process of the trial installation on a CCM of voestalpine Stahl Linz will be presented.

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Numerical Investigation of Air-Mist Spray in the Secondary Cooling during Continuous Casting of Steel

Author: Vitalis Anisiuba[1]

Co-authors: Armin Silaen [1]; Chenn Zhou [2]; Haibo Ma [1]

[1] *CIVS, Purdue University Northwest*

[2] *Purdue University Northwest*

Corresponding Authors: ma344@pnw.edu, czhou@pnw.edu, vanisiub@pnw.edu, asilaen@pnw.edu

Continuous casting is an important process to transform molten metal into solid. During secondary cooling of steel, arrays of spray nozzles are used to remove heat from the slab letting it solidify. Effective heat removal from the slab without causing slab cracking and deformation is desired. Air-mist spray is one of the promising technologies to achieve high-rate heat transfer due to the significant reduction in water droplet size, as a result of the strong air-water interaction in the spray nozzle. With the aid of three-dimensional computational fluid dynamics simulations, the present study would numerically analyze air-mist spray by a flat-fan atomizer and the impingement heat transfer between droplets and the slab surface during the secondary cooling process. Parametric studies would be conducted to investigate the effects of some important casting parameters such as air pressure, water flow rate, standoff distance and casting speed on the heat removal from the steel slab. A cooling water temperature and slab surface temperature of 300K and 1473K respectively would be used and the heat transfer coefficients would be evaluated for each of the casting condition to see the effect of these operating conditions on the spray cooling heat transfer coefficient. The numerical study would be done using ANSYS FLUENT 2020R1. The results from this study would provide useful information in the continuous casting operations and optimization.

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Temperature model for secondary metallurgical application

Author: Roman Rössler[1]

Co-authors: Stephan Natschläger [1]; Hannes Seyrkammer [1]; Stefan Fuchshumer [1]; Georg Grimm [1]

[1] *voestalpine Stahl GmbH*

Corresponding Authors: stefan.fuchshumer@voestalpine.com, hannes.seyrkammer@voestalpine.com, georg.grimm@voestalpine.com, roman.roessler@voestalpine.com, stephan.natschlaeger@voestalpine.com

Temperature control is crucial in metallurgical processes. The correct temperature regime during slab casting is essential from a high qualitative perspective. Moreover, incidents like casting abortion because of too low temperature or outbreaks have to be avoid for safety reasons as well. After reviewing the state of the art available temperature models the decision was made to develop a temperature model at voestalpine Stahl GmbH in Linz. A physical model based on thermodynamic equations of state programmed and put into operation at the secondary metallurgy in Linz.

The present paper describes the fundamental considerations based on the specific needs of the Linz steel plant with one- and two-strand casting machines. Aim and benefit were defined by the internal customer. The accuracy of the model was tested using an industrial dataset featuring several 1.000 heats covering the different metallurgical production routes and huge steel grades variety.

Based on the model a temperature prognosis is established and compared with production data. The limits of the prognosis are estimated by analytical and technical limits as well as metallurgical variations throughout the production. The temperature model was implemented in Dec. 2020. Since then it is operating successfully and permanently optimized.

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Numerical Simulation of Free Grain Sedimentation in Continuously Cast Billet

Author: Zhaohui Wang[1]

Co-authors: Miaoyong Zhu [1]; SEN LUO [1]; Weiling Wang [1]

[1] *Northeastern University*

Corresponding Authors: luos@smm.neu.edu.cn, myzhu@mail.neu.edu.cn, zhaohuineu@163.com, wwl4128281987@163.com

The free grain sedimentation is a common transportation phenomenon in molten steel during the continuous casting process and has great effects on the solidification structure and defects of as-cast. Based on our previously proposed multi-scale cellular automaton model (CA-FVM), the free grain sedimentation in the continuously cast billet is numerical simulated and its effects on the solidification structure of wire steel 82b cast by a bow-type caster with section size of 160 mm×160 mm are quantitatively analyzed. The results show that under the effect of gravity, the free equiaxed grains, which form ahead of the columnar grain, would settle down and block the columnar grain in the outer arc of strand. But the free equiaxed grain would be gradually away from the columnar grain tip in the inner arc of strand and remelt in the strand core with high temperature. Thus, the mechanical block of free equiaxed grain on the growth of columnar grain becomes weaker in inner arc than that in outer arc of strand, and asymmetric morphology of solidification structure in continuously cast billet of 82b with casting speed of 1.8m/min is quantitatively determined that the length of the columnar grains in the inner arc and outer arc of strand are 57.0 mm and 31.0 mm respectively.

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Using a Multiphase Model to Study the Solidification Structure and Macrosegregation in Continuous Casting Process

Author: Rui Guan[1]

Co-authors: Cheng Ji [1]; Miaoyong Zhu [1]

[1] *Northeastern University, China*

Corresponding Authors: jic@smm.neu.edu.cn, a609450750@163.com, myzhu@mail.neu.edu.cn

This study establishes an Eulerian columnar-equiaxed solidification model to study the solidification structure and macrosegregation in the continuous casting process by coupling fluid flow, macro-scale heat transfer, microstructure, and solute transport. The different phases include the extradendritic melt, the columnar solid dendrite, the interdendritic melt between columnar dendrites, the equiaxed solid dendrite, the interdendritic melt between equiaxed dendrites. The results demonstrate that the multiphase columnar-equiaxed solidification model corresponds well with the measured carbon segregation. This phenomenon can be exploited to improve the qualities of bloom and slab.

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On the modelling of channel segregation: from benchmark to steel ingots

Author: JUN LI[1]

Co-authors: Hongbiao Dong [2]; Jianguo Li [1]; Neng Ren [1]

[1] *Shanghai Jiao Tong University*

[2] *University of Leicester*

Corresponding Authors: lijg@sjtu.edu.cn, li.jun@sjtu.edu.cn, hd38@le.ac.uk, rennengneu@163.com

Channel segregation is one of the most frequently observed segregation patterns in large steel ingots, electro-slag remelting ingots, and as cast superalloys. These segregation defects are often referred to as 'A' segregate or lamellar-structured segregate in large steel ingots and 'freckles' in vertically solidified castings such as in the process of directionally solidification of superalloy castings. It is widely recognized that the channel segregation is formed by the thermol-solute-fluid flow instability during solidification process, therefore, it is important to gain better understanding of the fluid flow, heat transfer and species transport during solidification processing. Here, we employed the multi-phase solidification model to investigate the chimney behaviour and the evolution of channel segregation from the lateral heat dissipation Pb-Sn benchmark case to both nickel-based single crystal superalloy CMSX-4 and large steel ingot. Although channel segregations are caused by unstable convection of liquid melt into the mushy zone, channel segregations have different behaviors for castings of different materials and sizes, and their formation mechanisms are also different from each other, which will be discussed in current study.

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Distribution of TiN precipitates in high Ti UHSS grade conventional thick slab

Author: Hongbin Yin[1]

[1] *ArcelorMittal Global R&D*

Corresponding Author: hongbin.yin@arcelormittal.com

Development of Ultra High Strength Steel (UHSS) is a hot topic in recent years as demand for light weight automobile and machinery steels increases drastically. To understand the inclusion behaviors in a high Ti UHSS grade during casting and slab cooling, automated inclusion analysis tool was utilized to investigate the TiN precipitates distribution and their heterogeneous growth on oxide inclusions in conventional thick slab from surface to centerline. Precipitation size, number density and area fraction of TiN as well as complex heterogeneous TiN precipitates on oxide inclusions are studied at surface chill zone, chill to columnar transition zone, established columnar zone and centerline equiaxed zone. Thermodynamic modeling was made to understand the TiN precipitation under equilibrium condition in slabs at various temperatures during cooling. Kinetic modeling was made based on local solidification process from slab surface to centerline during casting and slab cooling. Attempt is made to utilize the TiN distribution from surface to slab center to back-calculate the segregation level inside a slab.

