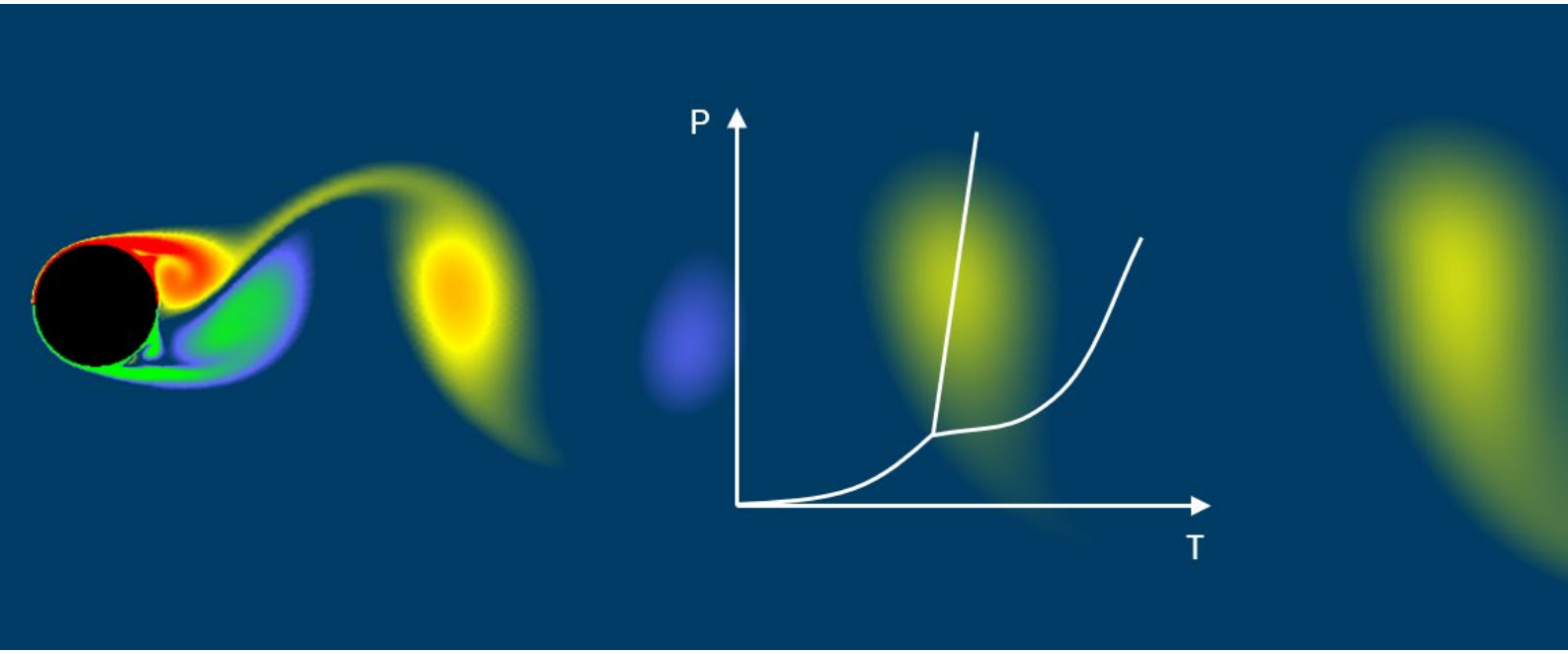
CFD 2024



15th International Conference on Industrial Applications of Computational Fluid Dynamics

Trondheim, June 11-13, 2024

Book of abstracts

SINTEF

Preface

This book comprises all accepted abstracts for the *15th International Conference on Industrial Applications of Computational Fluid Dynamics* is the 15th conference in this series of conferences initiated by CSIRO in 1997. CSIRO have hosted the conference every 3 years in Melbourne, Australia, as the *International Conference on CFD in the Minerals and Process Industries*. In 2005 SINTEF joined in as organizer and hosted conferences in Trondheim, Norway, named International Conference on Computational Fluid Dynamics In the Oil & Gas, Metallurgical and Process Industries. For the 15th conference the name was modified to reflect the challenges of the industry related to the green shift.

As can be seen from the program many CFD scientists apply their research related to the green shift. Green shift topics covered include water electrolysis, carbon capture, hydrogen, biofuels, reduced emissions and more. Advances in these technologies can be accelerated by improved CFD models and better understanding of the underlying physics of mass transfer, turbulence, reaction kinetics and other phenomena which is implemented in flow models. CFD is a generic technology that has applications in any process and where knowledge transfer between application areas can open new possibilities. The conference is organized with the objective to share knowledge on these topics, explore applications of CFD to new industrial challenges, and help make the CFD models more accurate and efficient.

Organizing committee:

Stein Tore Johansen, SINTEF
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Keynote speakers

Keynote: Learnings from 40 year of working with CFD - Stein Tore Johansen

Stein Tore Johansen
SINTEF Industry

CFD was mostly not known 40 years ago, and slide ruler and digital calculators were mostly used in engineering calculations. As digital computers became more powerful, together with software and numerical techniques, CFD rapidly offered new possibilities.

In this talk we will look briefly into the history of CFD, and how this developed in the SINTEF Flow Technology group. We will see that CFD is much more than just applying some CFD software. We look at CFD as one of many tool-box elements that we need to solve challenges. The user of the tool is the key element to successful results. As computers have evolved it is now possible to run simulations with billions of grid nodes. Does this indicate that we can do more accurate simulations and the need for models inside the CFD simulations will disappear? The knowledge needed to solve problems goes far beyond the CFD tool itself. We therefore look into some methods that should be considered in multiphase applications. Often, CFD may contribute with key input to simpler, pragmatic models, which may be used in digital twins or other type on models to analyze and optimize system behavior.

We finally discuss the possibilities and challenges with working with CFD. We have recently observed the new hype on artificial intelligence (AI). Will AI make CFD engineers superfluous in the future?

Keynote: Multiphysics aspects of the gas bubble evolution during water electrolysis - Gerd Mutschke

Gerd Mutschke
Helmholtz-Zentrum Dresden Rossendorf, Institute of Fluid Dynamics

Water electrolysis offers a way to produce hydrogen from renewable electrical energy. However, the details of gas evolution have a major impact on the energy efficiency of the process, as gas bubbles growing at the electrodes or floating in the electrolyte cause overvoltages and losses. It is therefore desirable to improve our understanding of gas evolution in order to further improve electrolysis processes. Gas evolution is influenced by a number of aspects, including electrolyte supersaturation and constitution, nucleation and wetting at the electrode, electrolyte flow, interfacial flow and capillary effects, coalescence with neighboring gas bubbles as well as temperature and electric fields. The presentation will summarize the knowledge gained in recent years, based on own work and recent literature.

Keynote: Towards manufacturing digital twins using GPU based physics simulations: a particles perspective - Nicolin Govender

Nicolin Govender
University of Johannesburg, Mechanical Engineering (South Africa) and Blaze Computing LTD (London, UK)

GPU computing is enabling groundbreaking innovation and enhanced efficiencies for a number of manufacturing industries. From digital twins that enable production automation and optimization, to finding unique patterns in material combinations that can lead to new formulations, simulation is transforming what's possible. Although significant success has been achieved with data-driven digital twins, inferences are limited when the underlying physics is complicated. Physics-based digital twins on the other hand offer far richer inferences but require access to verified and validated solvers and models that are computationally tractable. While there has been progress in applying AI to accelerate numerical methods themselves, industrial materials are complex with a mixture of fluid and solids for which there are no closed form solutions. In this talk progress towards physics based simulations of particulate materials using GPU computing will be presented along with a technical discussion on the art of utilizing GPUs for other solution methods ending with an outlook of the potential of AI for industrial simulations.

Keynote: Fast and simplified models to solve complex problems - Thomas Lichtenegger

Thomas Lichtenegger
Department of Particulate Flow Modelling, Johannes Kepler University Linz

Many fluid-mechanical systems exhibit spatio-temporal multi-scale dynamics. Detailed methods that resolve the smallest and shortest scales cannot reach the larger and longer ones. Phenomenological models, on the other hand, are connected to a larger degree of uncertainty. To overcome these limitations, hybrid models combine knowledge of the laws of physics with observational data to include mesoscopic information. Since high-fidelity data for large-scale flows are expensive to obtain, we developed the hybrid simulation technique “recurrence CFD” [1] that approximates the evolution of dynamic systems with relatively little data in a pragmatic fashion. For a given flow field, we determine the most similar reference state in a precomputed database and apply the corresponding evolution over a large time step. Upon iteration, long time series can be constructed from this reduced basis of flow states and slow transport processes simulated with little costs. Application examples include long-term investigations of (i) heat transfer in fluidized beds [2], (ii) heterogeneous reactions in moving beds [3] and (iii) species transport in turbulent flows [4]. In these cases, the processes of interest evolve over much longer time scales than those characteristic for the rapid dynamics of these systems. Finally, an outlook on our envisioned future research is given, which will focus on the generalizability to off-database conditions. To this end, a propagator formalism is introduced to systematically account for changes in the underlying dynamics [5].

[1] Lichtenegger T., and Pirker S. “Recurrence CFD – a novel approach to simulate multiphase flows with strongly separated time scales.” Chem. Eng. Sci. 153 (2016): 394-410. [2] Lichtenegger T., et al. “Dynamics and long-time behavior of gas–solid flows on recurrent-transient backgrounds.” Chem. Eng. J. 364 (2019): 562-577.
[3] Lichtenegger T., and Pirker S.. “Fast long-term simulations of hot, reacting, moving particle beds with a melting zone.” Chem. Eng. Sci. 283 (2024): 119402.
[4] Pirker S., and Lichtenegger T. “Efficient time-extrapolation of single-and multiphase simulations by transport based recurrence CFD (rCFD).” Chem. Eng. Sci. 188 (2018): 65-83. [5] Lichtenegger T. “Data-assisted, physics-informed propagators for recurrent flows.” Phys. Rev. Fluids 9.2 (2024): 024401.

Keynote: Mass transfer from bubbles: how to model realistic systems - Maike Baltussen

Maike Baltussen
TU Eindhoven

Modelling the mass transfer from bubbles to the liquid is challenging as the Schmidt numbers in real systems are generally in the order of 100-10.000. These high Schmidt numbers indicate that the mass transfer boundary layer is significantly thinner than the fluid dynamic boundary layer, i.e. the resolution requirement for the mass transfer is significantly higher than the resolution for the fluid dynamics. This limits the possibilities to simulate the mass transfer in realistic gas-liquid systems. The high gradients, which require the high resolution, are generally obtained in close vicinity of the gas-liquid surface. In this contribution, a method will be presented, which approximates the high gradients near the gas-liquid interface and thereby reduces the resolution requirements for the mass transfer. The method will be verified with analytical solutions in the limits of Stokes flow and potential flow. In addition, the method will be validated against high resolution simulations.

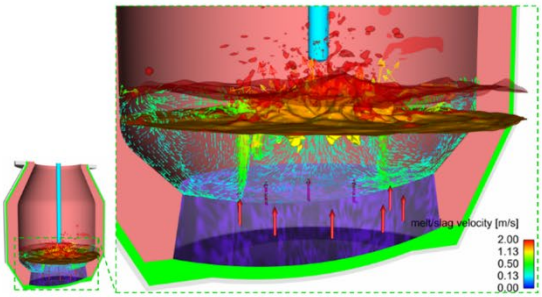
After validation and verification, the method will be used to determine the mass transfer from single bubbles in an infinite medium. The results will be compared to other numerical simulations and experimental correlations obtained from literature showing that the method is very well suited to simulate the mass transfer from bubbles in realistic gas-liquid systems.

Keynote: Challenges and solutions of CFD simulations for the steel and non-ferrous metals industry - Hans-Jürgen Odenthal

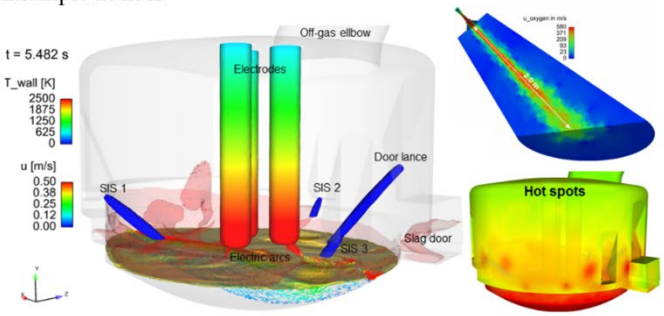
Hans-Jürgen Odenthal
SMS group GmbH, Am SMS Campus 1, 41069 Mönchengladbach, Germany

Worldwide, the steel industry and the non-ferrous metals industry follow a decarburization strategy to meet the green house gas emission reduction targets. Regardless of which route is used for the respective product - in the case of steel, for example, the route via the blast furnace-converter, the direct reduction plant or the electric arc furnace – the metallurgical aggregates can always be modified and improved. As a result of the enormous increase in computing power and progress of solution algorithms in recent years, it is possible to simulate fluid flow and thermal phenomena which could not yet been calculated so far; CFD provides insights into plant areas that cannot be observed or measured directly due to the extreme boundary conditions prevailing there. The presentation focuses on typical questions that the engineer is confronted within his daily work and illustrates the huge potential of CFD. Both, the difficulties in modelling and the practical solutions from the point of view of the plant builder and the analogue operator are discussed, but also the limits of today's simulation techniques are briefly dealt. The following metallurgical devices are discussed: - Basic oxygen furnace (BOF): Combined blowing converter with oxygen top blowing and inert gas bottom stirring. -Electric arc furnace (EAF): Supersonic oxygen jets and how they affect the melt/slag domain. -Steelmaking ladle: Bottom stirring and mixing effects in large-sized ladles. -Peirce-Smith converter: Copper matte refinement using convergent-divergent nozzles. -Vacuum inert gas atomization (VIGA): Physical and numerical simulation of the close-coupled atomization process in order to predict the metal particle size distribution. -Hybrid burner/injector: Replacement of natural gas with hydrogen in the EAF burner

Example 1: BOF converter



Example 2: EAF



AI/ML applications in CFD

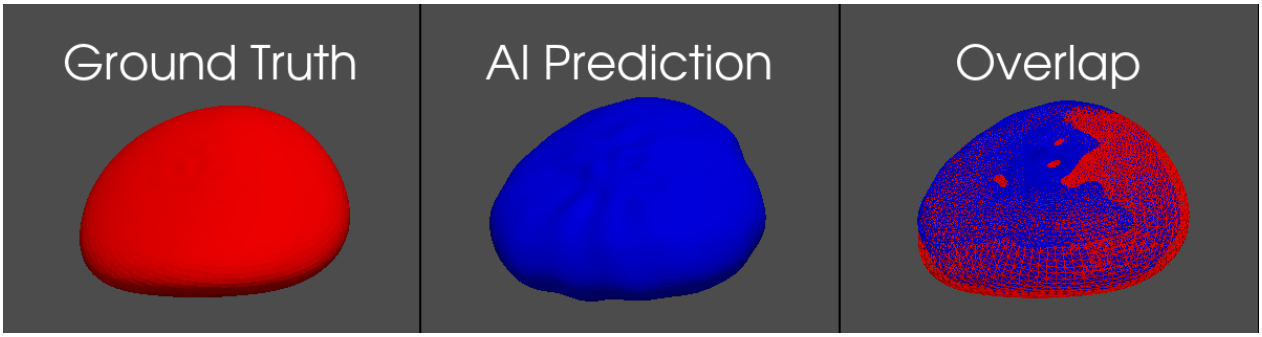
3D Bubble Shape Reconstruction from 2D Imagery Using CNNs

Ir. D.R. Orij*, Dr. Ir. I. Roghair, Prof. Dr. Ir. M. van Sint Annaland
TU Eindhoven

Session: AI/ML applications in CFD

The possibility to predict the 3D shape of air bubbles in air-water bubbly flows from 2D imagery contributes to accurate information on mass transfer properties. Achieving this goal is reached using Convolutional Neural Networks (CNNs). Trained networks accurately convert 2D images of single gas bubbles into the 3D shapes. The 3D shape output is represented as a weighted sum of spherical harmonic functions. Spherical harmonics are used for grid independence and dimensionality reduction.

The CNN input was generated by recreating a 20x20x100 cm gas-liquid bubble column in 3D software Blender. With Blender, images could be rendered for each of the 10.000 3D bubbles acquired from a front-tracking dataset. When comparing the renders with reference images an invisible edge around the bubble was discovered in both sets. The edge became visible when bubbles overlapped, or the lighting was dimmed. The cause is light reflection and refraction and was validated experimentally. This proof increases the validity of the input images used for training the CNNs. The results of the CNNs are accurate but not suitable for real-life applications yet. Before application, the training database should be more varied and noise handling must be improved.



Integration of Deep Learning and 3D CFD-PBM Model for Characterizing Mg(OH)2 Precipitation

Antonello Raponi*, Daniele Marchisio
Politecnico di Torino

Session: AI/ML applications in CFD

Contemporary research in reactive crystallization processes involves a multitude of phenomena spanning various scales. Notably, supersaturation is generated at the micro-scale due to chemical reactions. This heightened supersaturation level directly triggers primary nucleation and molecular growth (molecular processes) and indirectly leads to irreversible agglomeration (a secondary process). Modelling these phenomena requires assuming a functional form (kernel) and tuning the fitting parameters appropriately (eight in this contribution).