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Modeling Contact and Friction at the Mold-strand Gap through Lubrication and Contact Indexes

Authors: Hyunjin Yang[1]; Pavel E. Ramirez Lopez[1]

Co-author: Diana Vasallo [2]

[1] *SWERIM AB*

[2] *SIDENOR I+D*

Corresponding Authors: pavel.ramirez.lopez@swerim.se, hyunjin.yang@swerim.se, diana.mier@sidenor.com

Predicting contact conditions between the solidified shell and the mold wall is essential to simulate heat transfer and mold friction in continuous casting due to their significant impact on interfacial resistance and normal stress at the mold-strand gap. However, the multi-physics nature of continuous casting coupling fluid flow, heat transfer, solidification, and thermo-mechanical stresses makes it challenging to accurately predict local contact at the mold-strand gap. In this work, a new approach to model the local contact is proposed by considering the thermo-mechanical interactions between ferrostatic pressure, mold taper, and thermal shrinkage under steel solidification and slag infiltration. A newly introduced Contact Index classifies the contact area into three zones: 1) Compression dominant, 2) Ferrostatic dominant, and 3) Shrinkage dominant zones. With the Lubrication Index which divides into liquid and solid slag lubrication zones, normal stress applied on the mold wall or air gap formed at the gap is calculated according to six different scenarios. This approach is tested on a Digital Twin as a proof-of-concept. The simulation reveals that the influence of the thermal expansion coefficient of steel is substantial. A parametric study with different thermal expansion coefficients shows that the same casting process can cause the formation of air gap or excessive taper within a typical range of thermal expansion coefficients. Furthermore, the model demonstrates that the shell expansion by ferrostatic pressure plays an important role in mold friction in spite of its small magnitude compared to thermal shrinkage and mold taper.

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Roller geometry optimization in order to minimize unsteady bulging of slab casters

Author: Alija Vila[1]

Co-authors: Irene Watzinger [1]; Philipp Wieser [1]

[1] *Primetals Technologies*

Corresponding Authors: alija.vila@primetals.com, philipp.wieser@primetals.com, irene.watzinger@primetals.com

Process stability during continuous casting is an essential criterion to produce high-quality slabs. The meniscus is the most sensitive zone of the whole strand, as the initial strand shell is generated there. Unsteady bulging of the strand shell between two rollers is inducing feedback on the mold level position due to the liquid core of the strand. During unsteady bulging, heavy mold level fluctuations can build up and lead to surface defects and casting instabilities. Peritectic steels, which develop a rippled shell in the mold, are known for that effect. In addition, soft steels with creeping material behavior such as ultra-low carbon steels, silicon steels, and ferritic stainless steels show unsteady bulging.

The roller geometry of the casting machine has a high impact on the unsteady bulging affinity, as consecutive identical pitches lead to the superposition of the pumping effect. A new software tool has been developed in order to simulate the unsteady bulging effect and the generated level fluctuations. Therefore, a coupled simulation model combines solidification, shell transport, mechanical bulging, strand pumping, and mold level control. This tool offers new options to design the strand guide with an optimum distribution of the roller pitches in order to reduce unsteady bulging affinity. Each new caster built by Primetals Technologies has an optimized strand containment configuration in order to minimize mold level instabilities related to unsteady bulging.

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Influence Mechanisms of Processing Parameters on Solidification Structure of Continuously Cast Steel

Author: Weiling Wang[1]

Co-authors: Chen Meng [1]; Miaoyong Zhu [1]; SEN LUO [1]

[1] *Northeastern University*

Corresponding Authors: myzhu@mail.neu.edu.cn, wwl4128281987@163.com, luos@smm.neu.edu.cn, mengchen2001557@163.com

Continuous casting of steel typically consists of primary, secondary, and air-cooling zones, whose intensity is weakened in sequence. It promotes the transition of columnar dendrites to equiaxed ones, especially for middle and high carbon steels. However, due to the weak cooling rate, the inner solidification structure is prone to become coarsened deteriorating the solidification quality. So, it is necessary to clarify influence mechanisms of casting parameters on the evolution of solidification structure of the steel strand. With cellular automaton (CA) method, we developed a simple and efficient approach to connect the temperature fields at the macroscopic scale and the dendrite evolution at the microscopic scale. First, the thermal history of a high carbon steel strand was predicted and validated through comparison with measured surface temperature and shell thickness. Second, a 2D CA model for the dendritic growth of steel was developed and evaluated through comparison with in situ observation experiments. Then, the thermal history of a 4 mm × 40 mm region near the centerline of the strand was extracted and imported into the CA model to predict the dendrite evolution from the strand surface to the center under the critical conditions for CET including the nucleation undercooling, the nucleation probability, and the temperature gradient. The predicted dendritic arm spacing and CET location agree well with the actual results in the strand. The primary dendrite arm spacing of columnar dendrites decreases with increasing secondary cooling intensity, or decreasing superheat and casting speed. The CET is promoted as the secondary cooling intensity and superheat decrease. At weak secondary cooling intensity, some inner dendrites develop with extremely long and asymmetrical primary arms. The CET is not influenced by the casting speed, owing to the adjusting of the flow rate of secondary spray water.

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Modelling in Continuous Casting in the frame of the VALCRA RFCS project

Authors: Arianna Gotti[1]; Pavel Ramirez Lopez[2]

Co-authors: Edoardo D'Amanzo ; Michele De Santis

[1] *Rina Consulting - Centro Sviluppo Materiali Spa*

[2] *SWERIM*

Corresponding Authors: arianna.gotti@rina.org, pavel.ramirez.lopez@swerim.se

Internal and external defects are recurrent problems during Continuous Casting (CC) of steel due to the introduction of new grades that are often difficult to cast, as well as the everlasting pursuit for higher quality and improved yield.
Numerical modelling was introduced as an alternative to study CC defects in a more cost-efficient way than using traditional trial-error tests in the plant, starting in the late 70's and 80's with the advent of personal computers.
The RFCS dissemination project VALCRA, has reviewed the history of numerical modelling in the ECSC and RFCS projects over more than 20 years, which contributed to the development of this research field and which in turn largely benefited from it.
The present work proposes, after the overview about the role of models in continuous casting, a proactive outlook on the future of modelling, as an outcome of the discussions occurred during the dissemination events organised within the project with the European and world-wide steel community.

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Control of liquid metal flow in a laboratory model of a continuous caster with Electromagnetic Brake and Contactless Inductive Flow Tomography

Author: Ivan Glavinić[1]

Co-authors: Frank Stefani [1]; Sven Eckert [1]; Thomas Wondrak [1]

[1] *Helmholtz-Zentrum Dresden-Rossendorf*

Corresponding Authors: s.eckert@hzdr.de, f.stefani@hzdr.de, t.wondrak@hzdr.de, i.glavinic@hzdr.de

The quality of steel produced by a continuous caster depends on the flow condition during initial solidification in the mould. While the understanding of the flow and its effects is highly desirable, high temperature, opaqueness of the liquid steel and harsh conditions during the production limit viable measurement methods. Contactless Inductive Flow Tomography (CIFT) can provide information about the dominant flow structure in the mould in real time. This information can be used in a control loop for the Electromagnetic Brake (EMBr). Due to the inductive nature of CIFT, every change of the magnetic field strength of the EMBr has a strong influence on the measurements. Changing the strength of the EMBr alters the magnetization vector in its ferromagnetic yoke, which, in turn, generates a signal up to a thousand times higher than the flow induced magnetic field.

In this paper, we present a way to compensate these effects of EMBr on CIFT by filling a database containing compensation values. We will also present the preliminary results of a controller that utilizes CIFT and EMBr to actively control the flow in the mould during casting. The experiments are conducted on the Mini-LIMMCAST facility, a laboratory model of the mould of a continuous caster with the rectangular cross-section of 300×30 mm^2. It is operated with the eutectic alloy GaInSn.

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Experimental study of turbulent flow in a continuous casting mold under the influence of an EMBr at various positions

Author: Dennis Schurmann[1]

Co-authors: Bernd Willers [1]; Ivan Glavinic [1]; Klaus Timmel [2]; Sven Eckert [1]

[1] *Helmholtz-Zentrum Dresden-Rossendorf*

[2] *Helmholtz-Zentrum Dresden Rossendorf*

Corresponding Authors: d.schurmann@hzdr.de, k.timmel@hzdr.de, b.willers@hzdr.de, i.glavinic@hzdr.de, s.eckert@hzdr.de

Experimental investigations of the fluid flow in a continuous casting mold are performed at the Mini-LIMMCAST facility at HZDR, which is a liquid metal mockup operated with GaInSn at room temperature. Velocity measurements in the non-transparent liquid metal are performed by means of the ultrasound Doppler velocimetry (UDV), which enables the reconstruction of the complex flow pattern in the mold. The focus of our study is on the influence of different electromagnetic actuators like electromagnetic brakes (EMBr) or electromagnetic stirring (EMS) on the mold flow in slab and bloom geometries.
Flow measurements are carried out in a slab model for continuous casting of steel under the influence of a ruler type Electromagnetic Brake (EMBr). Two-dimensional velocity distributions in the center plane of the rectangular mold with a cross section of 300⊠35mm2 are determined by means of the ultrasound Doppler velocimetry. This study especially focuses on the influence of the vertical position of the EMBr and its magnetic flux density as well as the effect of different immersion depths of the submerged entry nozzle. The horizontal flow velocity just below the free surface can effectively be reduced by choosing an optimal position of the EMBr, while an improper positioning even increases the near-surface velocity compared to the case without activated brake. A general braking effect of the EMBr on the submerged jet is not observed. The decisive mechanism for controlling the near-surface flow results from a modification of the jet geometry and a reorganization of the flow field. In terms of an effective flow control an appropriate positioning of the EMBr has at least the same significance as the regulation of the magnetic field strength.

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Large eddy simulation of continuous casting process

Author: Katarina Mramor[1]

Co-authors: Bozidar Sarler [2]; Robert Vertnik [3]

[1] *University of Ljubljana, Faculty of Mechanical Engineering*

[2] *Faculty Of Mechanical Engineering, University of Ljubljana*

[3] *Štore Steel d.o.o.*

Corresponding Authors: katarina.mramor@fs.uni-lj.si, bozidar.sarler@fs.uni-lj.si, robert.vertnik@store-steel.si

This contribution presents the large eddy simulation applied to the 2D model of the continuous casting process. The flow of molten steel in the continuous casting process is approximated by an incompressible fluid flow, which is described with transport equations for mass, momentum, spices, and energy, that are closed with fractional step method for pressure-velocity coupling, Boussinesq approximation for buoyancy, and Darcy approximation for the mushy zone. The turbulence is solved by applying the Smagorinsky large eddy simulation model and VanDriest damping function. The application of a large eddy simulation model enables us to model the eddies at higher accuracy than in the RANS type of models and with a much lower computational cost than in the DNS model. For the solution of governing equations, the meshless method based on the collocation with multiquadric radial basis functions is used locally on five-noded subdomains.
The meshless continuous casting simulation system has been previously successfully tested on several benchmark test cases. The results with the large eddy simulation implementation are compared to the other turbulence models such as the low-Re k-epsilon turbulence model. The time-averaged flow field of a large eddy simulation solution is in good agreement with the steady-state solution obtained by the previously implemented and tested RANS models.

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The Physical Chemistry of Steel Deoxidation and Nozzle Clogging in Continuous Casting

Author: Rodolfo Morales[1]

Co-authors: Alfonso Najera [2]; Carlos Muniz [3]; Jafeth Rodriguez [3]

[1] *Instituto Politécnico Nacional*

[2] *Instituto Politecnico Nacional*

[3] *Universidad Autonoma de Coahuila*

Corresponding Authors: rodrigo.muniz@uadec.edu.mx, r.morales@utoronto.ca, alfonso_najera@yahoo.com.mx, jafethrodriguez@uadec.edu.mx

Nozzle clogging in continuous casting of steel originates by the adherence of alumina particles and other oxides, precipitated during the liquid steel deoxidation, on the refractory material's surface. Hence, these particles' nucleation and growth rates in supersaturated melts are analyzed considering, specifically, the role of the interfacial tensions between alumina, silica, and other oxides and the liquid metal. Weak steel deoxidizers like silicon do not need high supersaturations favoring high nucleation rates, giving particles' narrow size distributions thanks to fast diffusion and Ostwald-ripening coagulation. Strong deoxidizers, like aluminum, need high supersaturation levels leading to broad size distributions. Besides, the morphology of these particles depends on the nucleation and growth mechanisms. The adhesion forces among the deoxidation particles, forming clusters, depending on the morphology and the oxide's chemistry. The stability of the nozzle's clog, adhered to the nozzle's wall, depends on the interface tensions between the melt and the nozzle's refractory surface and between the melt and the inclusion. CFD simulations and velocity measurements in a full-scale water model predict great distortions in flow during the operation of a mold using a clogged nozzle. The results obtained here help set up basic recommendations in steel refining and materials specifications of casting nozzles.

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Continuous Casting Mold Flow with Gas Injection: Comparison of Physical and Mathematical Simulations

Author: Mirko Javurek[1]

Co-author: Raimund Wincor [2]

[1] *Johannes Kepler Universität Linz, Institut für Strömungslehre und Wärmeübertragung*

[2] *voestalpine*

Corresponding Authors: mirko.javurek@jku.at, raimund.wincor@voestalpine.com

The injection of inert gas in the inflow region of the continuous casting mold is a common measure in continuous casting to reduce clogging. Depending on the gas injection rate, the resulting gas bubbles can significantly influence the turbulent mold flow because of their buoyancy forces. The mold flow pattern can change from double to single roll as a consequence of high gas injection rates and can therefore influence the steel product quality. As a consequence, it is necessary to consider the gas bubbles in numerical simulations of the mold flow. Comparisons of physical and mathematical model results show that enhanced models are required to consider the complex interaction of flow, turbulence and gas bubbles. Therefore, reliable physical models are necessary to provide accurate validation data for numerical simulations. Measured results from a 1:1 scaled mold water model are compared with simulation results.

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Micro-segregation induced strain inhomogeneity in >900MPa UTS martensitic hot rolled advanced high strength steel

Author: Cameron Bee[1]

Co-authors: Carl Slater [1]; Claire Davis [1]; Didier Farrugia [2]

[1] *WMG, University of Warwick*

[2] *TATA Steel R&D UK*

Corresponding Authors: didier.farrugia@tatasteeleurope.com, claire.davis@warwick.ac.uk, carl.slater@warwick.ac.uk, c.j.bee@warwick.ac.uk

Advanced high strength steel (AHSS) strip used in the yellow goods sector needs a balance of high strength with good toughness and bendability. Cracking during bending can result in failure depending on radius to thickness ratio, in view of the relative low ductility and complex microstructure of these steels. This paper examines how local compositional inhomogeneity can affect bending performance in tempered martensite AHSS.