The most prevalent methodology for simplified models involves executing a multivariate optimization routine that identifies the optimal parameter set by comparing model predictions with experimental targets (e.g., characteristic sizes from Number Size Distributions). A randomly chosen initial point (or a swarm of initial points) is subjected to a local minimum search through an optimization method (such as conjugate gradient).

However, a simplified eight-parameter model reveals a plethora of local minima, making the optimization problem highly dependent on the initial candidate and, on the other hand, it becomes practically impossible to perform for 3D models. In this contribution, the authors propose an innovative, quick-responsive procedure that provides a data-driven model for computationally expensive 3D models employing Neural Networks. Initially, a Computational Fluid Dynamics (CFD) - Population Balance Model (PBM) describing the precipitation in a T-mixer (Figure 1) was employed to generate the numerical dataset. Solving partial differential equations, the CFD-PBM model associates parameter sets and operational conditions (e.g., initial concentrations of reactants) with corresponding sizes.

Subsequently, a Deep Learning Neural Network (DLNN) was trained using the dataset above, with the input-output order reversed: sizes and concentrations were given as input, and the parameter set was the output. Experimental sizes at five concentrations were then provided to the trained DLNN, and the predicted mean parameter set was tested with the 3D model. The resulting set successfully reproduced the experimental data to infer parameters and predict diameters in a Y-mixer. Furthermore, uncertainty in parameters was quantified and depicted in Figure 2.

This innovative approach attests to the effectiveness of integrating 3D CFD-PBM models and deep learning techniques to precisely and responsively characterize reactive crystallization processes. It paves the way for a deeper understanding and more optimized design of reactive crystallization processes.

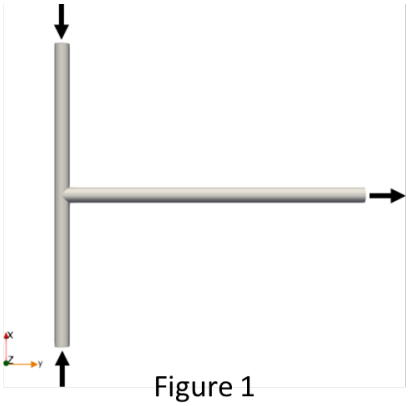


Figure 1

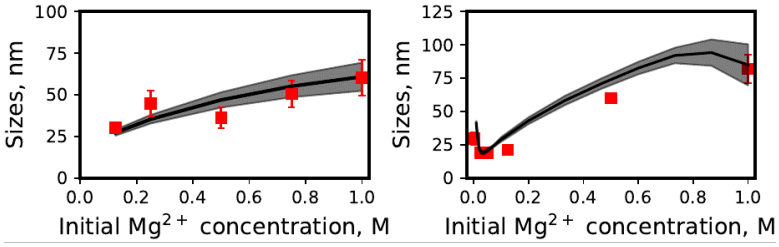


Figure 2

Hydrodynamics Improvement of a Pelletizer Chamber Using Computational Fluid Dynamics

Thiago Roberto Almeida, Alexandre Feoli Anele, Almir Guilherme Siqueira Lopes Ritta*
Braskem, Global Process Technology

Session: AI/ML applications in CFD

In underwater pelletizer, different factors in the process can impact the pellet quality and the good operability. Coming from a previous stage, under very high temperature and pressure conditions, molten thermoplastic is forced to pass through a die with numerous holes of circular profile. When the molten thermoplastic passes through the die holes it is cut by a set of knives attached to a rotatory piece (a.k.a. knives-holder). Immediately the pellets get in contact with water and solidify. After, water and pellets are conveyed to a drier, where the pellets are separated from the water stream. The water is pumped back to the pelletizer chamber, in a close circuit. Poor water hydrodynamics in the interface between the die and the knives-holder front face (where the set of knives are attached) leads to an insufficient temperature drop to ensure the pellet solidification and its proper formation, causing it to stick to the knives, to the knives-holder or to each other's, forming agglomerates and/or die holes plug. Such issues, consequently, lead to maintenance stops and/or equipment breakdown. Using Computational Fluid Dynamics (CFD), the present work provides a consistent analysis of the implementation of an apparatus, called Diffuser, to improve the hydrodynamics within the underwater pelletizer. The Diffuser main function, from the process perspective, is to drive a large amount of process cooling water against the interface between the die and the knives-holder front face. More water in this region tends to cool the pellet more quickly. In addition, the Diffuser promotes a shorter water residence time in the cutting and rotational regions. Consequently, the pellets, driving by the water, leave those regions faster, minimizing the probability of touch each other's while are with its surface cooling down. Using a transient single-phase Eulerian approach, the work focused in evaluate the most suitable Diffuser geometry align with the best process conditions possible to use. To evaluate the performance of each design, the amount of water passing through the pumping holes and the water residence time within the cutting and rotational regions were defined as variables of interest. The results showed that the amount of water, when compared the case with and without the Diffuser, jumps from 59% to 77%. In terms of local residence time, at the rotational and cutting regions, the numbers are good as well. The local mean water residence time is reduced by two seconds, meaning that the water and pellets leave those regions faster than the case without the use of Diffuser. Also, the study shows that optimal conditions can be reached for the cases evaluated, such as increase the rotation in 16% and reducing the number of knives in 17%. Playing with those two variables we can increase the so called 'pumping effect', which is the effect that leads more water to the interface of the die-plate and the front face of knives-holder.

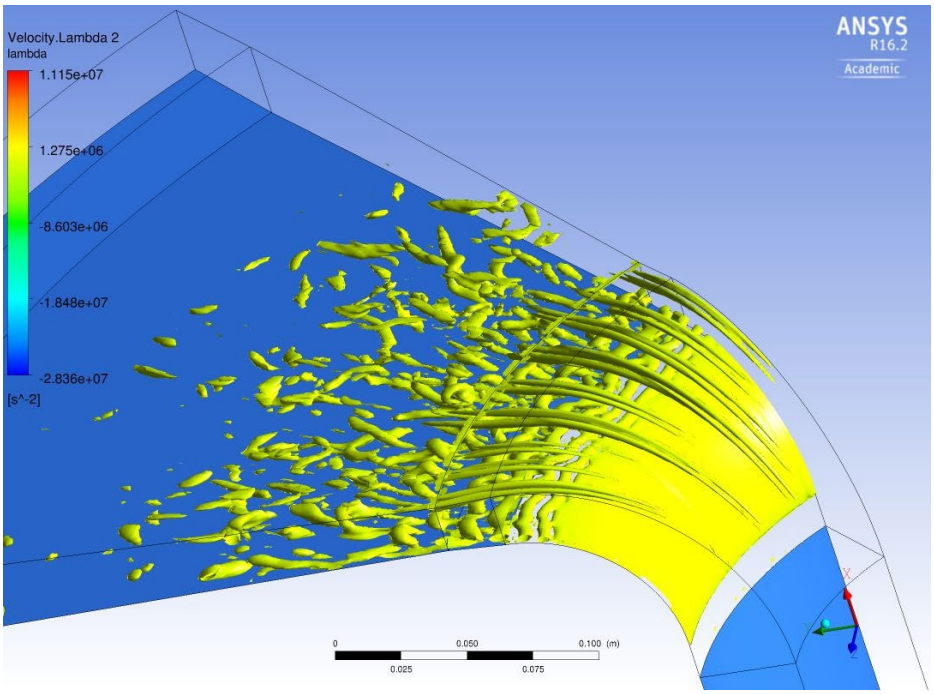
Applied CFD

LES study and comparison with experiments of an axial-radial difuser configuration

Are J. Simonsen
SINTEF Industry

Session: Applied CFD

The current work aims the flow in radial diffuser following an axial radial bend. This is a typical configuration turbo machinery as flow retardation is needed at the same time as available axial space is limited. Although a simple geometry this configuration represents several complex flow phenomena that are challenging for numerical solvers such as flow in a bend and adverse pressure gradient. The current study aims to quantify the agreement between experimental data and a high fidelity numerical model using a spectral based numerical solver, SEMTEX. The results can be used to improve and evaluate simpler and more cost effective RANS models for future design purposes.

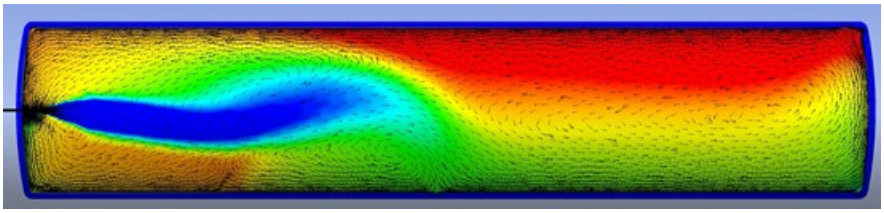


CFD simulation of the filling of a high-pressure hydrogen tank

Marcer Richard
PRINCIPIA, EDF, EIFER

Session: Applied CFD

To decarbonize the mobility sector, hydrogen is a relevant solution that continues to develop, particularly for heavy transport (trucks, trains, etc.). The speed at which hydrogen gas tanks in vehicles powered by fuel cells can be filled is a commercial and industrial challenge for manufacturers and operators of hydrogen refilling stations (HRS). For safety reasons, the heating kinetics of the gases due to their compression during the filling phase must be controlled so that the temperatures in the tanks remain at acceptable levels with regards to the mechanical strength of the structures. Hydrogen tanks are usually designed for 350 or 700 bar, making this challenge even more complex than for natural gas tanks. In addition, for operating constraints reasons, the duration of this filling phase must also be optimized. The filling speed, the associated heating of the compressed gases and the cooling of the gases by the cold filling jet are therefore key points of the issue. The pre-cooling of the injected hydrogen (usually between -40°C and 0°C) is necessary for reducing as much as possible the filling duration. Nevertheless, this aspect has an important economic impact on the cost of the HRS, and better understanding what is the optimal pre-cooled temperature is also a key aspect. Manufacturers and operators of hydrogen filling stations have simplified models (0D for the gas volume and 1D for the wall layers of the tank) whose set of physical parameters is based on manufacturer data or feedback. These models can still be improved because they do not reproduce all cases of interest, in particular cases for which the temperature field is not homogeneous. In this scenario, the difference between the mean temperature and the minimum and maximum temperatures should be available to complete the safety assessment. A 3D CFD model theoretically allows to take into account all the physical processes involved. More specifically, it provides the local dynamic/thermal fields, thus highlighting possible stratification phenomenon during the filling phase of the tank. The CFD model is based on a RANS approach with a two-equations model including buoyancy effects. A real gas (RK) state of the law is used, well adapted for high pressure compressible gas. Thermal fluid / solid coupling allows to consider thermal transfers between the hydrogen flow, and the liner / wrapper structure layers. Sensitivity studies are carried out especially on turbulence models (k-□ standard and Realizable), boundary conditions for the hydrogen filling (imposed pressure or flow rate) and the nozzle shape (mono or bi-nozzles). Overall, results show that after a stage of progressive and homogeneous increase of the hydrogen temperature and pressure during the filling, thermal fluctuations appear systematically with the development of (high pressure) flow vortices in the tank, eventually enhancing stratification processes.



CFD of a Flow Conditioning Unit

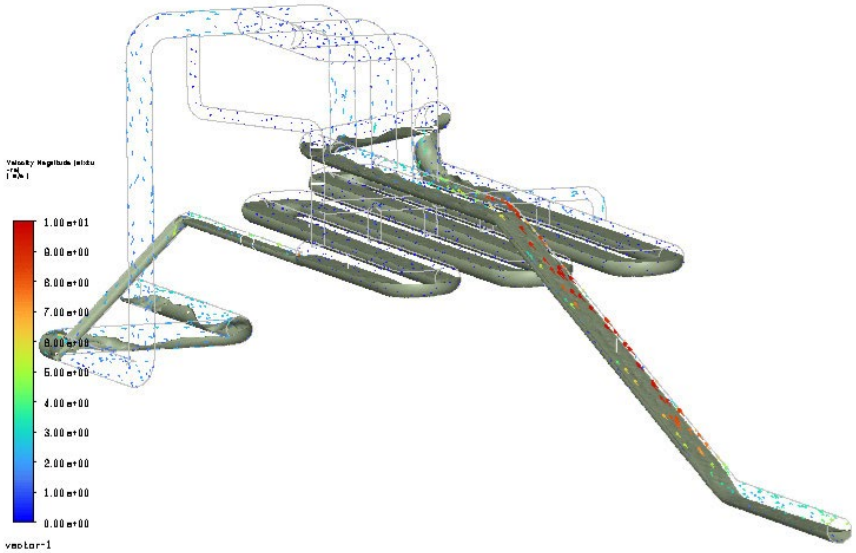
Pablo Matias Dupuy, Netaji Ravi Kiran Kesana
Equinor ASA

Session: Applied CFD

An open challenge related to subsea well compression is avoiding surges and slugs into a wet gas compressor station. A Flow Conditioning Unit (FCU) helps to dampen the sudden changes that are caused by variations in multiphase flow patterns. Computational Fluid Dynamics (CFD) transient simulations are performed on a high-performance computing cloud to verify and improve the design of the FCU in terms of sizing and liquid handling capacity. The simulations are performed using the Volume of Fluid (VOF) method, employing adaptive meshing approach to simulate complex gas liquid dynamics under various flow conditions. Ultimately, these simulations lead to optimized design of the FCU unit and its test facility. Furthermore, multiphase CFD simulations are further utilized during large scale experiments for better understanding of observed flow behavior.

Some of the phenomena to be shown are large liquid entrainment in gas harp and the presence of gas in liquid draining lines.

This work shares details on the CFD simulations performed, including the mesh size development, wall-time required, and post-processing tools utilized. However, the focus is to show how an industrial actor leverages CFD tools to iterate on expensive testing infrastructure, thereby reducing risk and cost.

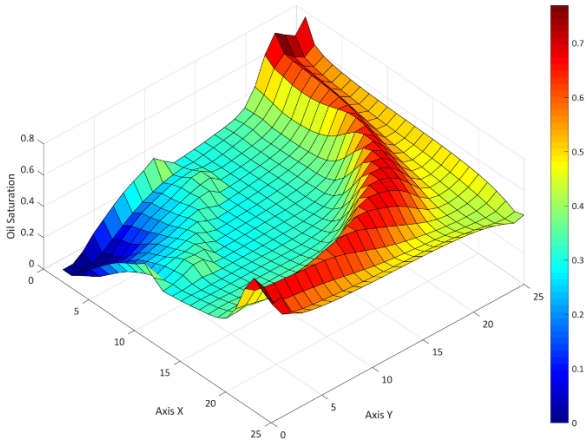


Surfactant-Polymer Interactions in a Combined Enhanced Oil Recovery Flooding

Pablo Druetta
Department of Chemical Engineering, Faculty of Science and Engineering, University of Groningen

Session: Applied CFD

The use of standard Enhanced Oil Recovery (EOR) techniques allows improving the recovery factors after traditional waterflooding processes. Chemical EOR methods comprise alkalis, surfactant or polymers, which modify different properties of fluids and/or rock in order to mobilize the remaining oil. A series of combined chemical flooding techniques has been developed in order to maximize the performance by using the combined properties of the chemical slugs. In the present research, a new model is developed to study a surfactant-polymer flooding. A novel compositional simulator is presented based on a two-phase, five-component system (aqueous and organic phases with water, petroleum, polymer, surfactant and salt) for a 2D reservoir model. Polymer and surfactant together affect each other interfacial and rheological properties as well as the adsorption rates. This is a phenomenon known as Surfactant-Polymer Interaction (SPI). New numerical models of these interactions show their effect on the recovery processes. The analysis of the chemical injection strategy was also included in the scope of this research. The latter plays a major role in the efficiency of the recovery process, including both the order and the time gap between the injection of each chemical slug. When the latter is increased, the combined flooding tends to behave as two separate chemical EOR processes. Best results were found when both slugs are injected overlapped, with the polymer in first place which improves the sweeping efficiency of the viscous oil. This also hinders the surfactant adsorption rates. This is because the latter is more sensitive to this phenomenon than the polymer. This novel simulator can be then used to study different chemical combinations and their injection procedure in 2D fields to optimize the EOR process.



Bubbly flow

Mass transfer in bubbly flows – Different configurations and varying bubble composition

Roland Rzehak, Haris Khan
Helmholtz-Zentrum Dresden - Rossendorf, Institute of Fluid Dynamics

Session: Bubbly flow

Mass transfer in bubbly flows is important in many engineering applications. Simulation of such processes on technical scales is feasible by the Euler-Euler two-fluid model, which relies on suitable closure relations describing interfacial exchange processes. In comparison with the pure fluid dynamics of bubbly flows however, modeling and simulation of bubbly flows including mass transfer is significantly less developed. In particular, previous simulation studies have focused almost exclusively on absorption in bubble columns without liquid flow. However, recent experiments on single bubbles suggest that the simultaneous desorption of dissolved inert gases in general cannot be neglected. This requires consideration of changing bubble composition in addition to bubble size. In addition imposing a liquid flow allows a steady state to be achieved also when the mass transfer is accompanied by a chemical reaction, which greatly simplifies the analysis of reactive mass transfer problems. Therefore, the present study first considers a larger variety of conditions including desorption and counter-current (downward) flow for which experimental data for a first comparison are available from the literature. Then a simple sandbox test case is used to illustrate how the bubble composition may be tracked as a secondary property in addition to bubble size within a population balance framework. An analytical solution can be found for this test case, which facilitates verification of the software implementation of the discretized population balance equation. In this way, further building blocks for a more complete numerical treatment of mass transfer in bubbly flows are now available. A thorough validation for realistic applications however requires yet further experimental work to provide suitable measurement data.