Localised inhomogeneity in the microstructure can generate regions of strain concentration during deformation, affecting the bending performance of the material. Inhomogeneity at the material scale includes inclusion distributions, mixed microstructures, compositional segregation and texture. Inclusions and other impurities in the steel have been reported to be dominating factors in formability. However, as advanced steels become cleaner, other factors become more influential in limiting bendability. When considering bending performance, the sub-surface region is of particular significance as it experiences the greatest strain and stress during bending. These are commonly the nucleation points for failure, primarily through the formation of rippling, micro-shearband, tensile triaxiality and cleavage fracture.

A range of multiscale characterisation methods including micro-XRF, SEM-EDS and nanoindentation have been combined with SEM in-situ mechanical tests to examine the scale and role of local

inhomogeneity. These techniques have been used to assess compositional inhomogeneity (Inter dendritic segregation of Mn formed during solidification subsequently hot rolled to give Mn enriched and depleted bands) on the local hardness (instrumented nano-indentation mapping) and therefore strength. Variation in the severity of segregation banding has been observed in strip steels of different thickness, and with respect to position through thickness. The influence of the different banding severity on strain partitioning and shear band formation during deformation has been identified using DIC. The significance of the correlation between these factors is discussed in the context of processability.

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Bolt forging process optimisation using simulation software with applied Avrami model for recrystallisation

Author: Michal Filipowicz[1]

Co-authors: Carl Slater [1]; Paul Lansdell [1]; Steven Hill [2]

[1] *University of Warwick*

[2] *WH Tildesley*

Corresponding Authors: stevenhill@whtildesley.com, michael.filipowicz@warwick.ac.uk, c.d.slater@warwick.ac.uk, p.lansdell@warwick.ac.uk

Fasteners are quite simple products but critical in most sectors. Bolt manufacturing is a large, well-established industry worldwide with a long history however, due to the low value nature of this product type, the production process has not been fully metallurgically optimised, increasing yield and production rates have instead been main areas of improvement. With modern analysis tools and understanding of recrystallisation, it is now much faster to implement these metallurgical principles into the simplest of parts that aid optimisation.
The nature of the bolt itself provides a complex distribution of temperature and strain with just the bolt head being heated and very little strain being imparted on the threaded section. This results in a barrelling/bulging type deformation of the bolt head during deformation, the strain pattern is dependent on the size of the head and the temperature at which deformation takes place (due to the differing constraints of the threaded section). Choosing an inappropriate temperature would result in very little strain in critical regions such as the shoulder and therefore result in a lower yield strength and therefore overall performance.
Through the combination of an instrumented power hammer and FE simulations, an understanding of the flow patterns of 316 stainless steel 20mm bolts is obtained. Variables such as temperature and deformation rate have allowed a systematic review of the spatial distribution of the grain growth and recrystallisation kinetics.
A series of mechanical tests, hardness mapping and microstructure examination were performed on a manufactured bolt. These results were then compared to the simulation and commercially available comparisons allowing for the bolt process to be optimised.

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Use of damage theory to improve material model and predict potential failures in a hot rolling simulation system

Author: Umut Hanoglu[1]

Co-author: Bozidar Sarler [1]

[1] *Institute of Metals and Technology*

Corresponding Authors: bozidar.sarler@imt.si, umut.hanoglu@imt.si

In this research, a previously developed hot rolling simulation system, based on novel meshless computing technology, is upgraded from the pure plastic to a more realistic elasto-plastic material model that allows to cope with damage mechanics. This enables a more detailed virtual testing of different rolling schedules. Helmholtz free energy is used to structure damage coupled constitutive equations and stiffness matrix on the basis of irreversible thermodynamics. Both the elastic and the plastic parts contribute to the free energy. For the elastic part, initial elastic stiffness tensor changes into damaged elastic stiffness tensor and the plastic part of the free energy is added due to the strain hardening. Effective stress tensor is redefined with the inclusion of the damage tensor. Damage variables are initialized through the density of the micro voids inside the steel billet. Instead of fracture mechanics, a continuum damage mechanics is considered here to analyze the mechanical behavior of the rolled steel before the occurrence of any crack. Therefore, a damage tensor is calculated during the hot rolling simulation, which is obtained based on the current deformation state. A two dimensional slice model is considered in the simulations. These slices are aligned parallel to each other and perpendicular to the rolling direction. Therefore, the components of the damage tensor towards the rolling direction are neglected. The main improvement of the upgraded simulation system represents a more realistic material model that considers the initial processing history of the steel and reveals the damage effects throughout the simulation. This provides a good virtual estimation where and when to expect failure.

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Digital Process and Product Twin for hot rolling

Author: Markus Widder[1]

Co-authors: Alois Seilinger [1]; Axel Rimnac [1]; Konrad Krimpelstaetter [1]

[1] *Primetals Technologies Austria*

Corresponding Authors: konrad.krimpelstaetter@primetals.com, axel.rimnac@primetals.com, markus.widder@primetals.com, alois.seilinger@primetals.com

A knowledge driven, physically based and reliable determination of process parameters during hot rolling is crucial for the accurate prediction of final product properties and for the precise layout and design of hot strip mills.
Based on known initial conditions of the material and accurate product tracking, the evolution of physical properties can be calculated based on the time-temperature deformation path. For this purpose, several detailed sub-models are required to describe, e.g. temperature evolution due to heat generation and heat radiation, convection and conduction or considering the effects of descaling. The same holds for the prediction of heat loss and phase transformations while passing the material through a transfer bar cooling unit, a heat cover its thermal equilibration inside a coil box or the impact of inductive heating and fast cooling along the cooling line.
Based on metallurgical process parameter settings, the calculated interaction between mill and material in terms of temperature evolution, deformation induced work hardening and resulting forces and torques provide direct input for dimensioning of the force and power requirements of mill stand and drives. Moreover, the model results are also utilized for dimensioning of several other components of a hot strip mill like shears, profile and flatness actuators, cooling equipment or downcoilers. Calculation of metallurgy relevant intrinsic parameters such as states of precipitates and microstructural morphology provide the basis for the prediction of phase transformation kinetics and physical properties such as yield and tensile strength.
A detailed analysis of the product mix enables throughput evaluations based on a variety of pass and cooling schedule optimizations allowing accurate predictions on operational expenses and return on investments to be expected. The feedback from existing rolling mills is used as an input for the fine tuning and continuous improvement of the detailed models.

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Recrystallization simulation and double-hit compression tests of microalloyed steel

Author: Evelyn Sobotka[1]

Co-authors: Erwin Povoden-Karadeniz [1]; Johannes Kreyca [2]

[1] *CDL-IPE, TU Wien*

[2] *voestalpine Forschungsservicegesellschaft Donawitz GmbH*

Corresponding Authors: erwin.povoden-karadeniz@tuwien.ac.at, johannes.kreyca@voestalpine.com, evelyn.sobotka@tuwien.ac.at

Temperature dependent strain induced precipitation of (Ti,Nb,V)(C,N) MX carbonitrides can retard static recrystallization. Predicting the role of microalloying elements on the recrystallization behavior by thermokinetic simulation is expected to support the technological process optimization and cost reduction of steel development. In this study, we assess the predictive power of recrystallization modeling for the effect of Ti, Nb, and V microalloying on recrystallization kinetics.

Isothermal double-hit compression tests are performed on a Gleeble 3800 thermo-mechanical simulator to investigate the microstructure evolution related to static recrystallization kinetics of microalloyed steel. By determination of the recrystallized fraction of austenite using the 5 % true strain method at different strains, strain rates and temperatures the static recrystallization critical temperature (SRCT) is derived for the studied microalloyed steel grade.