On a dissolving bubble plume from subsea release of CO2

Jan Erik Olsen*, Paal Skjetne
SINTEF Industry

Session: Bubbly flow

In the value chain for CCS pipeline transport of CO2 and storage of CO2 underneath the ocean floor are key aspects. Failures in these can cause a subsea release of CO2 which will result in a bubble plume of CO2 rising to the surface. This affects the pH levels in the ocean and potentially poses a safety concern if released into the atmosphere. A mathematical model assessing the bubble plume will be presented. It accounts for mass transfer into the ocean since CO2 is very soluble. It also accounts for evaporation of CO2 droplets since the phase diagram dictates that for most scenarios the release will be a mixture of gas and liquid.

Single bubble dynamics under the influence of Marangoni force

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Mahdi Saeedipour, Department of Particulate Flow Modelling, Johannes Kepler University Linz

Mark W. Hlawitschka, Institute of Process Engineering, Johannes Kepler University Linz

Session: Bubbly flow

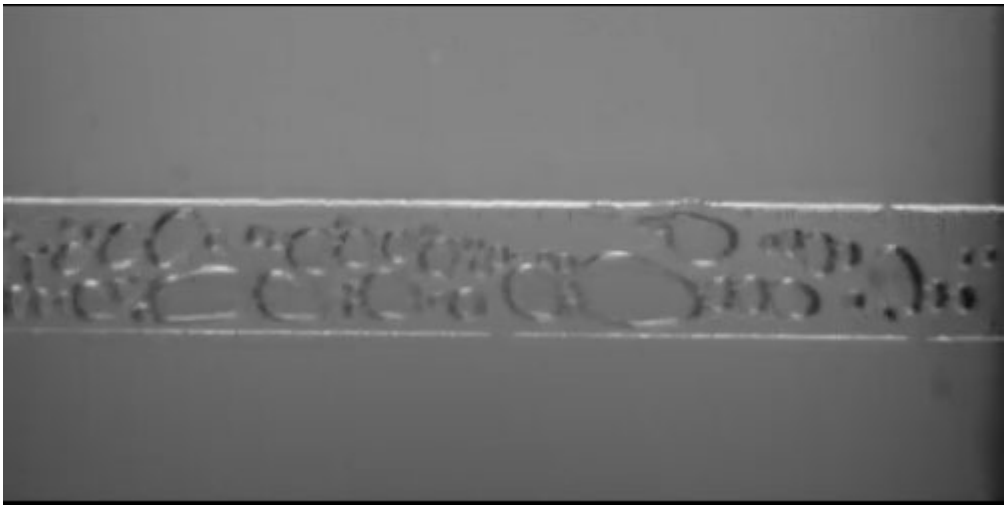
The accurate prediction of mass, momentum, and heat transfer across the liquid-gas interface is a fundamental concern in a great variety of industrial applications. Thereby, concentration gradients occurring in hydrometallurgy, chemical or biological industry towards the complex hydrodynamics are not fully understood, but play a major role for the final design. To overcome this, in-depth analysis for single bubble hydrodynamics is required. The Marangoni effect assumes significance in bubbly flows when temperature or concentration gradients exist in the domain. This study investigates the hydrodynamics of single bubbles under the influence of the Marangoni force induced by stratified fields of dissolved sugar, providing a numerical framework to examine these phenomena. A lab-scale bubble column and high-speed imaging were utilized to analyze the bubble behavior. An OpenFOAM-based geometric volume of fluid solver is extended by incorporating the solutocapillary Marangoni effect and a passive scalar transport equation for the sugar concertation was solved. To reproduce the sugar concentration gradient field in water, the passive scalar field of c is initialized with a linear rate in the vertical direction, and the physical properties of the continuous phase are accordingly linked to the concentration value. It is worth mentioning that an OpenFOAM function object called phaseScalarTransport is adopted to prevent the penetration of contamination into the bubble during the simulation, i.e., the contamination field is only transported inside the water phase. The dependency of surface tension on the concentration (β) is a unique value for each system, which is equal to 0.0038 in the case of an aqueous sugar solution ($c \leq 0.4$ w/w). To obtain an insight into the influence of β on the bubble behavior with the aid of CFD, three different values were assigned to this parameter (β=0.2,0.02,0.0038 and 0); among which, the 0.2, 0.02 and zero values are artificial values. In order to exclusively study the influence of Marangoni force on the bubble behavior, the artificial cases of β=0, in which the gradient of concentration is applied but the Marangoni force is set to zero manually, was considered. Results reveal that small bubbles entering regions of elevated sugar concentration experience deceleration, transitioning into linear paths, while those departing high sugar concentration areas exhibit fluctuation and meandering. Furthermore, the concentration gradient leads larger bubbles to meander throughout the entire column, without a notable increase in their velocity. The intensity of these behaviors is governed by the magnitude of the Marangoni force. In fact, regarding the influence of β magnitude, this study reveals that it increases the aspect ratio of the bubble throughout the column and enhances the zigzag behavior in cases with positive concentration gradients where impurity concentration is below 20%w/w. Consequently, it elevates the velocity when the impurity concentration exceeds 20%w/w. Therefore, impurities causing a substantial increase in surface tension result in higher average bubble velocities, potentially unfavorable for prolonging contact time between the two phases.

Multiphase flow dynamics in mini-channels used in water electrolysis

Paul Roger Leinan*, Paal Skjetne, Loïc Duffo
SINTEF Industry

Session: Bubbly flow

Objectives and Scope: Broadly water electrolysis can be divided into alkaline electrolysers (AEL), proton exchange membrane (PEM) electrolysers, and solid oxide electrolysers (SOE). All water electrolysers are exothermic and consume water and electricity. As unit costs are high it is imperative that cells operate as efficiently as possible. Thermal management is usually over-designed as thermal degradation will rapidly reduce unit performance. Due to this flow field design for PEM electrolysers in particular focus on achieving low pressure drops. Due to constraints such as e.g., material properties, material consumption, size and geometry, manufacturing tolerances to name only a few challenges, little attention has historically been focused on optimal flow field design. Popular designs found in the literature can have twice as much flow [in ml/s] in certain parts of the cell compared to other parts of the cell. PEM cell sizes are typically of the order 10 cm. Thus, flow paths are relatively short, but have very large aspect ratios with channel width and height being of the order 1 mm. At the entrance to these channels pure water is pumped in, and reactants (hydrogen or oxygen gas) enter the flow channel through the gas diffusion layer (GDL. Thus, the holdup in the channel is not constant and the resulting flow is an accelerating and developing multiphase flow. Consequently, pressure drop correlations for fully developed multiphase flow may not be suitable. This makes it questionable to apply single phase design principles when optimizing flow fields for PEM cells. We investigate experimentally and numerically the multiphase flow in mini channels with continuous gas injection along the channel length. Methods: To experimental investigating multiphase pressure drop and phase distribution in a relevant electrolyser cell geometry, a flow cell with a single mini channel was fabricated using acrylic pressure lamination technique. The flow channel (0.5 x 1.5 mm cross section) had small holes at regular intervals along the bottom wall of the channel to simulate the porous structure of a GDL. Four pressure sensors were used to measure the pressure drop from inlet to the start of the flow channel, across it and in the outlet section. High speed video recordings were obtained and analysed using a novel PIV algorithm. Simulations were performed using a Eulerian-Eulerian multiphase model in a commercial CFD code. Results and Observations: A matrix of test points for the air and water flow velocity was chosen based on relevant scenarios for electrolysers, i.e. superficial velocities (air and liquid) from ~0.1 to 1m/s and stochiometric ratios 125, 250 and 500. In total 18 flow conditions were tested, with multiple repeated experiments. Accelerating flow was observed in the flow channel and mainly two flow remiges, bubbly, and Taylor bubble flow. In the Taylor bubble flow interesting bubble coalescence dynamics was observed. The pressure drops were compared to available simplified known models in the literature.Simulation showed good comparison with selected experiments both with respect to predicting pressure drop and void distribution.



Electrochemical systems

Solutal Marangoni flow around a growing hydrogen bubble: An immersed boundary simulation study

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Session: Electrochemical systems

Improving the efficiency of industrial water electrolysis for hydrogen production is a critical aspect of energy transition. During water electrolysis, hydrogen is produced at the cathode, resulting in the formation of bubbles. The reaction creates a gradient of the electrolyte concentration that causes local surface tension variations along the bubble surfaces. This leads to a shear stress that causes convection, which is called the solutal Marangoni effect [1]. Marangoni convection can affect the gas evolution process during water electrolysis by improving the mass transfer [2]. In this study, we simulate solutal Marangoni flow occurring near a single hydrogen bubble attached to an electrode in an alkaline electrolyte in a narrow channel with a relatively high current density. Furthermore, we investigate the effect of Marangoni flow on the velocity field, bubble growth rate, species concentration, potential, and (local) current density. To solve the governing equations including the Navier-Stokes equations, the mass transfer equations, and the potential equation for the tertiary current density, we use a sharp interface immersed boundary method. An elegant method for applying the Marangoni stress boundary condition at the bubble interface using the immersed boundary method is proposed and implemented. We find a significant Marangoni flow. Figure 1 compares the velocity fields for the case with(out) Marangoni flow at the x-y plane in the center of the computational domain when the bubble grows to a radius of 25 µm. In the case of no Marangoni flow, the maximum fluid velocity value is 2.4 mm/s, while in Marangoni flow, it is 20.2 mm/s.

[1] S. Park, L. Liu, C. Demirkır , O. van der Heijden , D. Lohse, D. Krug, M. T. Koper, Solutal Marangoni effect determines bubble dynamics during electrocatalytic hydrogen evolution, Nature chemistry, 15(11), pp. 1532-1540, 2023.

[2] X. Yang, D. Baczyzmalski, C. Cierpka , G. Mutschke , K. Eckert, Marangoni convection at electrogenerated hydrogen bubbles, Physical Chemistry Chemical Physics, 20(17), pp. 11542-11548, 2018.

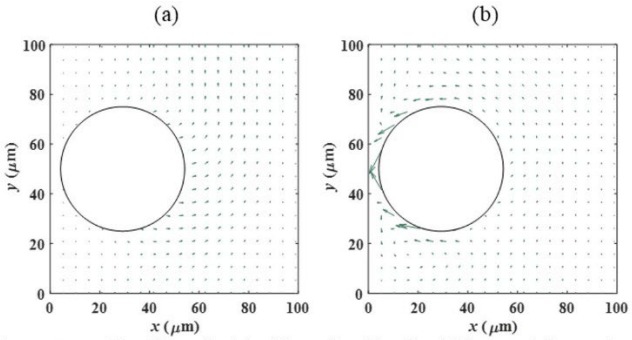

Figure 1: Velocity vectors at R = 25 µm for (a) without (b) with solutal Marangoni flow at the central x-y plane.

Computational Modeling of Plasma Jet

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Session: Electrochemical systems

The plasma jet generated by a non-transferred plasma torch may appear steady and laminar, but it undergoes significant turbulence. Initially, within the plasma torch, the jet begins as laminar, but upon interaction with the surrounding atmosphere at the outlet, it transforms into a turbulent flow. As it exits, the jet extends into a long structure and evolves into a wavy, fully turbulent flow. This paper delves into the intricacies of computational modelling for non-transferred plasma torches, outlining the challenges associated with simulating multiphysics and multiphase interactions at the outlet, and detailing the development of the plasma jet. The computational analysis is executed using the COMSOL Multiphysics software. Steady-state computational analysis is conducted on a 2D axisymmetric geometry, employing various turbulent models. A comparative analysis of results from each turbulent model is presented. Additionally, a transient study is undertaken using the optimal turbulent model to capture the jet's structure and its evolution. The paper concludes by validating the computationally obtained jet structure through a comparison with experimental data, ensuring the accuracy and reliability of the simulation results.

A CFD parametric study for the optimized catalyst layer's thickness and porosity based on the performance of a zero-gap alkaline water electrolyzer (AWE) cell

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Session: Electrochemical systems

One of the most promising technologies for successfully integrating renewable energies into the grid is the production of hydrogen through electrolysis to store surplus electric energy. Low-temperature alkaline water electrolysis (AWE) technology, with greater maturity and the larger commercial outreach, has been in use for several years for hydrogen production. Mostly the preceding research primarily focus on the conventional AWE which is based on two non-porous electrodes separated by a liquid electrolyte in which gas bubbles moves freely. However, this design has a drawback since it has a high ionic (ohmic) resistance due to the relatively wide bubble containing electrolyte gaps between the electrodes and the separator membrane. In recent trends, modern AWE electrolyzers are based on zero-gap configuration in which position of two porous electrodes are directly adjacent to a hydroxide ion conducting membrane or separator. This configuration forces gas bubbles to be escaped from the backside of the porous electrodes, thereby, considerably lowering the ohmic resistance contribution from the electrolyte between the two electrodes. Unfortunately, there is a scarcity of research on two phase modeling of zero-gap AWE combined with electrochemical reactions, and thus, accurate hydrodynamic modelling of the gas-liquid flows is necessary since the local distribution of gas affects the amount of electrical energy needed to produce hydrogen. A two-dimensional (2D) two-phase model of zero-gap AWE cell containing 30% potassium hydroxide (KOH) solution has been developed using COMSOL® software. The model embodies electrochemical kinetic for both cathode and anode electrode, the two-phase flow model for gas and electrolyte, and the transport model for species including diffusion/convection/migration. A numerical two-phase model based on the extended Darcy approach was used to simulate two-phase flow in the porous media during the cell's operation. This multiphysics approach allows the model to simultaneously evaluate the electrochemical, fluid flow, and species transport phenomena occurring in an electrolysis cell. A comparative study was conducted to investigate the effect of two-phase flow on zero-gap AWE performance while considering various cell parameters. In particular, the electrical response was evaluated in terms of polarization curve (voltage vs. current density) at different catalyst layer thickness and porosity. Furthermore, the gas crossover across a separator which is considered as a critical aspect related to AWE performance was studied. Simulation results showed that the cell with a large catalyst layer thickness and high porosity, and small catalyst layer thickness and low porosity exhibited better electrical response. Besides that, the gas crossover across a separator lied well below the critical limit for the typical AWE's current density 0.3 A/cm2. The current full 2D AWE model provides a comprehensive information of the electrochemical and transport phenomena, making it a viable tool for large-scale AWE cell and multi-megawatt stack design.

Modelling of Flow through Multi-Phase Porous Media for Fuel Cells

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SIEMENS

Session: Electrochemical systems

Flow through porous media occurs in many industrial systems like geological, biological, etc. In recent times, with the advent of Polymer Electrolyte Membrane Fuels Cells, the CFD modelling of the transport process within the fuel cells has become very critical. Additionally, the presence of multiple phases within the fuel cell adds to the complexities of modelling. Traditionally, many flow solvers have used the simplified approach towards modelling porous media by providing viscous and inertial resistance terms within the Navier-Stokes momentum equation which is an interpretation of the Darcy-Forchheimer law. However, within this simplification, there can be numerous effects associated with modelling of the permeability within the porous media. In the current paper, we demonstrate a model to simulate multiphase flow through porous media using different formulations for relative permeability. We validate the model with Buckley- Leverett method for Air-Water and Water-Oil solutions. Finally, we simulate a case which is representative of the flow of liquid through the various porous zones inside a PEM Fuel Cell, namely the Catalyst layer (CL), the Membrane (ML) and the Gas Diffusion Layer (GDL). We will study the effect of different permeability formulations on flow through the three porous layers, namely CL, ML, and GDL.

Fluidized beds

Experimental Study on Sticking Behavior during Iron Oxide Reduction for the Metal Fuel Cycle.

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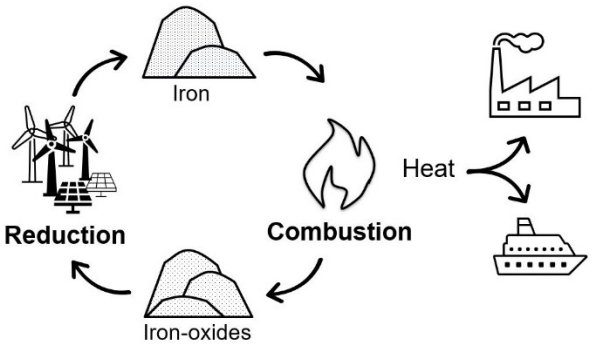
Eindhoven University of Technology

Session: Fluidized beds

Electrification is seen as a promising solution to the transition towards sustainable energy. However, the operation of the electricity network, is disrupted by intermittency of these sustainable energy sources. Therefore stockpiled fuels are needed to deal with supply disruptions and variability of these clean sources. One of these storable energy sources is metal, that can be used as a recyclable dense energy carrier of green energy. Metals like iron can be burnt with air or react with water to release its chemical energy even up to industrial scale with a high power output. The thermal energy which is released during this process provides heat to high energy- and emission- intense industries. After combustion the generated metal oxides are captured and reduced back to metal. It is also possible to export the metal over long distances, or store it indefinitely with minimal loss. The main issue is that our scientific knowledge to support the metal fuel combustion/regeneration cycle is largely missing and needs to be developed. While the oxidation element of the cycle is a widely studied part of the metal fuel cycle, the regeneration of the energy carrier is still in a starting point of development. Study of the reduction process is essential for the future success of the metal fuel cycle. One application which can be used for reduction is the fluidized bed. The fluidization of particles depends on the type of gas, gas density, as well as solids characteristics, such as bed porosity, particle size and particle density. In this experimental study, we aimed to investigate and understand factors contributing to the sticking phenomenon and its impact on the reduction process within a fluidized bed. Pressure drop measurements were monitored throughout the reduction process, and it was observed that after a certain amount of time, there was a significant decrease in fluidization due to partial defluidization of the bed. To further comprehend the sticking behavior and its underlying causes, the reduction reduction reaction was stopped for different time intervals. This to analyze the powder composition with X-ray diffraction (XRD) and the size distribution of the powder using a Particle size Analyser (PSA). Next to this, the particle morphology is analyzed using Scanning Electron Microscopy (SEM). Initial findings from the powder composition analysis revealed the presence of metallic iron and various iron oxides in the iron ore feedstock. Over time, as the reduction process progressed, the abundance of metallic iron increased, while the iron oxide phases diminished. These changes in the powder composition could be linked to the sticking behavior observed during the reduction process. The analysis of powder composition and size distribution provided valuable information on the changes occurring within the particles, highlighting the potential causes of sticking. Understanding and mitigating the sticking behavior can contribute to the improved efficiency and effectiveness of the iron ore reduction process, facilitating the advancement of the metal fuel cycle for sustainable energy production.



Three Phase Modelling of a Coarse Particle Flotation Machine

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CSIRO Mineral resources

Session: Fluidized beds

The recovery of coarse particles by flotation is a long-standing challenge for the mineral processing industry. Recent developments in flotation cell design have produced a flotation machine specifically designed to enhance the recovery of ultra-coarse composite mineral particles. The flotation machine is part liquid fluidised bed and part traditional flotation machine and uses a three-phase fluidised bed as the contact zone for particles and bubble within a mineral slurry.

A three phase CFD model of a laboratory scale cell was developed to model the liquid-solid-gas flow and gain an insight into the hydrodynamic phenomena in the cell. Two modelling approaches were used to predict the liquid-bubble-particle flow. The model predicted three distinct regions with a packed bed in the base of the cell, a region above the liquid-gas sparger where the particles are well fluidised with bubbles interacting with the particles above which is a fairly quiescent liquid with slow rising bubble plumes. Results show that key flow patterns can be captured by the model, but that bed expansion was over predicted when compared to measurements.

A Comparative Study of Different CFD-codes for Fluidized Beds

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Per Fredrik Daun, Hydro
Kristian Etienne Einarsrud, Department of Materials Science and Engineering NTNU

Session: Fluidized beds

Fluidized beds are a crucial component of modern process industry and chemical engineering. Over the decades, Computational Fluid Dynamics (CFD) has been playing a key role in the design and optimization of fluidized beds. However, CFD modelling of fluidized beds is not without challenges, partly due to the scarcity, incompleteness, or inconsistency of experimental data for validation. Moreover, CFD models involve many parameters and assumptions that introduce uncertainty and sensitivity in the predictions, even with seemingly identical conditions in different CFD codes. In the current work, we aim to address these intra-code subtleties by comparing results from the open-source software packages MFIX and OpenFOAM, and the commercial software package ANSYS FLUENT to experimental data. The gas-solid flow is simulated with a Eulerian-Eulerian framework, utilizing the kinetic theory of granular flow (KTGF) to determine solid-phase properties. The classical drag-laws of Gidaspow and Syamlal-O'Brien, along with the various available options, have been investigated in detail through a parametric study.

Gas-Solid Injection in Fluidized Beds for Biomass Wastes Valorization

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Session: Fluidized beds

The processing of biomass and biomass wastes towards renewable energy and green fuels plays an important role for the decarbonisation of global economy and mitigation of climate change. The injection of solid fuels into fluidized bed reactors for thermochemical conversion is challenging due to the inherent complexity of the multiphase system, related to the fast gas-solid transport and jet interaction with bed bubbles. Ultimately, solid feeding impacts on process reliability, conversion efficiency and design robustness. In this study, the gas-solid transport and pneumatic injection in gas-solid systems was investigated. A pressurized air feeder was used to inject a batch of sawdust powders into fixed and fluidised beds at lab scale. First, the horizontal feeder was characterised as a function of the operating parameters (feeder pressure, secondary gas velocity, initial biomass content), which showed an impact on the solids flux and flow concentration. Then, these parameters were used to define a transport regime operation map for the injection line. The experimental results were used to evaluate the CPFD approach MP-PIC (Multiphase Particle in Cell) with the software BarracudaTM. The gas-solid transport simulations under different feeder operating conditions showed a fair agreement with the experimental results, in terms of solids flux and flow concentration. Finally, different tracking techniques (fluorescent particle tracking, pitot tubes, and electric capacitance tomography, ECVT) were used and compared to assess the penetration and dispersion of the biomass into fixed and fluidized beds. The jet propagation was captured with transient/3D images with the ECVT, and the biomass concentration across the jet length was quantified with the fluorescent particle tracking technique. Similar jet penetration lengths were obtained with the different techniques, and it was generally more under higher solids flux from the injector. Ultimately, the pros and cons of each tracking technique were highlighted.

Lagrangian methods and particles

Numerical Study on Transport of Respiratory Droplets in Ventilated Indoor Environments

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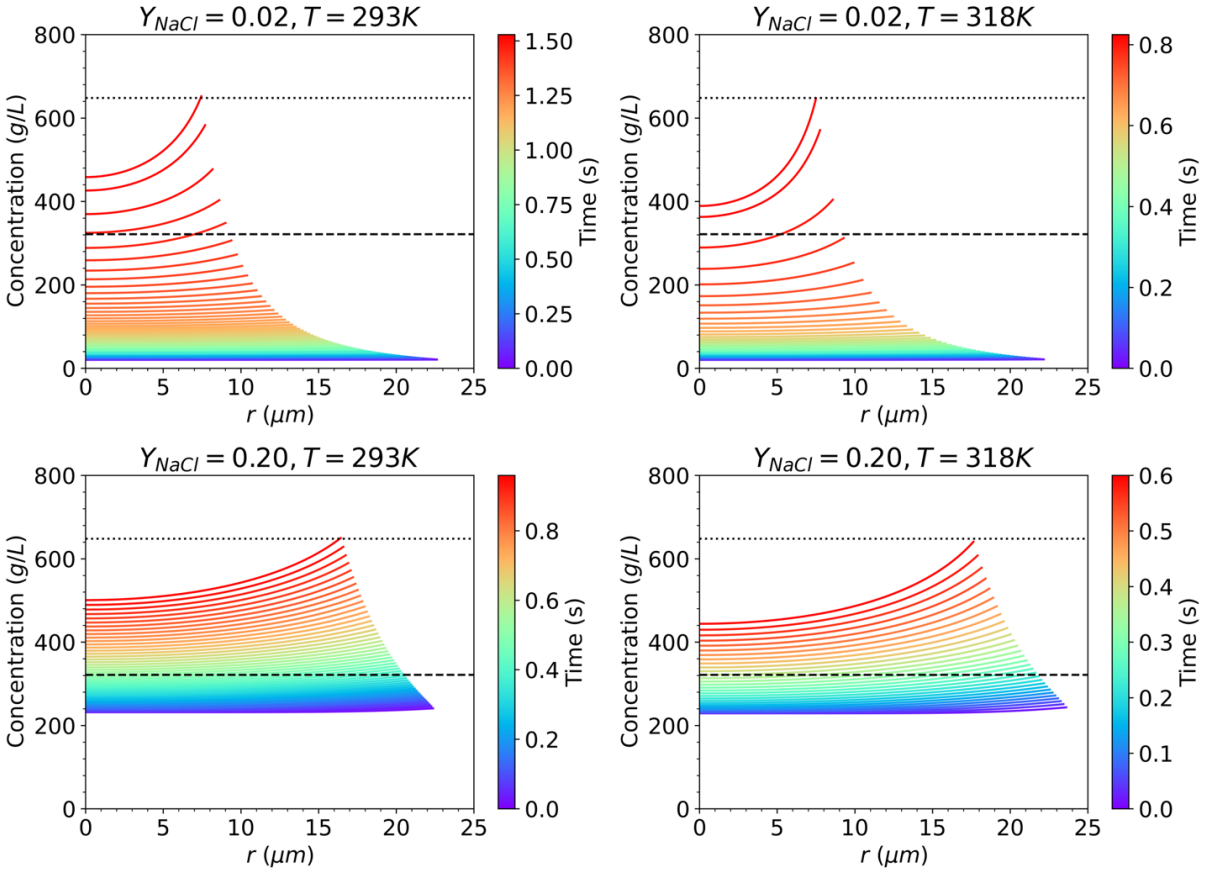
Session: Lagrangian methods and particles

Infectious diseases, such as COVID-19, can be transmitted by the exhaled virus-laden respiratory droplets. In indoor environments, ventilation systems are widely used to dilute or remove such droplets. To improve their performance and lower the infection risk, investigations on droplet transport under ventilation systems are of great importance. Respiratory droplets in indoor environments constitute a complex multiphase system. The sizes of droplets, affecting the balance between aerodynamic and gravitational forces acting on them, play an important role in their trajectories. In addition, the respiratory droplets are multicomponent, containing volatile and non-volatile substances. They can evaporate, which causes changes in size and significantly affects droplet transport. Computational fluid dynamics (CFD) provides a powerful tool to investigate the droplet transport. To consider the effect of evaporation, a zero-dimensional (0D) evaporation model for the salt-water droplets, which assumes salt is homogeneously distributed inside a droplet, is widely used to resemble the respiratory droplets. However, the salt is found to be not homogeneously distributed inside the droplets [1]. A salt shell may form due to the enrichment of salt in the droplet surface, resulting in the droplet residue larger than the prediction of 0D model. Therefore, the one-dimensional (1D) evaporation model, considering the salt diffusion inside the droplets, was adopted by some researchers [1, 2]. This, however, increases the computational costs. Therefore, in this study, the factors affecting salt distribution inside the droplets are analyzed using the 1D model. Based on the results, a simple 0D model with corrections considering the non-homogeneous salt distribution is developed. The corrected model is validated with experiment [1]. Then it is coupled with the CFD-population balance modelling (CFD-PBM) approach to trace the transport of respiratory droplets in ventilated indoor environments. An example of the obtained information is shown in Figure 1, where the evolutions of salt concentration profiles inside the NaCl-water droplets are presented. The setups are from the work of Gregson et al. [1], and the results agree well with their simulations. It can be seen that increasing ambient temperature or decreasing the initial salt concentration leads to a more non-homogeneous salt distribution inside the droplets. This is because such measures cause a higher evaporation rate so that the salt enriched in the droplet surface does not have enough time to diffuse to the center of the droplet.

References

[1] Gregson FKA, Robinson JF, Miles REH, et al. Drying kinetics of salt solution droplets: Water evaporation rates and crystallization. The Journal of Physical Chemistry B, 2018, 123(1): 266-276. [2] Ozler G, Grosshans H. Airborne virus transmission: Increased spreading due to formation of hollow particles. Environmental Research, 2023, 237: 116953.


$Y_{NaCl} = 0.02, T = 293K$
$Y_{NaCl} = 0.02, T = 318K$
$Y_{NaCl} = 0.20, T = 293K$
$Y_{NaCl} = 0.20, T = 318K$
Concentration (g/L)
r (μm)
Time (s)

CFD simulation of organic dust deflagration in a vertical channel

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Session: Lagrangian methods and particles

Deflagration describes the subsonic combustion wave propagating through a premixed mixture of gaseous and/or particulate fuel and oxidizer. In dust deflagration dust particles are typically levitated in gas flows. Consequently, any deflagration event is closely coupled to the characteristics of the fluid-dynamical behaviour of dust particles. Dust deflagration poses a serious safety risk in any industrial process involving fine combustible dusts. For the numerical analysis of deflagration of a typical volatile organic dust represented by maize starch, we employed a Euler-Lagrangian method, where the trajectories of the dust particles are tracked by representative parcels. Since the combustion of dust particles involves relatively high temperatures radiation is considered as well. Radiation is especially important during the initial phase of electric spark ignition for the energy transfer of spark energy to the surrounding particles. Furthermore, combustion of particles is considered a two-stage process. First, particles are heated by an ignition source (e.g., electric arc) triggering pyrolysis degassing mostly carbon monoxide and methane. The pyrolysis model was established via Thermogravimetry and gas analysis of a maize starch sample. Second, these pyrolysis gases combust in the gas-phase. Turbulent gas-phase combustion is modelled via the eddy dissipation model. Fuel conversion and a chemical timestep are modelled by a four-step mechanism proposed by Jones and Lindstedt [1]. Comparisons between predicted dust cloud evolution and flame speeds and experimental observations of deflagration events of organic dust in a vertical channel [2] reveal fairly good agreement. Finally, such numerical simulations enable the detailed investigation of deflagration events, which, in turn, allows the considerable improvement of process safety.

References

[1] W. P. Jones and R. P. Lindstedt, “Global reaction schemes for hydrocarbon combustion,” Combust Flame, vol. 73, pp. 233–249, 1988. [2] S. Puttinger et al., “Dust cloud evolution and flame propagation of organic dust deflagration under low wall influence,” J Loss Prev Process Ind, vol. 83, no. February, p. 105042, 2023, doi: 10.1016/j.jlp.2023.105042.

CFD-DEM simulation of chemical looping gasification of biogenic residues at 1 MWth scale

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Session: Lagrangian methods and particles

Chemical looping gasification is an innovative process for chemical recycling of residues. Two circulating fluidized bed reactors are coupled with a metal oxide as oxygen carrier that circulates between the reactors. In the fuel reactor, the feedstock is converted to syngas. Heat and oxygen for the gasification are provided by the oxygen carrier. In the air reactor, the oxygen carrier is re-oxidized using air. Thus, the production of an almost nitrogen free syngas is possible without the need for a costly air separation unit. In this work, a CFD model was developed for the fuel reactor in ANSYS Fluent 21R2. The multiphase flow is modeled based on Euler-Lagrange methodology using the discrete element method (DEM). To the authors knowledge, this is the first model for biomass chemical looping gasification using CFD-DEM. Drag forces acting on the particles from the gas are modeled with an EMMS model. Biomass gasification is a complex process including many species and parallel and consecutive reactions. To make a simulation of the fuel reactor feasible, a reduced reaction network was defined. The model consists of 14 species and 9 reactions including pyrolysis of feedstock particles, gasification, oxygen carrier reactions as well as tar decomposition by steam reforming and water gas shift. Custom kinetics specific to the feedstock and oxygen carrier used in this study were implemented. In 2022, the first demonstration of autothermal chemical looping gasification at MW scale was achieved at TU Darmstadt using biogenic residues as feedstock and ilmenite, a natural titanium-iron-oxide as oxygen carrier. The CFD model was applied to selected operating points from the pilot operation and validated with measurement data. The reactor hydrodynamics and thermodynamics could be predicted accurately. The pressure profile was in good agreement with the experimental measurements in both, the dense bed at the bottom of the reactor and the upper lean zone. Oxidation degree of the oxygen carrier at reactor outlet corresponded well with experimental samples indicating a correct representation of oxygen transfer to the reactor. Syngas composition correlated reasonably well with the experimental measurements.

Unprecedented Insight into the Thermal Processing of a Blast Furnace

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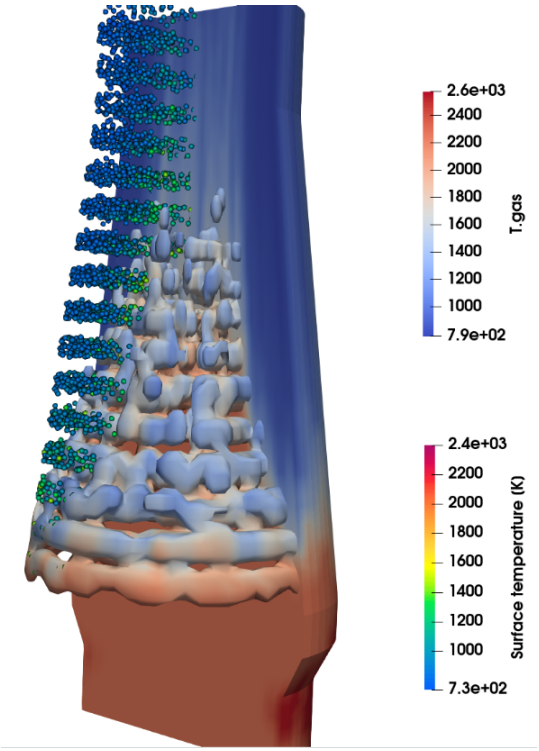
University of Luxembourg

Session: Lagrangian methods and particles

Two-thirds of the world's crude steel output of 1.95 billion mt in 2021 came from traditional blast furnace-based steel production, despite the inevitable shift to "green" steel to make it commercially viable and lessen the steel industry's carbon footprint. Conventional blast furnaces, on the other hand, are intricate multi-phase and multi-physics processes that only very slightly permit experimental access. The extended discrete element method (XDEM) is the primary representative of advanced multi-physics simulation technology (AMST), which is the recommended tool for gaining a deeper understanding of the complexity of these processes. The particulate phase - whether it be iron or coke particle - is handled as a discrete entity in this simulation framework, complete with motion and thermodynamic state. The latter in particular includes a multitude of chemical reactions that can be linked to particles, including phase changes like melting or combustion, drying, and reduction by the reducing agents hydrogen and carbon monoxide. The aforementioned processes involve a significant exchange of mass, momentum, and energy between the discrete and continuum phases. The latter is based on conventional computational fluid dynamics (CFD) and describes the flow of gases or liquids in the void space between the particles. The temperature and species distribution within a particle are determined by heat and mass transfer between the particle surfaces and the embedding gas phase, while an exchange of momentum, such as drag forces, creates a corresponding pressure drop over the reactor's height. Results from using the XDEM technique to resolve the particulate and continuum phases are extremely detailed. The underlying physics of steel production, in particular the formation and shape of the cohesive zone as depicted in fig. 1, are revealed through an analysis of the results, which is crucial for design, operation, and addressing environmental challenges. Decision-makers are assisted by these findings in making well-informed choices.