A recrystallization model, recently implemented into the simulation software toolbox MatCalc, is used to reproduce the experimentally determined SRCT-values. In addition, the softening fractions are evaluated as a function of time by adapted Avrami equations. Results from the MatCalc recrystallization model and the Avrami model are subsequently compared and their predictive power is assessed.

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Flow stress modelling considering dislocation density and recrystallization kinetics during hot deformation of API X70 pipeline steel

Author: Nabi Allah Razani[1]

[1] *deputy of planning and development-Khouzestan Oxin Steel Company- Ahwaz-Iran*

Corresponding Author: n.razani@oxinsteel.ir

ABSTRACT
Flow behavior constitutive equations have been widely used in FE analysis and parameter's optimization in thermomechanical processes of micro alloy steels. Flow curves of API-5L X70 pipeline micro alloy steel were analyzed to determine the material genome. Hot compression tests were performed over the different temperatures of 850-1150 ℃ and the strain rate range of 0.001-1 sˆ(-1) to obtain the kinetics of dynamic events. Using an inverse analysis (IA) technique, including a set of a finite element model of the hot compression process and the experimental data, the flow curves ware predicted. Constitutive equations of flow stress and time-dependent dislocation density comprising of work hardening, dynamic recovery and kinetic of dynamic recrystallization were presented as the material genome. The coefficients of the constitutive equations were extracted using regression analysis. The Arrhenius equation was applied to calculate the activation energy and verifying the validity of the calculation results. The predicted flow curves of the proposed model were manifested with a good agreement with the experimental results.

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Steel strip hot runout table simulation and high temperature electromagnetic measurement for phase transformation monitoring

Author: Russell Hall[1]

Co-authors: Claire Davis ; Lei Zhou [2]; Mohsen Aghadavoudi Jolfaei [2]

[1] *Warwick Manufacturing Group*

[2] *University of Warwick*

Corresponding Authors: mohsen.jolfaei@warwick.ac.uk, lei.zhou@warwick.ac.uk, r.hall.5@warwick.ac.uk

Quality control for efficient steel processing is extremely important with the need to decarbonise production, produce steels to tighter material property constraints. Thermo-mechanical controlled processing and the models for predicting microstructural development need input from smart sensing technologies to improve their capability, particularly for advanced high strength steel grades that are demanding to produce. Real time control of steel production requires sensors that can withstand and measure at high temperatures during processes such as hot rolling and run out table cooling.

Direct measurement in-situ during processing of steel microstructure is challenging, with electromagnetic (EM) sensors now being regularly employed during strip production, primarily for inspection during cold strip processing. EM sensors have, more recently, been used for hot strip steel monitoring. Physical simulation of industrial run out table conditions combined with high temperature electromagnetic sensing, along with advanced modelling techniques, is needed to support and expand this development to wider applications. For example, electromagnetic sensor arrays are in development that can be used for assessment for varying strip widths, thicknesses and products with complex geometries such as rod and wire. This paper reports on a laboratory demonstration furnace-roller table with embedded EM sensors where variable flowrate water cooling regimes can be imposed to generate specific steel phase transformation behaviour. The EM sensors can be used for monitoring of phase transformation, and with feedback for control of cooling to achieve specific microstructures. Trials using different steel products and chemistries have been completed and related to modelling results. It has been shown that it is possible to measure phase changes at high temperatures during steel cooling from normalising temperatures for plate, strip, rod and wire applications. EM sensor feedback can be used by steel processors to integrate into mill control systems for accurate product metallurgy and mechanical property control.

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Identification of the 3D cellular automata model of static recrystallization based on the inverse analysis

Author: Mateusz Sitko[1]

Co-authors: Grzegorz Cios [1]; Lukasz Madej [1]; Lukasz Rychłowski [1]; Mateusz Mojzeszko [1]; Piotr Bala [1]

[1] *AGH University of Science and Technology*

Corresponding Authors: rychlowski@agh.edu.pl, mmojzesz@agh.edu.pl, msitko@agh.edu.pl, lmadej@agh.edu.pl, piotr.bala@agh.edu.pl, grzegorz.cios@agh.edu.pl

Identification of the three-dimensional cellular automata (CA) model of static recrystallization (SRX) based on the inverse analysis concept is the primary goal of the research. The developed CA model is a full-field approach that captures local heterogeneities in grain morphology, crystallographic orientation, and distribution of stored energy after deformation. The identification stage is based on the inverse analysis concept that combines a direct problem numerical model, corresponding experimental data, and optimization algorithm. Experimental data revealing the recrystallization fraction evolution during heating of the deformed samples are extracted from extensive scanning electron microscopy (SEM) analysis. To distinguish between recrystallized and unrecrystallized grains, electron back scattered diffraction (EBSD) capabilities are used. The goal function is based on the square root error between measured and calculated recrystallization fractions as well as final grain sizes. Finally, the minimization of the defined goal function is based on the nature-inspired technique. As a result of the inverse approach, a set of identified model coefficients for the SRX simulations for the commonly used in the industry ferritic-pearlitic steel is provided. Examples of microstructure evolution under heat treatment conditions are also presented to highlight model predictive capabilities.

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Automatic unstructured quadrilateral mesh generator based on a direct method

Authors: Filippo Avellino[1]; Silvia Mancini[1]; Luigi Langellotto[1]

[1] *RINA SpA*

Corresponding Authors: luigi.langellotto@rina.org, filippo.avellino@rina.org, silvia.mancini@rina.org

Mesh quality is a fundamental issue with the Finite Element Method. Structured meshes are quite common: however, they usually have some problems when it comes to change rapidly the element size in the adaptive mesh. For this reason, to usage of unstructured mesh is more appropriate when the target is the creation of an adaptive mesh using quadrilateral elements. This work aims to present a Finite Element unstructured quadrilateral mesh generator based on a direct method. The algorithm starts from an initially ordered series of points (loops) discretizing the continuous edge of the computational domain to be meshed. Then the algorithm generates internal layers of elements, based on the segment connecting two consecutive nodes, thus increasing the mesh quality on the boundary, where the higher thermal, strain, stress gradients are placed. After the regular external layers are generated, the meshing procedure starts the direct decomposition of the domain, until the section meshing is completed. To enhance mesh quality, if it is necessary, a mesh smoothing is operated. After the 2D mesh of the section has been created, an extrusion along the rolling direction allows the generation of a complete 3D mesh.

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Effect of sample geometry on strain uniformity and double hit compression tests for recrystallisation kinetics determination

Author: Nusrat Tamanna[1]

Co-authors: Carl Slater [1]; Claire Davis [1]

[1] *University of Warwick*

Corresponding Authors: c.d.slater@warwick.ac.uk, claire.davis@warwick.ac.uk, nusrat.tamanna@warwick.ac.uk

Since its first implementation in the 1950's thermo-mechanically controlled rolling has proven to be invaluable in steel industry for giving grain size refinement and hence improved strength and toughness. This led to widespread use of lab based thermo-mechanical simulators, such as Gleeble and ServoTest machines, to reproduce the strain, strain rate and temperatures of hot deformation and support the optimisation of rolling schedules for improved microstructures and steel grade development. These machines use compression samples (typically plane strain or uniaxial) to investigate the key fundamental metallurgical processes such as recrystallisation, where precise temperatures, strains and hold times can be imparted before quenching of the sample to reveal the prior austenite grain size, which is not possible on full scale plants. Whilst several research has been carried out to correct for friction and temperature variations on the flow stress behaviour, strain variation within the samples is a problem, particularly for microstructural assessment. However, as initial recrystallisation studies mainly focused on average grain size and kinetic predictions the strain non-uniformity did not give significant error. Modern recrystallisation studies focus on full grain size distribution predictions, which generally require characterization of >700 grains to give smooth histograms, in order to assess phenomena such as grain size bimodality, influence of segregation etc.