Location and shape of the cohesive zone are identified by an iso-surface that represents the mass transfer rate of molten iron from the iron bearing particles to the liquid phase of the Euler solver in a blast furnace. In addition, the gas temperature and ore particle layers with its surface temperature are depicted in a reduced size for better visibility.

A CFD-CPM model for the simulation of the fluidization of fine-grained ores

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Session: Lagrangian methods and particles

Fluidized bed and moving bed reactors are one of the most important technologies in several branches of process industry. Especially, it is known since decades that fine iron ores can be reduced rapidly and efficiently from iron carrier materials using such devices. Within the next decades, most of the carbon-based steel production will be transformed to hydrogen-based technologies. Fluidized beds have the potential to become a key technology for this green steel production. The key advantage in using fluidized beds is that the process step of agglomeration of fine or finest grained iron ores is saved. Nowadays most high-quality iron ores are only available in this form (before agglomeration). Due to the limited accessibility for measurements, simulation methods have become one of the most important tools for optimizing the iron making processes. While continuum models, such as the two-fluid model [1]or the filtered two-fluid models [2] would be good candidates to attack the simulation of large-scale multi-phase processes it lacks from a proper representation of the particle size distribution and the related physical phenomena. This, in turn, favours particle-based approaches, such as the coupling between CFD and DEM methods, which can easily handle, for example, gas-particle reactions and particle morphology. However, CFD-DEM approaches require considerably large computational resources, since particle-particle collisions have to be resolved. Thus, CFD-DEM is restricted to very small fluidized beds. The situation gets even worse in the case of fine-grained ores. Following Verma and Padding [3], we implemented a continuum particle model (CPM) into the Opensource code CFDEMcoupling [4]. CPM is a recent approach to multiphase-particle-in-cell (MP-MIC). In contrast to DEM, CPM does not picture individual particle collisions, these are rather modelled by a continuous particle stress tensor. This simplification allows, for example, larger time steps for the particle integration. However, the drawback of CPM is the appropriate definition of the particle stress tensor, which considerably depends on mapping and interpolation schemes. Thus, we introduce a novel face-based mapping/interpolation scheme allowing the determination of a smooth particle stress tensor. Results show that this new CFD-CPM approach is able to reproduce the fluidization behaviour (i.e. pressure drop, velocity profiles) deduced from reference CFD-DEM simulations but at much lower cost. Finally, CFD-CPM is coupled with a recently proposed reduction model [5] revealing the applicability of this approach for the simulation of the direct reduction of fine-grained ores.

References

[1] S. Schneiderbauer et al., Chem Eng Sci, vol. 80, pp. 279–292, 2012. [2] S. Rauchenzauner and S. Schneiderbauer, Chem Eng Sci, vol. 247, p. 117104, 2022. [3] V. Verma and J. T. Padding, Chemical Engineering Science: X, vol. 6, p. 100053, 2020. [4] C. Kloss et al., Progress in Computational Fluid Dynamics, vol. 12, no. 2/3, pp. 140–152, 2012. [5] M. E. Kinaci et al., Chem Eng Sci, vol. 227, p. 115858, 2020.

Towards predicting cavitation collapse effects in Eulerian CFD model

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Session: Lagrangian methods and particles

As the liquid pressure drops below the vapor pressure, liquid-to-gas phase change occurs, and vapor filled cavities emerge within the liquid phase. Once the vapor-filled cavities are subjected to higher liquid pressures again, they collapse violently and generate shockwaves and local high temperature (>5000 K) and pressure (>500 bar) values, which in turn results in erosion on the nearby solid surfaces and harm turbomachinery. Due to this harmful nature of cavitation, it has been historically seen as an unwanted phenomenon in many industries. Although these concerns still hold today, researchers showed that the intense conditions created during the collapse of cavitation bubbles can also be used to intensify several processes, including wastewater treatment, hydrogen production through electrolysis, and biofuel production, by employing cavitation assisted reactor technologies. Modelling such devices is proven to be computationally challenging due to their complex geometries and significantly different time and length scales encountered in a cavitating flow. Thus, the current state-of-the-art in modelling of cavitating flows consists of studies that emphasize either the dynamics of a single bubble under cavitation conditions or the accurate representation of the geometry and the flow field, while over-simplifying the other. The existing Eulerian cavitation closures in CFD software follows the latter approach by neglecting several key characteristics of the phenomenon, such as the impact of shockwaves or the bubble chemistry following the dissociation of water molecules. Therefore, although these models are computationally inexpensive, they fail to meet the needs of the modelling efforts for the emerging cavitation-assisted reactor technologies, where especially the collapse conditions and the resulting bubble chemistry plays a significant role. This work will start by discussing the drawbacks of the current CFD methods for modelling cavitation when applied to cavitation-intensified reactors. Next, results from a recent study solving single bubble dynamics equations on Lagrangian cavitation bubbles tracked on a Eulerian flow field are discussed. Such an approach allows cavitation collapse conditions to be predicted while considering the detailed flow behavior of the cavitation reactor. However, several challenges were encountered with this approach, especially when it comes to coupling the effect of the bubble volume change to the Eulerian pressure field. In addition, results from a recent study focusing on single bubble dynamics are shown to illustrate how simple algebraic expressions can be obtained for predicting the reactive species formed under bubble collapse. These expressions could be introduced into CFD models as closures to include the outcome of cavitation bubble collapses without resolving the short timescales of the collapses, greatly reducing the computational cost compared to the aforementioned Lagrangian approach. In conclusion, possibilities are discussed for including cavitation collapse effects in Eulerian cavitation models to facilitate improved usage of CFD models to design cavitation-intensified reactors.

A particle scale model of charge and slurry behaviour in SAG mills including coarse particle breakage, attrition and slurry phase grinding and transport

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Session: Lagrangian methods and particles

Prediction of grinding mill performance, throughput and product size distribution in full 3D SAG mills with feed and discharge is now possible using a multi-physics, particle-scale model which combines charge and slurry behaviour, breakage and attrition of resolved coarse particulates, and grinding of unresolved fines in the slurry phase. This uses a fully two-way coupled DEM+SPH model to represent the behaviour of the coarse solids (DEM) and fine slurry (SPH) phases as well as the interactions between these phases. Size reduction of feed material is included in the DEM sub-model through four inter-related comminution mechanisms. These include body breakage and surface attrition (via chipping, rounding and abrasion) which create explicit size and shape modification of the resolved coarse (DEM) particles. Body breakage makes use of a particle-replacement method and breakage characterisation data to pack super-quadric progeny into each fracturing parent particle. Fine unresolved fragments either in the feed or resulting from coarse fracture are transferred to the SPH slurry phase where the viscosity then spatially varies with fines content. Collisions and shear due to the motion and stressing load of the coarse DEM particles generate local energy dissipation. which is used to calculate size-dependent grinding rates. The slurry size distribution and its time evolution are then predicted by solving a coupled set of population balance equations for each SPH particle. This allows prediction of mass transfer between size classes due to grinding. Dispersive fluid phase transport of unresolved fines (in the SPH fluid) is represented as diffusion whilst advection is automatically treated by the SPH.

The ability of this particle scale model to predict SAG mill performance is explored for an industry standard 1.8 m diameter by 0.6 m long pilot SAG mill. The model demonstrates that rock with a size invariant elastic threshold E0 for incremental damage accumulation leads to a coarsening of the rock charge as smaller particles are preferentially broken. The flow inside the grinding chamber is complex and fully three dimensional with strong axial flow away from both the feed end and the grate as well as the traditional cascading and cataracting flows from the belly lifters. These mixing and transport behaviours interact with the breakage and grinding to give a complex spatial distribution for both the coarse rocks and for the slurry phase fine rocks. Flow of both smaller resolved rocks and slurry through the grates into the pulp chamber is predicted by the model. The model is able to show which parts of the grate allow flow into the pulp chamber and which parts have retrograde flow back into the grinding chamber. Finally, discharge flow from the mill and a final product size and throughput are predicted.

Blockage prediction in multiphase flow with cohesive particles using machine learning

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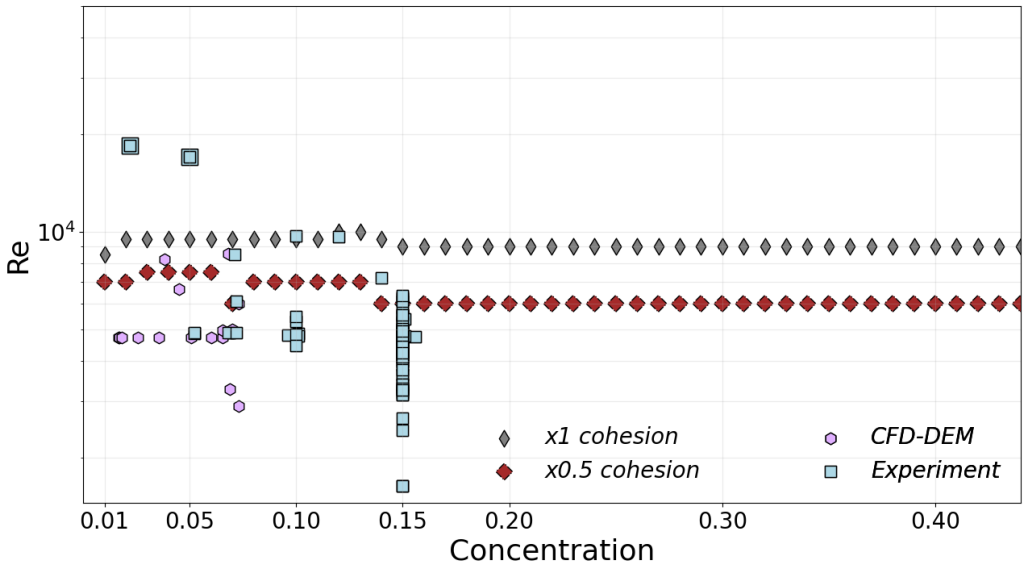
Session: Lagrangian methods and particles

This study presents a machine learning (ML) approach using a random forest classifier to predict blockages in multiphase flows with cohesive particles. The machine learning model aims to predict blockage under varying parameters, using binary classification as the result. We chose the random forest classifier because it can handle complex datasets with many variables, which is suitable for our research with multiple parameters and features. We applied a classifier using the Scikit-learn library in Python. The model is trained using a combination of datasets from flow loop experiments with ice slurry in decane and Computational Fluid Dynamics with the Discrete Element Method (CFD-DEM) simulations. Experiments and simulations provided a complete view of the dynamics of the considered multiphase system, including the effects of parameters. The collected dataset contains parameters like the Reynolds number, concentration, capillary number, and an indication of blockage. The model is evaluated using a cross-validation method with a parameter k=5, repeating this process five times with different fold combinations to verify its performance. Each model was trained on 80% of the data and tested on the remaining 20% in each iteration. Some parameters were adjusted, including a fixed random seed, the number of estimators, and the maximum depth of decision trees, while all other parameters were at their default values. After finalising the hyperparameters, the final random forest classifier was trained on the complete dataset to construct the blockage boundaries. The model's performance was evaluated using precision, recall, and F1-score metrics, demonstrating high values. Notably, the model achieved a maximum precision score of 1 and a recall of 0.8 for blockage cases. The key result of our study is the flow map, which compares machine learning boundaries with experimental and CFD-DEM simulation results. The flow map demonstrates that the results of the applied model closely align with the upper boundaries observed in simulations and experiments, especially at high Reynolds numbers. Furthermore, we considered how changes in cohesion affect blockage boundaries, observing an increase in cohesion. In conclusion, our method combines experiments and simulations to create an accurate predictive ML model. The successful application shows how machine learning can benefit fluid dynamics and blockage prevention, indicating possibilities for advanced models.



Metallurgical applications

A practical computational model to estimate PAH emission from furnaces

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SINTEF Industry

Session: Metallurgical applications

Due to the large computational overhead associated with simulating the PAH chemistry, predicting the PAH emission from industrial furnaces based on detailed CFD simulations is impractical. To address the lack of tools for practical estimation of PAH emissions from furnaces, a novel approach based on CFD+0D PSR reactors to predict PAH generation rate is proposed in this work. The proposed approach uses the results of the CFD simulation of the major process gases based on a reaction mechanism as the input to PSR reactors (which is run on each cell in the domain) using detailed PAH chemistry. The proposed model is used to simulate various operationally relevant scenarios like variations in the inflow (composition and velocity) of gases emanating from the charge surface and flue gas recycling levels. The model is seen to be able to capture the overall trends in the PAH emission predicted by the detailed reaction mechanism based CFD for cases simulated. As the PAH emission is chemistry driven, the choice of reaction mechanism used to CFD simulation of the major species in the proposed approach is seen to be critical as it provides a distribution of reaction intermediates relevant for PAH chemistry.

Understanding the continuous casting process with CFD modelling: the impact of microscopic dynamics on macroscopic scales

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Session: Metallurgical applications

In this contribution, we will present recent advances in the CFD modelling of the continuous casting process in the framework of K1-MET projects in Austria. Physical phenomena on both microscopic and macroscopic scales have been investigated, and the resulting dynamics in the metallurgical process sequence of continuous casting has been modelled. Non-metallic inclusions (NMIs), their microscopic dynamics and their interaction with macroscopic flows in casting vessels have strong impact on the final steel quality. If NMIs are not properly treated in the tundish of a continuous caster, e.g., captured by or dissolved in the covering slag, these particles can cause clogging in the submerged entry nozzle (SEN) and lead to harmful defects in the cast steel slab. Therefore, K1-MET has made great effort to model the NMI behavior using CFD tools to depict their behavior in a multiphase fluid flow, i.e., their removal from the steel into the slag phase in a tundish, their subsequent advance into the SEN and impact on clogging, as well as their behaviour in the mold during the casting and solidification. Detailed simulations of the NMI behaviour have been developed, characterizing their tendencies of dissolving into a slag phase at the steel-slag interface or adhering to the vessel walls. Considering the wettability and size of the particles, as well as local capillary motion and Marangoni convection, an effective removal rate of NMIs from steel into a slag phase has been derived. These simulations have been validated with laboratory experiments determining separation dynamics as well as material properties, for different combinations of NMI and slag materials. Subsequently, transport of NMIs in the SEN, nozzle clogging considering the transient clog growth and its interaction with the multiphase flow are modelled. Laboratory investigations of clogged SENs with different material compositions have been compared to the simulations for a validation of the CFD model. Based on these detailed simulations, effective models for the NMI behaviour in tundish and SEN have been developed, and effective NMI removal rates and clogging rates, respectively, have been incorporated into larger-scale simulations to simulate a realistic flow behaviour in vessels like tundish and SEN. Ultimately, the SEN clogging model has been used as a boundary condition for the effective flow behaviour of steel into the mold, and the resulting impact on the solidification and potential casting defects in the steel slab has been investigated. The different modelling approaches and their respective validation by experiments have been successfully brought together to achieve a comprehensive image of the dynamics governing the complete continuous casting process and are an impressive showcase of the insights into complex industrial processes that can be gained with CFD modelling.

Prediction of mass transfer regimes in a steelmaking ladle.

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Session: Metallurgical applications

Steel composition can depend on mass transfer with slag. It is typically the case during the secondary metallurgy step for the desulfurization of steel. In a continuous casting mold, the lubrication efficiency is strongly affected by the slag viscosity, which is dynamically modified before reaching the chemical equilibrium with steel. To correctly predict the time-evolution of the steel or slag composition, the mass transfer coefficient should be correctly assessed.

The aim of this work is to detect and explain the occurrence of different mass transfer regimes in an industrial ladle when the argon flow rate used for stirring is increased. Those regimes are already observed in different water models, see Kim and Fruehan (1987) or Joubert et al. (2022). OpenFOAM software is used for the flow modelling and the compressible multiphase VoF solver is selected, with static refinement in the interface region (steel / slag and steel / bubbles). Turbulence is described by a hybrid RANS-LES approach, as developed by Shur et al. (2008).

A set of 12 argon flow rates from 106.5 to 1200 STL is chosen. We check that the prediction of the open eye geometry is in correct agreement with published visualizations in an industrial configuration. For each of the gas flow rates, it is possible to get the local mass transfer coefficient k (m/s) and the local surface area A (m2). In this work, k is obtained by a correlation based on the local shear stress, Banerjee (2004). Specific algorithms are developed to get the gradient of tangential velocity at the steel slag interface and the local surface area.

When they are averaged over the steel/slag interface, opposite behaviors are observed for k and A. As expected, A continuously increases with argon flow rate. But a significant increase of A is detected above a critical flow rate corresponding to the creation of a large amount of slag droplets. Same phenomenon is observed in water model simulations, Joubert (2022). For k, non-intuitive results are predicted since k, globally, decreases with the gas flow rate. Even if, locally, important shear stresses are produced with high gas glow rate, the progressive intumescence development when the gas bubbles cross the top interface diverts the flow into the core region of the ladle. Then, dead regions are created near the slag / steel interface outside the open eye, accompanied by low values of the shear stresses. When averaged over all the interface, the contribution of these dead zones is predominant and drives the k value. Regarding the surface mass transfer kA, which is ultimately the main coefficient affecting the chemical kinetics, it is predicted to have the same behavior as A.

Prediction with OpenFOAM can reproduce complex phenomena in a ladle. Similar mass transfer regimes are observed in water models and industrial configurations. Significant differences are detected for k and A when gas flow rate increases.

Interface-resolved large eddy simulations of primary breakup in metal melt gas atomization

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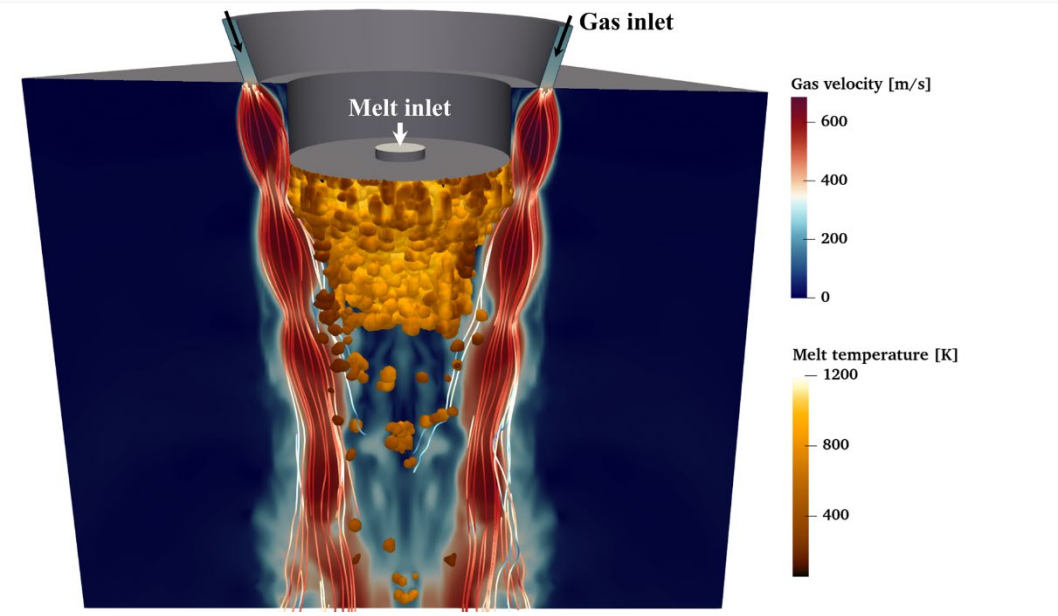
Session: Metallurgical applications

Bed-based additive manufacturing (AM) techniques, in which thin layers of metal powder are locally fused together by a laser, allow for the production of components with complex designs. While the metal AM technology is relatively matured, flexible and accurate production of high quality metal powder is less developed. Gas atomization is a production technique for metal powder, in which high pressure gas jets rupture a molten metal stream into fine droplets, which subsequently solidify into a powder. A small scale gas atomization process for the production of high-quality metal powder can greatly enhance the versatility and sustainability of powder bed AM techniques. The gas atomization process is typically described in terms of a primary and secondary breakup stage. This work focuses on the modelling of the primary breakup of the metal melt, covering the initial breakup into large droplets and ligaments. The secondary atomization describes the further breakup of these droplets into fine elements. High local Weber and Reynolds numbers are encountered as a result of supersonic gas jets impinging on the melt stream. Large velocity and temperature gradients increase the computational complexity of the breakup process. While in previous studies mainly the gas dynamics were studied, the current modelling strategy is aimed at understanding the primary breakup process for both the melt and gas phase. To this end, the gas-melt interface is modelled using a geometric Volume of Fluid (VOF) method for compressible flow in the open-source OpenFOAM software. Large Eddy Simulations (LES) are applied, in order to partially resolve the local turbulent flow structures. Special attention is devoted to the local resolution of the computational grid, with respect to requirements of both the VOF and LES. Adaptive mesh refinement is applied at the phase interface to ensure sufficient resolution of the VOF method. The numerical methods are validated separately prior to application in primary atomization. A parameter study is performed based on design of experiments principles. Statistics of the droplets are collected at several locations in the spray, in order to analyze the impact of process parameters on the primary breakup process. The gathered droplet statistics allow to separately model the secondary breakup process using less computationally intensive modelling techniques in the future.



Direct numerical simulation of mass transfer at the oil water interface in a model metallurgical ladle.

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Session: Metallurgical applications

We investigate mass transfer between liquid steel and slag during a metallurgical secondary refinement process through a reduced scale water experiment which reproduces the dynamics seen in an argon-gas bottom-blown ladle. The three-phase flow modelling includes a container filled by water, modelling the molten metal, topped by a thin layer of oil, modelling the slag. The system is agitated by the injection of air at the bottom, creating a bubble plume that merges into the air on top of the system (Fig.1). A tracer material, dissolved in the water, acts as a passive scalar that is progressively absorbed into the oil layer. The numerical results obtained for the hydrodynamics and the mass transfer properties of the system are then compared with theoretical and experimental studies for two differently shaped ladles: a cubical ladle as investigated by Joubert[1,2] and a truncated cone ladle as in the experiments by Kim[3]. The numerical study of the ladles is made difficult by the large values of the Peclet number Pe=U_0h_w/D_w involved, where U_0 is the typical large scale velocity in water, h_w is the height of the water layer and D_w is the tracer diffusion coefficient. Peclet numbers of the order of $10^{6\text{-}10}7$ are obtained even at the lowest flow rates in the experiment, leading to extremely thin boundary layers of size δ∼h_w*Pe^(-n), with n=1/3∼1/2. Such small boundary layers require numbers of grid points that are prohibitive even with advanced octree simulation methods. To circumvent this difficulty, we proceed in two steps. First, the hydrodynamics of the flow is investigated, then in a second step we analyze how the momentum boundary layers drive concentration boundary layers. For the hydrodynamics the numerical results recover two regimes: a laminar regime at low flow rates in which the oil-water interface remains relatively quiescent and an atomizing regime at large flow rates where the oil layer sheds into ligaments and droplets. The numerical results in a range of relatively small Peclet numbers are extrapolated to large Peclet numbers using a theory of the boundary layer with shear, the final results are in agreement with the experiments at low flow rates. In Fig.2(a) the average Sherwood number, the ratio between convective and diffusive mass transfers is plotted against the Froude number N, that compares the flow inertia to the external gravitational field, for the cubic ladle experiment and for two simulations at different minimum grid size. Fig. 2(b) shows instead the instantaneous local Sherwood number on the oil water interface, showing how the majority of mass transfer occurs in an annulus surrounding the open eye.

[1]N.Joubert. Liquid-liquid mass transfer characterization applied to metallurgical process.

[2]N.Joubert, P.Gardin, S.Popinet, S.Zaleski. Experimental and numerical modelling of mass transfer in a refining ladle.

[3]S.Kim and R.J.Fruehan. Physical modeling of liquid/liquid mass transfer in gas stirred ladles.

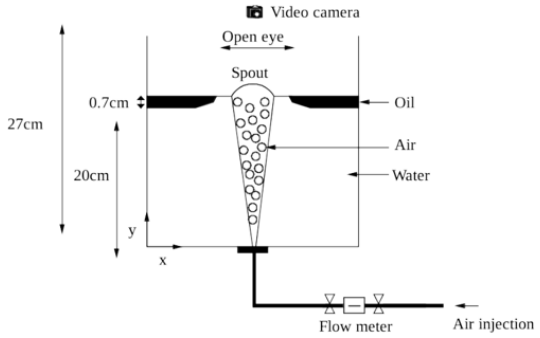
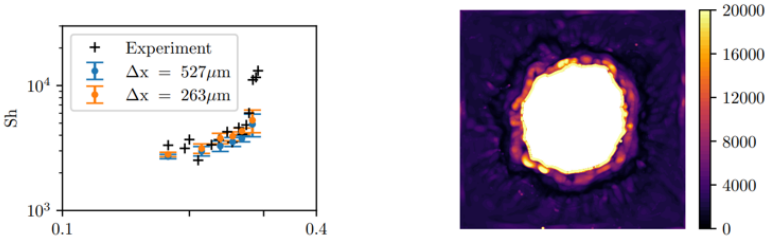


Figure 1: Schematic representation of the cubic ladle experiment . |



(a) (b)

Figure 2: (a) Numerical and experimental Sherwood number for different Froude numbers. (b) Instantaneous Local Sherwood Number on the oil water interface for a flow rate of 0.6L/min.

Optimization of mesh coupling between nozzle and mould for modelling turbulent flow during continuous casting

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LTU and Swerim

Session: Metallurgical applications

Continuous research and development ensure the production of high-quality steel which is a key component in society and people's everyday lives. Computational fluid dynamics is used in R&D to optimize the flow control during production. Generating a high-quality mesh while maintaining a reasonable cell count has significant impact on the equilibrium between computational cost (i.e., time and memory) and accuracy. The traditional approach when meshing the nozzle and mould is using a combination of hexahedral elements for the simple mould geometry and tetrahedral elements for the complex nozzle. However, building the coupling between these cell types is challenging and inefficient. The present study examines the possibility of using a hexahedral-polyhedral combination or a full polyhedral mesh instead of tetrahedral cells to decrease the amount of elements and improve accuracy (e.g. improved skewness, smoothness, orthogonality, etc.) with less computational cost. Finally, the resulting mesh is tested as part of a state-of-the-art digital model of a real industrial caster with the aim of facilitating the flow optimization.

Simulation of melt flow in steel continuous casting considering transient clogging of submerged entry nozzle

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K1-MET GmbH

Session: Metallurgical applications

Clogging of the submerged entry nozzle (SEN) in continuous casting of steel occurs due to the solid material build-up on the inner wall of the SEN. Different mechanisms have been proposed for clogging but attachment of solid non-metallic inclusions (NMIs) is supposed to be the dominant mechanism. In this work, effects of clogging on the melt flow and non-metallic inclusions (NMIs) distribution in the mold region were investigated transiently using a numerical model. In this model, inclusions are considered as solid spherical particles and their motion is calculated in a Lagrangian frame of reference; the turbulent melt flow is simulated with an Eulerian approach. NMIs attach on the inner wall of SEN due to the turbulent melt flow to form clog material and the clog growth changes the melt flow field simultaneously. With two-way coupling between clog growth and melt flow, transient behavior of the melt flow in the mold region can be investigated. The simulation results showed an asymmetric flow pattern and consequently an asymmetric inclusion and temperature distribution in the mold region. Effects of transient clogging on dynamic flow direction on the meniscus were also addressed. Using this numerical model, the effects of clogging on the different parts during the casting process can be predicted.

Metallurgy

Investigating Thermal Dynamics in Submerged Arc Furnaces through Numerical and Water Modeling

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Session: Metallurgy

In the pursuit of cleaner and more sustainable steel production methods, innovative approaches such as Direct Reduction of Iron by Hydrogen (DRI) have emerged. However, these advancements also present unique challenges. While DRI can be effectively melted in an Electric Arc Furnace (EAF), this requires high grade ores and extensive secondary metallurgy processes. Alternatively, Submerged Arc Furnaces (SAFs) offer a promising avenue for producing high-quality steel from BF grade ores while adhering to the Basic Oxygen Furnace (BOF) route. SAFs operate similarly to EAFs, albeit with a critical distinction: the arc is submerged within a thick layer of liquid slag. Consequently, heat transfer in SAFs differs substantially, as radiation from the arc is replaced by Joule heating within the slag. Efficiently transferring this heat to the liquid metal beneath the slag layer poses a significant challenge. Molecular conduction is inherently slow and insufficient for achieving economically viable production rates. Thus, convective heat transfer becomes paramount. However, buoyancy-driven flow within the furnace is typically weak, imposing limitations on the heat exchange between the heat source and the liquid metal. In tackling such challenges, a deeper comprehension of the flow dynamics and associated phenomena within SAFs becomes imperative. Numerical modeling stands out as a pivotal tool in unraveling the effects various parameters exert on thermal energy transfer within these environments. The development of such a model necessitates rigorous validation. Validation from industrial processes is extremely difficult, due to harsh conditions in the furnace. Thus, water models are an invaluable resource for validation purposes. To this end, a physical model containing water and oil, mimicking the properties of hot metal and slag, respectively, is designed and constructed. Within this setup, a constant temperature heater with two concentric coils is submerged in the oil while local cooling is applied to mimic heat losses. Particle Image Velocimetry (PIV) is employed to investigate the buoyancy-driven flow field within the water. Multiple thermocouples are placed in the water and the oil to record temperature variations over time. Additionally, thermocouples are also placed in the air above the oil. Throughout a series of experiments, two key parameters – heater temperature and water height – are independently varied to discern their effects on the system. Concurrently, Computational Fluid Dynamics (CFD) simulations are executed. The laminar nature of the flow poses inherent challenges to numerical simulations. Factors such as low diffusivity and the presence of multiple phases make the thermal energy conservation challenging. While the temperature profile exhibits close agreement with experimental data, further refinement is warranted to enhance the accuracy of the velocity field. By elucidating the intricate dynamics of heat transfer within the water-oil system representative of SAFs, this work contributes significantly to the understanding of steel production methodologies.

Numerical modeling of the submerged arc furnace

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Session: Metallurgy

As part of the European Green Deal, many material production processes need to be adapted. Reduction processes in particular nowadays mostly use carbon carriers such as coal, coke or natural gas as reducing agents. One of the biggest CO2 emitters is the steel industry. In the classic process route, iron ore is reduced to pig iron in the blast furnace using coke. As the coke also performs static tasks in the furnace, it is difficult to defossilize the blast furnace. An alternative route, which is currently being promoted by many steel manufacturers and plant builders, consists of direct reduction of the iron ore with hydrogen and subsequent melting in the electric smelting furnace (ESF). The latter can be designed as a submerged arc furnace (SAF) or open slag bath furnace (OSBF), which means differences in the charging of the raw material. In this presentation a CFD model of a SAF will be presented and it will be shown how the relevant process areas and phenomena (arc, radiation, chemical reactions, etc.) were modeled.

Modeling a pilot furnace for manganese alloys.

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NORCE Norwegian Research Centre

Session: Metallurgy

This paper presents the advancements in developing a 2D-axisymmetric finite element method model for a pilot-scale furnace used in the production of manganese alloys. The model is specifically designed to simulate furnace runs and predict the production of both ferromanganese and silicomanganese alloys, along with acid and basic slags. The multiphysics model incorporates several intercoupled phenomena, including material flows, physical-chemical transformations, electrical conditions, and heat transfer. It enables the investigation of both steady and transient states through time-dependent simulations. The model provides valuable insights into the distribution of materials within the furnace, temperature profiles, current paths, energy balances, and the rates and compositions of alloy and slag production.

Computational modelling of electric arc behaviour in direct-current smelting furnaces using hydrogen as a reductant

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Session: Metallurgy

Direct-current (DC) electric arc furnaces are used extensively for the recycling of scrap steel as well as primary production of many industrial commodities such as ferro-alloys, titanium dioxide, cobalt, and platinum group metals. The latter processes typically make use of carbothermic smelting, in which raw materials are reacted with a carbon-based reductant such as metallurgical coke to produce the alloy products of value. Although well-proven and economical, such processes are becoming increasingly undesirable due to their significant emissions of carbon dioxide and other harmful materials. Many alternatives to carbothermic smelting are currently being explored, including the replacement of part or all of the furnace reductant feed with hydrogen. A DC smelting furnace using hydrogen reductant has the potential to operate at zero carbon emissions provided renewable resources are used for both electricity and hydrogen production.

The primary heating and stirring element in a DC furnace is the electric arc, a high-velocity, high-temperature jet of gas which has been heated until it splits into a mixture of ions and electrons (a plasma) and becomes electrically conductive. The plasma arc completes the circuit between the tip of one or more graphite electrodes which enter vertically through the roof of the vessel, and the molten bath of process material underneath them. The arc acts as the engine room of the furnace, efficiently transferring thermal and mechanical energy to the process from the electrical power supply as well as facilitating exotic chemistry through the introduction of highly reactive species such as free electrons and monoatomic and ionized species.