This paper reports on FE modelling and experimental verification of strain distribution in commonly used plane strain and uniaxial compression test sample geometries. Local strain was determined in the deformed Fe-3Si alloy samples by EBSD misorientation indexing, calibrated against samples with known (tensile deformed) strain. Significant strain inhomogeneity is seen for the standard compression samples, therefore a new plane strain geometry has been designed to minimize strain variability, and optimize the amount of material that exhibits uniform strain (for microstructure assessment) that matches the overall imposed macrostrain.

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DEVELOPMENT OF A THICK STEEL PLATE MANUFACTURING ROUTE

Author: Jean-Christophe Gebelin[1]

Co-authors: Andrew Dunsmore [1]; Biao Tao [2]; Bogdan Nenchev [1]; Chinnapat Panwisawas [3]; Hongbiao Dong [3]; JUN FU [3]; Ming Li [4]; Qing Tao [1]; Xiaoan Yang [3]; Zihui Dong [1]

[1] *NISCO-UK Research Centre, The University of Leicester, UK*

[2] *NISCO Research Institute, Nanjing Iron and Steel United Company, China*

[3] *University of Leicester*

[4] *NISCO Research Institute, Nanjing Iron And Steel United Company, China*

Corresponding Authors: bn55@leicester.ac.uk, hd38@le.ac.uk, xy149@le.ac.uk, liming1@njsteel.com.cn, taobiao@njsteel.com.cn, acd33@leicester.ac.uk, qt15@leicester.ac.uk, zihui.dong@leicester.ac.uk, jg499@leicester.ac.uk, jf320@leicester.ac.uk, chinnapat.panwisawas@leicester.ac.uk

Industry 4.0 promotes the use of digital twins to improve manufacturing efficiency. In this paper we report work being carried out at the NISCO-UK Research Centre at the University of Leicester, UK, looking at steel plates manufacturing. Physics-based models of the production of slabs by continuous casting and subsequent rolling are used to further improve the understanding of the impact of Key Process Variables on the formation of defects such as linear cracking and abnormal grain structures. The continuous casting model takes into account liquid steel flow within the slab, solidification of the steel and the mechanical effect of the rolls acting on the slab as it is being cast. The rolling model include the modelling of the pre-heating and its resulting temperature distribution, followed by the thermomechanical modelling of the slab as it is being rolled.
As an example, a slab of thickness 160mm is produced using a continuous caster, then rolled to a final thickness of 40mm. Some variations of the KPVs are then considered and their impacts on process outcome highlighted.

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Using alloy design, modelling and rapid alloy processing validation to improve through-thickness microstructural uniformity during the production of large section components

Author: Carl Slater[1]

Co-authors: Claire Davis [1]; Matthew Green [2]; Russell Hall [3]

[1] *University of Warwick*

[2] *Liberty Speciality Steel*

[3] *Warwick Manufacturing Group*

Corresponding Authors: claire.davis@warwick.ac.uk, r.hall.5@warwick.ac.uk, c.d.slater@warwick.ac.uk, matt.green@libertysteelgroup.com

High-value speciality steels are often designed for specific large component engineering applications. These steels, which are typically heavily alloyed, offer excellent properties in terms of fatigue, toughness, high-temperature strength and corrosion resistance. However, due to the fact steelmakers are at the start of a multi-partner supply chain, feedback regarding component manufacture and performance in service is often limited. The high cost of production scale material manufacture can make the cost of development trials prohibitive. For this reason, it is desirable to use laboratory-scale trials and computer alloy design to optimise properties and process parameter selection.
In the speciality steel market there is a requirement for large diameter bar. Producing large diameter bar from ingot by hot rolling comes with many challenges including difficulties in achieving through-thickness uniformity. In order to achieve sufficient reduction during hot working larger ingots can be used, but increasing ingot size does not guarantee improved uniformity across the full bar section. During rolling, strain levels, strain uniformity and thermal homogeneity all decrease as bar diameter increases. These factors may manifest themselves in the final product as variation in grain size, second phase distribution and/or segregation levels.
Alloy design coupled with process modelling has been used to predict the extent of segregation during casting and reheating together with strain histories through the thickness of bar stock and microstructural development during hot working with the aim of optimising the process route to consistently achieve specification requirements throughout the product. The modelling predictions have been verified using rapid alloy processing facilities: laboratory ingots of 8kg were cast, homogenised and characterised. Samples were thermo-mechanically processed according to both surface and core time/temperature/strain conditions using a Gleeble HDS-V40. This paper presents case studies demonstrating the alloy design, modelling and RAP route.

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Numerical modelling of thermal evolution and phase transformation during high-heat input electro-gas welding of marine steel

Author: JUN FU[1]

Co-authors: Biao Tao [2]; Bogdan Nenchev [1]; Chinnapat Panwiswas [1]; Hongbiao Dong [1]; Ming Li [2]; Qing Tao [1]

[1] *University of Leicester*

[2] *NISCO Research Institute, Nanjing Iron and Steel United Company*

Corresponding Authors: qt15@leicester.ac.uk, chinnapat.panwisawas@leicester.ac.uk, liming1@njsteel.com.cn, jf320@leicester.ac.uk, hd38@leicester.ac.uk, bn55@leicester.ac.uk, taobiao@njsteel.com.cn

The high heat input welding method can improve the efficiency of manufacturing, but the impact toughness of the heat-affected zone (HAZ) is reduced seriously during the welding process. Thermal profile evolution in HAZ is the key factor affect microstructures and resulting mechanical properties of welded joints.

In this study, we coupled heat transfer, solid mechanics and solid-state evolution to simulate the electro-gas welding (EGW) process of ultra-high-strength marine steel plate using COMSOL multiphysics software. The real welding geometry, process variables and materials are used with a three-dimension heat source as a sinusoidal function with various heat inputs up to 200kJ/cm. The simulation results reveal that microstructure can be optimized by varying the welding source movement path and the cooling rate of sliding copper shoe, to improve the properties of HAZ.

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Predicting the change in strength properties of heavy plates due to the levelling operation

Author: Thomas Kaltenbrunner[1]

Co-authors: Daniela Gaith [2]; Erik Parteder [1]; Michael Liebrecht [2]; Rupert Egger [1]; Stefan Falkner [1]

[1] *voestalpine Grobblech GmbH*

[2] *MathConsult GmbH*

Corresponding Authors: stefan.falkner@voestalpine.com, michael.liebrecht@mathconsult.co.at, daniela.gaith@mathconsult.co.at, t.kaltenbrunner@voestalpine.com, rupert.egger@voestalpine.com, erik.parteder@voestalpine.com

In the processing of heavy plates, the leveling operation aims at improving the plate flatness and minimizing residual stresses, but is also the last process step influencing the strength properties in a significant manner. To this end, the roller-leveling machine applies multiple cycles of plastic bending with a strain sequence depending on the actual leveler setup to the plate cross section . The plastic deformation, in turn, affects the strength properties of the heavy plate. In consequence of the bending deformation, the strength contribution due to leveling varies across the plate thickness direction. In a previous work, a model to predict the local change of the strength properties across the thickness direction due to the leveling process was developed. The present work focuses on how these locally different strength changes across the plate thickness contribute to the plate's final overall strength . This modelling concept enables the implementation of a high performance automation application that is not only able to compute the levelling forces and power consumption but also to predict the degree of plastification and the change of the strength properties dependent on the leveler setup parameters.