Due to the extreme conditions inside operating DC furnace units, studying arcs experimentally is difficult and hazardous. The use of computational models coupling electro- and magneto-dynamics, chemical reactions, thermodynamics, kinetic theory, and fluid flow is therefore of great value in building an understanding of how arcs work under different process conditions. In this work, the authors present a coupled computational multiphysics solver incorporating fluid flow, heat transfer, and electromagnetic fields. Plasma thermodynamic and thermophysical properties – calculated using statistical mechanics principles – are also presented for a range of mixtures of hydrogen and water vapour that might be expected in the gas space of a smelter using pure hydrogen as a reductant. The properties are combined with the multiphysics model and used to generate predictions of the arc dynamics and electrical parameters that can be expected in hydrogen-fed DC smelting furnaces.

Metallurgy and furnaces

On Model Assisted Measurements and Applications

Eirik Manger,
Norsk Hydro ASA

Session: Metallurgy and furnaces

The developments in computer hardware combined with more sophisticated modelling tools have during the last decades created a wealth of new possibilities for understanding and explaining physical phenomena in complex systems. This is indeed true also for the aluminium industry, where the processes range from “simple” gas flow all the way to multi-phase flow with phase changes coupled with electromagnetic forces. Models are however still only approximations of the real processes, and comparison with measurements is still crucial and necessary. Previous presentations (Manger 2014 and Manger 2017) showed the importance of correct problem descriptions, as well as access to experimental data with good quality. On the other side, among the possibilities within digitization is also the ability to obtain real time data such as e.g. pressure and temperature from processes being continuously monitored. The true value of these measurements does however not appear before combining the data with models and theoretical understanding. By utilizing all available knowledge, important and useful characteristics on the physical system of interest can be obtained. In this paper the combination of simulations, theoretical knowledge and measurement equipment is explored and used to design an online system for monitoring flow through a Gas Treatment Center (GTC) line. By developing a CFD model and using the results from this, suitable positions for measuring differential pressure can be found. The principles for selecting and, if necessary, constructing geometries enabling such points correctly are described. Later the model, together with known physical principles, are used to establish a correlation between measured differential pressure, temperature and flow. This relationship is then used to monitor the flow rates online and in real time, also providing information on the fluctuations in the system and give warnings if experiencing large deviations/changes due to e.g. equipment failure.

References

MANGER, E. (2014), “CFD in Problem Analysis and Optimization – the Importance of Correct Boundary Conditions”, Proc. CFD 2014 – 10th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries, Trondheim, Norway, June 17th – 19th, 2014. MANGER, E. (2017), “Modelling and Measurements in the Aluminium Industry – Where are the Obstacles?”, Proc. CFD 2017 – 12th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries, Trondheim, Norway, May 30th – June 1st, 2017.

CFD Simulation of Melt Flow in a Pilot Container Glass Furnace: Investigation of the Influence of the Ratio of Electrical Power to Burner Power on the Melt Flow

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Session: Metallurgy and furnaces

Against the background of increasingly stricter national and international climate protection regulations, the energy-intensive container glass industry in Germany must reduce its energy consumption and CO2 emissions. In addition, energy prices are rising and the availability of natural gas as a fuel is partially limited. The “ZeroCO2Glas” research project, funded by the German Federal Ministry for Economic Affairs and Climate Action, is addressing this issue: Within the scope of the project, a highly flexible pilot glass furnace for the CO2-neutral production of container glass is being developed and commissioned. The hybrid-heated furnace generates its melting capacity through the oxyfuel combustion of hydrogen and electrical heating with six pairs of electrodes. Conventional container glass furnaces operate at 12 to 20% of their melting capacity with electrical heating. The pilot furnace, however, allows the level of electrical heating to be flexibly varied between 20 and 80%. The increased electric power affects the flow of the glass melt in the area of the electrodes and therefore the residence time of the glass particles in the furnace. This can have a significant impact on the quality of the finished container glass product. Due to the high temperatures and poor accessibility, the ability to analyse the melt flow in the pilot tank is very limited. For this reason, a simpler and more cost-effective method of investigation was used: In order to simulate the melt flow, a CFD model of the lower furnace of the pilot plant was developed to simulate the melt flow. The numerical model allows setting different electrical power/ burner power ratios in order to investigate their influence on the glass melt flow. In the presentation, the simulation results of the limit cases 20%/80% and 80%/20% will be presented and compared.

Investigation of submerged massive gas injection into liquid: numerical simulations and experimental observations

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Session: Metallurgy and furnaces

Submerged massive gas injection into liquid is a process intensification method that enhances the reaction rates through better stirring and mixing. Particularly, in metallurgical processes such as argon-oxygen decarburization (AOD) converter, high-speed injection of gas into molten metal facilitates the reduction of dissolved carbon. The gas injection velocity in such applications could reach the speed of sound and in several cases even constitute a supersonic gas flow penetrating high-density liquid. Such extreme conditions usually involve various sources of physical complexity such as gas compressibility, instabilities at the liquid-gas interface, and shock dynamics that eventually determine different flow regimes. This study presents a small-scale interface-resolved LES simulation of air-to-water injection at the near-nozzle region pursuing a validation strategy with water-based experiments. Using the compressible volume of fluid (VOF) method, we have simulated submerged massive gas injection into the water at different injection pressures. The simulations show reasonable agreement with macroscopic quantities obtained from flow measurement and high-speed imaging e.g. the mass flow rate and Mach numbers. We identified different regimes during gas penetration: at lower injection pressures, the flow becomes slightly supersonic with oscillatory shock wave structure inferring a bubbling regime, and as the pressure increases the flow encounters higher Mach numbers with stronger shocks establishing a more stable jetting regime. The total interfacial area, that is an indicator of gas fragmentation, increases with the injection pressure. This could be attributed to the Richtmyer-Meshkov instability during the shock-interface interactions. We also observed in both experiment and simulation that the probability of back-attack phenomenon decreases with the injection pressure which is consistent with the previous findings in existing literature. This may be explained by the dynamics of traveling shocks, their reflection at the liquid-gas interface, and their interference inside the compressible gas core. Due to the limitation of the optical measurement techniques in this context, this highly-resolved simulation study offers a basis for the physical interpretation of compressibility effects during massive gas injection in metallurgical plants.

Modelling Effects of Lancing into Process Material Through Furnace Tap-Holes

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Samancor Chrome, University of Pretoria

Session: Metallurgy and furnaces

Pyrometallurgical furnaces are integral for extracting valuable metals from ores, operating at temperatures exceeding 1600°C. These furnaces represent complex multiphase systems, posing significant challenges for direct industrial-scale study. In most furnaces, materials are charged, smelted, and accumulated, followed by a tapping process. The furnace features a 'tap-hole', a channel through the steel and brickwork, used for periodically opening and closing. The opening process involves lancing to remove refractory clay, akin to using a cutting torch. High temperatures are achieved by oxygen reacting with the steel lance. Once the lance penetrates the clay, unburned oxygen gas can enter the furnace, potentially impacting the molten material inside. Although an full model combining thermochemistry to study chemical interaction with a multiphase fluid flow would be ideal, combining these into a model that can be solved in a sensible amount of time would not necessarily yield a better set of answers than studying the problem in a systematic way from both angles.

In this paper, the authors explore different elements of gaining insight into the effect of lancing inside open-bath DC furnaces through multiphase fluid flow modelling for different situations in the furnace prior to tapping. The results from the fluid flow modelling is used to inform some of the other modelling done pertaining to potential refractory wear, etc. in the furnace as well.

Non-newtonian flows and polymers

Towards the understanding of the effect of non-Newtonian liquids in binary droplet collisions

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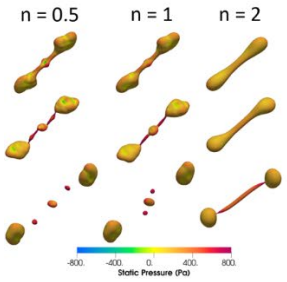
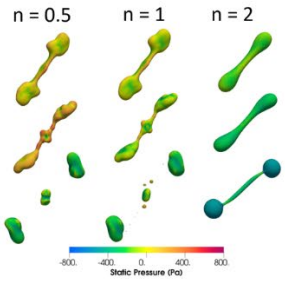
Session: Non-newtonian flows and polymers

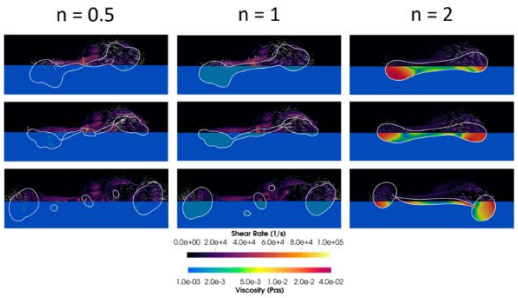
In many industrial processes, the collisions of droplets play a vital role in their performance. The fluids encountered in these applications often exhibit non-Newtonian behavior. These effects have a large effect on the outcome of the process and are currently not fully understood. To gain further knowledge, numerical simulations are performed using the Volume of Fluid Method and the Local Front Reconstruction Method. The non-Newtonian behavior exhibited by the droplets is the Ostwald-de Waele equation, including both shear-thinning and shear-thickening behavior. Earlier work shows this numerical setup is well equipped to simulate reality based on comparison with experiments for Xantham gum. The droplet collisions are performed until Weber numbers 300 for both head-on and off-center collisions. The rheology ranges from shear-thinning (n=0.5) to shear-thickening (n=2). For collisions at low Weber numbers, both simulation methods produce similar outcomes, whereas at higher Weber numbers the disintegration of the droplets follows a different mechanism, induced by the difference in numerical treatment of both methods. The transitions between the different outcome regimes were shown to be largely dependent on the power-law index. Our results further show that the expansion of the ring and the related diameter increases for higher Weber number and decreasing power-law index. In the case of off-center collisions, the detachment of the ligament is delayed for increasing Weber numbers and more shear-thickening fluids. This is accompanied by a higher critical ligament length. The results show there is a significant difference in collision dynamics for shear-thickening and shear-thinning fluids.



a) LFRM



b) VOF



c) Velocity field, shear rate field and viscosity profile LFRM

Enhancing Extrusion Performance: Macroscopic Analysis of Dispersive Mixing Sections

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Session: Non-newtonian flows and polymers

Dispersion is a critical process within the extrusion industry. Our focus is drawn to the deficiency in dispersive mixing quality in single screw extruders compared to their twin screw counterparts. This study outlines an approach that is used to evaluate and quantify the quality of dispersive mixing sections, which are commonly added to single screw extruders to compensate for this inherent lack of dispersive mixing quality.

Our study focuses on employing micro-level dispersion models that describe the macro-breakup of agglomerates—specifically, rupture and erosion. These models are integrated with Computational Fluid Dynamics to quantify the particle size of solid additives before, during, and after traversing these crucial mixing sections.

Using a non-isothermal Generalized Newtonian Fluid model with particle tracking and dispersion kinetics modeling, our methodology facilitates swift analysis of mixing sections and offers a fresh pathway for studying and optimizing the extrusion process.

Improving Flow Balancing: Employing GNF-X(M) for Predicting Flow Profile

Jakob Buist, Jordin van ’t Veld,
Windesheim University of Applied Sciences

Session: Non-newtonian flows and polymers

Flow balancing is the process of changing the geometry of a die in order to achieve a specific geometry for the extrusion profile, whilst minimizing the internal stresses in the material. In order to properly balance the flow in a die, the flow itself must first be accurately described.

Often, Generalized Newtonian Fluid (GNF) models are used to compute the flow profile of polymers above their melting points in the die. These models have the benefit of stability for the numerical process and low computational requirements. The drawback of these models is that extensional effects, which are present in converging flows such as in dies, are neglected.

Recently, the GNF-extended (GNF-X) model has been introduced, providing the stability and low computational requirements of non-viscoelastic models whilst implementing extensional stresses and viscosity. In this research this model is implemented into the ANSYS CFX software employing a Finite Volume Method. This aims to improve the accuracy with which the flow inside the die is described and thus the process of flow balancing. The outcome of this study is a comparison between the GNF and GFN-X models.

Numerics and methods

Development of a CFD model for supersonic gas flow in a close-coupled atomizer

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Session: Numerics and methods

Additive manufacturing (AM) opens the possibility to make lighter and more complex geometries using less material and shortens the time from idea to prototype. This requires a better understanding of the atomization process to produce high quality metallic powder as a feedstock. The atomization process requires a better understanding how the gas and melt interact to optimize the breakup of the metal stream. Computational fluid dynamics (CFD) is used to visualize fluid flow phenomena to create a model representation of the supersonic gas in the atomisation process in a close-coupled atomizer. Results show the transient behavior of the gas flow including turbulent fluctuations and typical flow structures such as shock waves, Mach discs, local density, and pressure changes, etc. The model developed is validated with Schlieren imaging and frequency analysis (FFT). A parametric study on the turbulence models available, mesh density, time stepping, sub-grid models as well as geometry assumptions such as 2D vs 3D ¼ section vs full 3D is carried out to determine the appropriate parameters for the simulations. The final aim is to empower the powder producers with a fast and reliable model which allows testing of geometry, pressure, and temperature variations for optimization of the atomization process.

CFD analysis of ultrasonic vibrations in enhancing recycled polymer extrusion efficiency

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(b)Windesheim University of Applied Sciences, Professorship for Polymer Engineering,

Session: Numerics and methods

The use of circular materials (recycled polymers) within the field of extrusion is difficult due their often-inconsistent viscosity related to variations in composition and molecular weight of the recycled polymers. Such variations lead to fluctuations in die pressure and flow balance, necessitating continuous adjustments in the extrusion process. Our study explores the use of ultrasonic vibrations to regulate extrusion die pressure, aiming to improve the quality of recycled plastic profiles. Employing Ansys CFD, we investigated the complex interaction of ultrasonic waves within extrusion dies, focusing on their impact on a non-Newtonian polymer melt. The presence of shear and pressure waves in a non-Newtonian polymer melt leads to shear thinning, effectively reducing die pressure. Consequently, this leads to more precise and effective pressure control within the die. The ultrasonic waves have a short penetration depth, which allows for local control of the flow resistance and therefore potentially flow balancing. This results in a more uniform and optimized extrusion process, highlighting the potential for improvements in the extrusion of recycled polymers.

MultiMorph - A Morphology-Adaptive Multifield Two-Fluid Model

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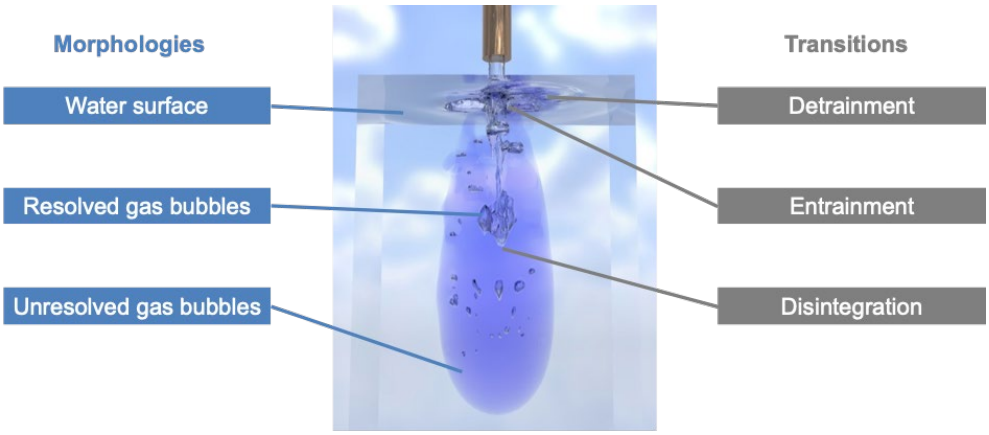
(a), Helmholtz-Zentrum Dresden-Rossendorf e.V.
(b)Reactor Engineering Division of Jožef Stefan Institute

Session: Numerics and methods

Industrial multiphase flows are typically characterized by coexisting morphologies. Modern simulation methods are well established for dispersed (e.g., Euler-Euler) or resolved (e.g., Volume-of-Fluid) interfacial structures. A simulation method that requires less knowledge about the flow in advance would be desirable and should allow describing both types of interfacial structures – resolved and dispersed – in a single computational domain. Such methods that combine interface-resolving and non-resolving approaches are called hybrid models. A morphology adaptive multifield two-fluid model, named MultiMorph Model, is proposed, which is able to handle dispersed and resolved interfacial structures coexisting in the computational domain with the same set of equations. For large interfacial structures an interfacial drag formulation is used to describe them in a volume-of-fluid-like manner. For the dispersed structures, the baseline model developed at Helmholtz-Zentrum Dresden - Rossendorf e.V. (HZDR) is applied. The functionality of the framework is demonstrated by several test cases, including a single rising gas bubble in a stagnant water column. Recent developments focus on the transition region, where bubbles are over- or under-resolved for Euler-Euler or for Volume-of-Fluid, respectively. The contribution will focus on an overview about the fundamentals of the MultiMorph Model and recent simulation results for a plunging jet, a stratified counter-current air-water flow and a column tray of a distillation column. The figure shows the numerical simulation of a plunging jet with the MultiMorph model with marked morphologies and phase transition regions.



Numerical prediction of flow morphologies in horizontal feed pipes

Thomas Höhne
Helmholtz-Zentrum Dresden-Rossendorf

Session: Numerics and methods

Two-phase flows in feed pipes of thermal separation columns have complex flow patterns and are difficult to predict during sizing and design for geometries with non-straight pipes. Numerical simulation codes have only been validated for very few pipe geometries. This work benchmarks the state-of-the-art Volume of Fluid model (VOF) and the Algebraic Interfacial Area Density model (AIAD) for the simulation of two-phase flow with the Euler/Euler CFD approach for straight pipes and horizontal bends as well as for different pipe diameters and flow rates. Both models are compared and shortcomings of the predicted velocity fields from AIAD in the vicinity of horizontal bends are highlighted. Predicted average phase fractions agree reasonably with experimental data. From the numerical results, recommendation for the selection of feed inlet device are derived.

Pragmatic modelling

On the importance of numerical calibration in recurrence CFD simulations

Hannes Lumetzberger, Daniel Queteschiner, Thomas Lichtenegger and Stefan Pirker
Johannes Kepler University, K1-Met

Session: Pragmatic modelling

Recurrence CFD (rCFD), aims at an efficient representation of long-term processes which slowly evolve on highly-dynamic pseudo-periodic flow fields. In the framework of rCFD, short-term full CFD simulations deliver recurrence databases of the governing flow. Based on statistical reasoning, rCFD then exploits these databases in order to evolve generic flow fields, which subsequently serve as basis for the long-term process under consideration.

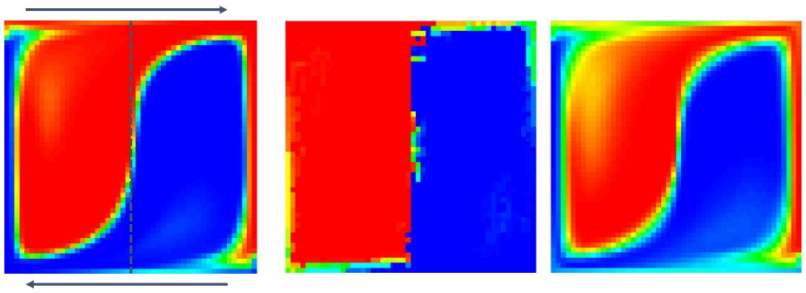
In transport-based rCFD, transport processes are modelled by a time-series of cell-to-cell shift patterns and face swap patterns, representing convection and diffusion. In applying rCFD to a set of single-phase and multiphase flows, we experienced a computational speed-up of up to four orders of magnitude.

Despite these successes, rCFD still faces open challenges, especially in cells of slow velocity where convection can hardly be represented by cell-to-cell shifts. In such cells, propagation of information is only enabled by isotropic face swaps, which might deteriorate rCFD predictions.

In this talk, we therefore present a novel numerical calibration method, aiming at levitating this existing limitation of rCFD. Based on a continuous displacement fields, which are extracted from full CFD simulations, we calibrate our cell-to-cell shift patterns such that information propagation is guaranteed in all cells, regardless of their flow velocity (see **Fig.1**).

After presenting this novel calibration methodology and thoroughly discussion first results of a lid-driven cavity test case, we apply our calibrated rCFD to the industrial process of grade change in a steel tundish.

Fig.1: Numerical simulation result of species propagation in a cubical lid-driven cavity – initially the left side was filled with red and the right side was filled with blue: **(left)** full CFD simulation, **(middle)** standard rCFD simulation with unfavorably small time-step width and **(right)** calibrated rCFD simulation with the same time-step width.

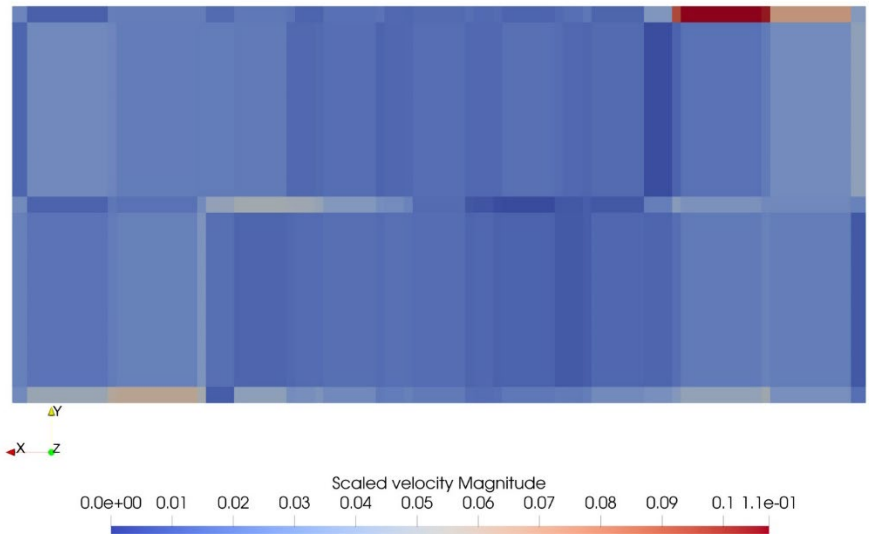


A pragmatism-based model of alumina distribution in industrial Hall-Heroult cells

Stein Tore Johansen,
SINTEF Industry

Session: Pragmatic modelling

We present a pragmatic computational model, which can be employed as a physics-based digital twin, and is used to simulate Alcoa's aluminium reduction cell. The model predicts the evolution of dissolved and particulate alumina in the electrolytic bath. In addition, we may solve for passive tracer distribution and the bath temperature. The model also includes simplified treatment of anode effects and loss of alumina due to sludge formation. The bath flow in the model is based on a detailed magnetohydrodynamic CFD simulation that is corrected to be mass conserving. The model predictions, using relevant initial conditions and operational settings (e.g., feeding patterns), are compared with detailed measurements of dissolved alumina and tracer during two industrial measurement campaigns. The comparison of the spatial and temporal evolution of tracer predicted by the model matches quite well with the experimental data. The model is able to predict the experimental observations of dissolved alumina by using a sludging coefficient. The simulations also indicate that the sludging and a corresponding self-feeding mechanism is a very local and very slow transient phenomena. The model has also been used to simulate the evolution of representative bath temperatures in the cell. Despite the simplifications, the model has been shown to be able to reliably model an industrial aluminium reduction cell at a low computational overhead.



A practical approach to calculating inertial forces for non-trivial subsea structures using CFD simulation

Maciej Kryś
TechnipFMC, Krakow, POLAND

Session: Pragmatic modelling

Subsea production systems often need extra protection to prevent equipment damage from dropped objects or trawling. This protection can be integrated into the foundation or provided as standalone equipment. One case of standalone protection structure is a Glass Reinforced Plastic (GRP) cover, which has the advantage of being lightweight, reducing manufacturing and installation costs. Low weight can however pose risks, especially in shallow water regions where storm events have a greater impact on flow conditions near the seabed. To prevent uncontrolled displacement of the GRP covers, they must be stabilized using rockdumps. However, it may be challenging to optimize the volume of rocks needed to mitigate the risk. The ballast weight must overcome the forces from the sea current and waves. On the other hand, excess of rocks will increase installation costs. [1] offers guidelines for computing forces on subsea structures, but the drag and inertia coefficient formulas are limited to simple geometries. Therefore, accurate force computation for more complex structures requires CFD simulations or experiments. When estimating forces, it's important to consider both drag - and inertia force generated by the oscillating velocity field from ocean waves. In fact, in storm conditions the inertia force is dominant. Although modern CFD tools typically have little trouble estimating drag force for similar geometries, inertia force may present a greater challenge in generating simulation inputs, solving, or post-processing stages. A simple procedure has been developed to calculate the maximum horizontal force that a GRP cover may experience during extreme weather conditions. Using the Morison equation and a simple curve-fitting procedure, it is also possible to estimate both drag and inertia coefficients for a specific geometry.

References

[1] DNVGL-RP-N103 "Modelling and analysis of marine operations"

A novel practical approach to cool down time thermal analyses in the oil and gas field

Mateusz Szubel, Damian Dywan
TechnipFMC

Session: Pragmatic modelling

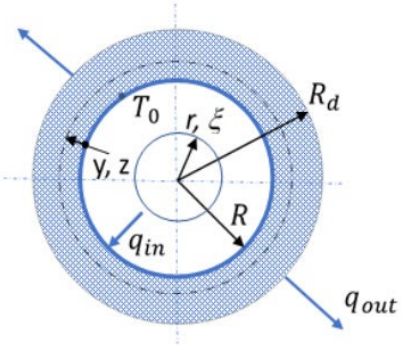
Over the years, physical tests have been pivotal in evaluating the thermal performance of subsea Oil and Gas production systems. However, the substantial costs associated with these tests have consistently driven efforts towards more cost-effective alternatives. Consequently, numerical modeling has become an indispensable tool in the subsea oil and gas production sector. A prevalent challenge in this field revolves around the risk of hydrate formation within subsea production systems (SPS) exposed to low temperature and high pressure. While Computational Fluid Dynamics (CFD) offers insights into production fluid cooling within the SPS, it remains computationally expensive. Conversely, Finite Element Analysis (FEA) lacks the ability to solve fluid movement, rendering it impractical for this purpose. This paper introduces an innovative 'iterative-FEA' approach aimed at maintaining the accuracy of SPS cool-down simulations, typical for CFD, while significantly reducing calculation time to a level akin to FEA modeling. To assess this method's effectiveness, the authors modeled flow system test cases using both CFD and iFEA methods. The CFD models were solved using Ansys Fluent, while iFEA simulations were conducted with the Ansys Thermal module alongside a set of original APDL scripts. To validate the computational results, a full-scale experimental rig was constructed, incorporating a dummy SPS section immersed in a water container and equipped with a comprehensive data measurement and acquisition system. The rig simulated the system's operation and underwent experimental testing using three distinct working fluids: water, air, and diesel oil. In analyzing the dynamics of fluid temperature change, the iFEA simulation results aligned with the experimental data as accurately as the CFD cases but within significantly shorter simulation times. This achievement represents a breakthrough in industrial SPS thermal simulations.

A Model of Freezing a Sea-Water Droplet Moving in a Cold Air

Dmitri Eskin, University of Alberta, Canada
Georgii Fisher, Mikhail Vulf,Svyatoslav ChugunovSkolkovo Institute of Science and Technology, Russia
Stein Tore Johansen, SINTEF

Session: Pragmatic modelling

A rapid freezing of a sea-water droplet moving in a cold air is modeled. A droplet freezing model is a key component needed for computational forecasting of ice accretion on surfaces of ships and other equipment operating in low-temperature regions. The freezing process consists of the three stages: 1) water cooling to the incipient solidification temperature; 2) liquid solidification; 3) further freezing of the primarily solidified droplet. An icy region, being formed during the 2nd stage, initially represents a slurry, composed of ice crystals suspended in water. Further cooling is associated with an increase in the crystal concentration that at a certain threshold causes slurry transformation into a spongy (porous) ice. The solidification stage model is composed of the three coupled differential equations formulated in the moving coordinate system. All the thermo-physical parameters, required for modeling droplet freezing, are calculated by using the empirical correlations. The set of the equations is solved numerically. The solidification process is illustrated by computational examples for different droplet sizes and water salinities. The computed icy region thickness vs. time, as well as temperature distributions and porosities along droplet radius at different time moments are shown.



Multiphase CFD model of plugging in cohesive slurries

Boris Balakin*, Pavel Struchalin
Høgskulen på Vestlandet

Session: Pragmatic modelling

Plugging of flow channels by cohesive particles is a critical problem in medicine, energy technology, petroleum, and communal water distribution. Plugging risk management would benefit from reliable numerical models of the process. However, only simplified models incapable of reproducing the entire process at industrially-relevant scales have been reported so far. Bridging the gap, in this paper, we present a pragmatic Eulerian-Eulerian model of plugging in pipes with local flow restrictions. The model accounts for the cohesion of particles via rheological expressions. The model consists of several user-defined modules incorporated in the commercial STAR-CCM+ and adaptable to other CFD packages. We further demonstrate how this model validates against flow loop experiments on plugging in ice-in-oil slurries.

Reactive Flows

Development of a CFD model for a gas-lift chemical reactor

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Session: Reactive Flows

1-Hexene serves as a pivotal constituent in the fabrication of industrial polyethylene materials. Functioning as a precursor, 1-Hexene facilitates the production of superior-quality polyethylene products while concurrently mitigating plastic consumption through its provision of barrier properties to thinner films. The utilization of ethylene trimerization reaction within a tubular gas-lift reactor configuration1, encompassing gas distribution volumes, reactor dimensions (riser-lower tube assemblies), and a gas-liquid separator, emerges as a promising technology for the synthesis of 1-Hexene. Nonetheless, this technique necessitates further hydrodynamic scrutiny to optimize its operational efficiency. In pursuit of this optimization, a comprehensive industrial plant 3D Computational Fluid Dynamics (CFD) model has been devised to forecast gas hold-up, liquid circulation dynamics, and localized concentration profiles of constituents within a 1-Hexene production gas-lift reactor. Methodological frameworks for multiphase hydrodynamics have been preliminarily investigated through a single-tube model (Fig. 1). Calibration of model parameters has been performed in accord with equation of state formulations, Henry's law principles, mass transfer criteria, diffusion models, viscous flow laws, multiphase modeling techniques, and both single-step and multi-step chemical kinetics, alongside considerations for heat transfer dynamics. Subsequently, the validated parameters have been extrapolated to a full industrial-scale steady-state CFD model. Validation of the model has been undertaken against experimental and analytical datasets acquired from a pilot plant reactor. Encouragingly, the CFD model exhibits a reasonably close agreement with pilot experimental data, with the accuracy of mass fraction predictions for outflow components in vapor and liquid phases falling within a range of ±10%. The progression toward a transient model promises to deliver insights into pivotal operational parameters such as the circulation ratio of the mixture within tubes, the uniformity of gas saturation across the entire volume, and the conversion rate under prescribed operating conditions. [1] Kulchakovskii, P.I. and Arkatov, O.L. (2021) 'Process for trimerization of ethylene and apparatus for trimerization of ethylene'.

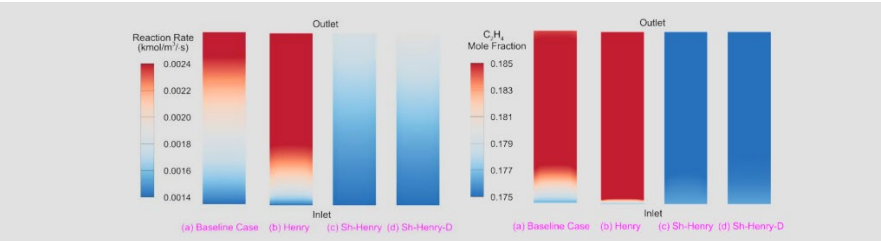

Figure 1: preliminar investigation of the computational framework.

CFD Simulation of Natural Gas and Hydrogen Oxyfuel Combustion: Comparison of kinetic mechanisms, combustion mechanisms and WSGG radiation models

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Department for Industrial Furnaces and Heat Engineering, RWTH Aachen University

Session: Reactive Flows

Oxyfuel Combustion is a well-known technique to enhance energy efficiency and CO2-emissions compared to conventional air-fired combustion. To not just reduce on-site fuel consumption but eliminate the combustion related CO2-emissions in accordance with the European Green Deal, switching to hydrogen as a fuel is an option, especially for energy intensive and hard to abate industries like steel and glass making. CFD simulation is an established method for quick and cost-efficient investigation of the influence of parameters on processes and identifying an opti-mum parameter set with less complex and expensive experiments. But many of the existing models used in CFD codes are developed and validated for natural gas combustion with air. A literature review was carried out to identify suitable models for oxyfuel combustion. The present paper gives an overview over the available kinetic mechanisms, the combustion mechanisms and the Weighted-Sum-of-Gray-Gases radiation models applicable for Natural Gas respectively Hydrogen oxyfuel combustion. CFD simula-tions of a 25 kW oxyfuel furnace with selected model combinations were carried out and compared and validated against experimental data collected from the furnace. An efficient and sufficiently accurate modelling approach for both fuels under oxy-fuel conditions is identified which then can be safely used for hard-to-validate simu-lations of industrial processes under oxyfuel conditions.

Comparison of dimethyl ether and natural gas combustion in a swirl-stabilized industrial burner using CFD simulations

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The European Green Deal aims to make Europe the first climate-neutral continent by 2050, necessitating the European Union to transform its energy system for affordability, efficiency, and circularity. Biofuels will play an important role in this energy transition. One such biofuel is Dimethyl ether (DME). It is a hydrocarbon that can, among other things, be synthesized from waste and residual feedstocks. The DME produced in this way is also called “renewable dimethyl ether” (rDME) and can reduce the carbon footprint of energy-intensive processes by replacing fossil fuels. Another advantage of DME over fuels such as hydrogen is its good transportability. Similar to LPG, DME can be liquefied at pressures below 10 bar. This allows for easy handling at comparably low pressures. The combustion of DME within internal combustion engines is well researched. In addition, there are initial studies that deal with the combustion of DME within industrial burners. This paper builds on this work. First, a literature research was carried out on the existing kinetic mechanisms of DME combustion and examined in relation to the set requirements. Subsequently, CFD simulations of a baffle and swirl-stabilized industrial burner within a burner test rig were carried out. In addition to DME, natural gas was also used as fuel in order to compare the combustion characteristics of DME and natural gas in an unmodified burner.