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Ultrafine grained high C steel bars obtained by multi-pass warm caliber rolling

Author: Claudio Guarnaschelli[1]

Co-authors: Filippo Dionisi Vici ; Francesco Papini [2]; Ilaria Salvatori [3]; Matthias Schmidtchen ; Nico Kaden [4]; Ulrich Prahl

[1] *Rina Consulting - CSM S.p.A.*

[2] *JSW Steel Italy*

[3] *Rina Consulting - CSM S.p.a.*

[4] *Technische Universität Bergakademie Freiberg*

Corresponding Authors: ilaria.salvatori@rina.org, f.papini@jswitaly.com, claudio.guarnaschelli@rina.org, nico.kaden@imf.tu-freiberg.de

Warm Caliber Rolling (WCR), a thermomechanical operation carried out in the ferritic domain in the range of temperatures 500-700 ℃, can lead to a strong grain refinement through mechanisms as dynamic recrystallization or recovery induced by accumulation of strain. Under proper conditions, it is possible to obtain ultrafine grained microstructures, which can significantly improve the mechanical properties, especially for those engineer applications – as special steel bars – where high toughness levels are required in combination with high strength.

In this work, thermomechanical cycles with temperatures 600-700 ℃ and high strain have been designed for a high carbon steel with C=0.80%, by means of preliminary Gleeble tests. WCR experiments were then performed on a pilot scale. As a key requirement for the formation of ultrafine microstructure is very high strain, multi-pass caliber rolling has been used to impart heavy deformations avoiding excessive rolling forces.

Starting from common lamellar pearlite typical of high-C steel, microstructures consisting of ultra-fine ferrite matrix (˜1 m) and finely dispersed spheroidized cementite (˜ 0.5 m) have been achieved under the optimized process conditions.

The tensile strength of the bars subjected to WCR results in general lower than that of the conventionally hot rolled materials, while a significant improvement (from 30 to 60 J) is found in terms of impact toughness. In addition, an increase of fatigue limit – evaluated by means of tension-compression fatigue tests – of about 10 %, has been found with respect to the reference steel.

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Role of cooling rate on microstructure evolution of Zn-Al-Mg based coatings via phase-field approach

Authors: Sai Pavan Bhogireddy[1]; Vanessa Quaranta[2]

Co-authors: Denis Saraev [2]; ILARIA IACONETA [3]; Jerzy Gawad [2]

[1] *NLMK Belgium Holdings*

[2] *NLMK Group*

[3] *NLMK Belgium Holdings S.A.*

Corresponding Authors: d.saraev@eu.nlmk.com, i.iaconeta@eu.nlmk.com, j.gawad@eu.nlmk.com, sp.bhogireddy@eu.nlmk.com, v.quaranta@eu.nlmk.com

Hot-dip galvanizing (HDG) Zn coatings represent a low cost and effective way of protecting steel against corrosion. In recent years, Zn coatings containing Mg became a promising next generation of Zn-based coatings due to their superior performance compared to pure Zn coatings in terms of corrosion resistance, formability, weldability and paintability [1].

These properties are strongly influenced by the microstructure which develops during the solidification process of the coating [2-3]. In this regard, computer-aided simulations represent powerful tools for a deep understanding of the microstructure evolution of HDG-Zn coatings as a function of the process conditions.

In this work, we systematically investigate the microstructure, in terms of surface morphology and surface phase fraction, of Zn+1.2%Al+1.2%Mg (ZAM) coating by means of phase-field approach. Our simulations enable understanding how the coating microstructure is influenced by the cooling rate. In particular, we investigate how cooling conditions determine the final eutectic structure and primary phases. First insights into the role of micro-alloy elements (i.e. elements added to the reference Zn+1.2%Al+1.2%Mg composition) on the surface microstructure are also discussed.

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Rapid alloy processing approach for ductility enhancement in commercial dual-phase steels through industrially relevant process and composition changes.

Author: Bharath Bandi[1]

Co-authors: Carl Slater [1]; Claire Davis [1]; Didier Farrugia [2]

[1] *Warwick Manufacturing Group, University of Warwick, Coventry, UK*

[2] *Tata Steel Europe, Rolling Finishing & Measurement Department, United Kingdom*

Corresponding Authors: c.d.slater@warwick.ac.uk, claire.davis@warwick.ac.uk, didier.farrugia@tatasteeleurope.com, b.bandi@warwick.ac.uk

Dual phase steels are extensively used in automotive safety and structural components because of their low alloying costs, relatively easy processing and optimum combination of strength and ductility. This good combination of properties is attributed to the presence of soft ferrite phase and hard martensite islands in the microstructure. More specifically, the mechanical properties are dependent on the martensite volume fraction (increases strength), ferrite grain size (increases strength and ductility), martensite distribution and morphology (affecting UTS and ductility uniformity), and nano-precipitate characteristics (increases strength).

To increase strength in the dual-phase family then typically the martensite fraction is increased, but this comes as a cost to ductility. This paper reports on the use of a Rapid Alloy Processing (RAP) facility to systematically investigate different composition and process parameter modifications designed to improve the ductility / strength balance. The RAP route involves the production of cast ingots (around 8kg), thermo-mechanically processing and annealling followed by mechanical property and microstructure chatacterisation. In this research work, RAP produced DP 800 steel has been benchmarked with respect to full scale commercial product to confirm upscalability and alloy / process modelling and predictions have been made to propose DP variants with enhanced properties. This paper reports on a number of DP variants based on process / composition parameter changes, within the range constrained by commercial production, of a) heating rate variation during the continuous annealing cycle to modify ferrite recrystallization and austenite nucleation locations to promote the formation of isolated martensite islands, b) controlled coiling to generate a ferrite-bainite hot rolled microstructure followed by cold rolling and annealing to modify austenite nucleation and subsequent martensite distribution, c) modified composition (variations in Nb and Mn) to refine ferrite grain size without increasing hot rolled product strength, and d) modified composition (increased vanadium) to give precipitate hardening.

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Multiscale homogenization of elastic properties in hypereutectoid steel

Author: Marko Vogric[1]

Co-author: Erwin Povoden-Karadeniz [2]

[1] *CDL-IPE, TU Wien*

[2] *TU Wien*

Corresponding Authors: erwin.povoden-karadeniz@tuwien.ac.at, marko.vogric@tuwien.ac.at

Hypereutectoid steels are of major importance for the railway and cable industry due to their good hardness and toughness. In-depth understanding of the link between their microstructure and mechanical properties presents therefore a significant industrial relevance. We have realized the multiscale modelling of macroscopic elastic properties of hypereutectoid steel based on the elastic properties of its constituent phases cementite and ferrite.

The presented model works through successive homogenization steps using the Eshelby matrix-inclusion approach and the definition of representative volume elements following quantitative microstructural criteria. Four different types of hypereutectoid steel microstructures are considered: lamellar or spheroidized globular pearlite, surrounded by a continuous or fragmented proeutectoid cementite film. Depending on the considered microstructure, various homogenization approaches

are used at the different homogenization steps: 1) Mori-Tanaka approach, describing matrix-inclusion composites – spheroidized pearlite in this study, 2) Classical self-consistent scheme, describing polycrystalline aggregates – here lamellar pearlite or combination of pearlite and fragmented cementite, and 3) Generalized self-consistent scheme, describing aggregates of phases surrounded by matrix films – here used for pearlite surrounded by a continuous cementite film.

The influence of microstructural parameters such as the pearlite colony size or the thickness of the cementite film on Young's and shear moduli and on the coefficients of the stiffness tensor is simulated, and the expansion of our multiscale approach to plasticity is considered. A proof of concept is obtained by comparing the calculated macroscopic elastic behavior of the material and experimental results from the literature.

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Prediction and optimization of the mechanical properties of Q&P Steel using process – property correlation via multiscale modelling

Authors: ILARIA IACONETA[1]; Sai Pavan Bhogireddy[2]; Vanessa Quaranta[3]

Co-authors: Denis Saraev [3]; Jerzy Gawad [3]; Maksim Moschenko [3]; Philippe Hernaut [3]; Xavier Cornet [3]

[1] *NLMK Belgium Holdings S.A.*

[2] *NLMK Belgium Holdings*

[3] *NLMK Group*

Corresponding Authors: d.saraev@eu.nlmk.com, i.iaconeta@eu.nlmk.com, m.moschenko@eu.nlmk.com, p.hernaut@eu.nlmk.com, sp.bhogireddy@eu.nlmk.com, v.quaranta@eu.nlmk.com, j.gawad@eu.nlmk.com, x.cornet@eu.nlmk.com

Quenching and partitioning (Q&P) process [1] is a heat treatment to produce steels with high strength and ductility. Chemical composition and process parameters control the final phase composition of a Q&P steel, thereby influencing its mechanical properties [2]. The objective of this work is to analyse computationally the effect of the composition and process parameters on the mechanical properties of Q&P steel.

The chemical composition is initially optimised in terms of alloying elements that strongly affect hardness. A set of most promising compositions are then used to evaluate the impact of process parameters by simulating different stages of the Q&P process. For the quenching process, the phases evolved at the end of the quenching process are predicted based on a coupled Finite Element- Thermo-kinetic approach. As a second step, the results of the quenching process are used as input for simulating the partitioning process. Here, a thermo-kinetic approach is employed to predict the microstructure evolution by varying parameters, such as prior austenite grain size, stop quenching temperature, and the partitioning time. The mechanical properties of the steel are estimated using the final phase fractions and their corresponding carbon contents obtained from the simulations.

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Unravelling the competing effects of chemical composition and grain size in affecting austenite stability in high carbon steels

Author: Adriel Wong[1]

Co-authors: Vikram Bedekar ; Enrique Galindo-Nava ; Rohit Voothaluru

[1] *University of Cambridge*

Corresponding Author: atcw2@cam.ac.uk

This work presents novel results on factors influencing austenite stability in carburised high carbon bearing steels. We have conducted a series of experimental and computational studies targeted at understanding these factors, including chemical composition, austenite grain size, stress/strain partitioning, and grain orientation.
In-situ neutron diffraction in steels with different nickel contents show that nickel increases austenite stability in the elastic regime but has no effect on the transformation rate; we also show that austenite grains with <200> direction parallel to the loading direction were the most susceptible to martensite transformation, and that these grains were most likely transformed into martensite with <211> direction parallel to the loading direction. Data from the neutron diffraction studies are coupled with a crystal plasticity finite element formulation to predict the mechanical responses of various multi-phase bearing steels, and estimate the stress/strain partitioning ratio as the austenite transforms into martensite.
Selected alloys were subjected to different heat treatments to study the relationship between the prior austenite grain size (PAGS) and the martensite start temperature (Ms); it is found that the Ms does not always increase with PAGS, as typically reported in literature for low/medium carbon steels, and that the resulting trends are due to competing effects of grain size and chemical composition. A limitation in the CPFE model is that the critical driving force for martensite transformation was originally assumed to vary linearly with the initial volume fraction of retained austenite. Predictions based on this method may be inaccurate if the austenite fraction falls outside the accepted range. Subsequently, the Ms, which is an indicator of austenite stability, is used to establish the critical driving force. Based on these results, correlations on the effect of chemical composition and PAGS towards austenite stability have been established.

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The Introduction of a Boundary Intensity Factor to Cellular Automata Modelling to Improve Prediction of Recrystallisation in Hot Rolled Steel

Author: Gabriel Ekoja[1]

Co-authors: Carl Slater [1]; Ces Bos [2]; Claire Davis [1]

[1] *WMG/University of Warwick*

[2] *Tata Steel Europe*

Corresponding Authors: claire.davis@warwick.ac.uk, kees.bos@tatasteeleurope.com, c.d.slater@warwick.ac.uk, g.ekoja@warwick.ac.uk

The mechanical properties of steels are influenced by their microstructure and particularly the grain size, with a small grain size giving high strength and toughness. A significant process for grain size control is recrystallisation during hot rolling, where the recrystallisation kinetics and recrystallised grain size are affected by the material's initial grain size, alloy content, temperature, strain and strain rate. It is desirable to be able to model the recrystallisation process to optimise hot rolling schedules and to provide a known microstructure for subsequent prediction of phase transformation on cooling.
A physically based 3D cellular automata model, developed for predicting recrystallisation kinetics and phase transformation in hot rolled steels, has been modified to give accurate predictions of recrystallised grain size distributions for different deformation strains and temperatures. Modification was required to correct for predicted temperature sensitivity for the recrystallised grain size that is not seen in experimental results.
In order to correctly model both the recrystallisation kinetics and resultant grain size distribution,

accurate representation of recrystallisation nucleation and nucleus growth to critical size are essential and these are driven by the local conditions. This paper reports on the implementation of a boundary intensity factor (BIF), giving a higher dislocation density at the grain boundary than grain interior, to drive the recrystallisation nucleation event and subsequent growth to exceed the critical nucleus. The concept of a BIF is supported by EBSD misorientation data, related to dislocation density, on deformed samples, which have been used to define the boundary intensity factor magnitude and boundary width. The effect of the BIF on the recrystallisation kinetics and recrystallised grain size distribution has been assessed using a model Fe-30Ni steel, with a starting grain size of 160 μm, deformed at a strain of 0.3 at 900 ℃ and 950℃.

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From ladle to wire: Integration of calphad-based design and traditional through process modelling approaches

Author: Johannes Kreyca[1]

Co-authors: Ernst Kozeschnik [2]; Matthew Galler [3]; Sabine Zamberger [1]

[1] *voestalpine Forschungsservicegesellschaft Donawitz GmbH*

[2] *Institute of Materials Science and Engineering, TU Wien*

[3] *voestalpine Wire Rod Austria GmbH*

Corresponding Authors: matthew.galler@voestalpine.com, ernst.kozeschnik@tuwien.ac.at, johannes.kreyca@voestalpine.com, sabine.zamberger@voestalpine.com

Johannes Kreyca*, Sabine Zamberger – voestalpine Forschungsservicegesellschaft Donawitz GmbH, Kerpelystr. 199, A-8700, Austria
Matthew Galler – voestalpine Wire Rod Austria GmbH, Drahtstraße 1
8792 St. Peter-Freienstein, Austria
Ernst Kozeschnik – TU Wien, Getreidemarkt 9, 1060 Wien, Austria

*Corresponding: Johannes.kreyca@voestalpine.com

ABSTRACT

The combination of traditional semi-empirical through-process modelling techniques covering temperature evolution during production, recrystallisation and grain growth, and a sound thermodynamic framework (e.g. CALPHAD) is necessary for the accurate prediction of actual production processes and mechanical properties of the final product. In this work, an integrated approach, comprising the production steps of continuous casting and wire rolling, is developed and demonstrated on the basis of the wire production process at voestalpine. The essential sub models are presented and areas of recent research activity are detailed. Special emphasis is laid upon the matrix phase transformation from austenite to low temperature microstructures such as ferrite/pearlite/bainite/martensite or a mixture of these.

Keywords: through process modelling, calphad, matrix phase transformation, wire rolling