## **BOOK OF ABSTRACTS FOR CFD2017**

The program serves as a list of contents. All program titles serves as links to an abstract.

#### Monday May 29th

1800-1930 Conference reception (drinks and snacks) at Scandic Nidelven (conference hotel)

### Tuesday May 30th

	Auditorium 1	Auditorium 2	Auditorium 3
0730-0815	Registration		
0815-0830	Opening		
0830-0930	Keynote: Jørn Kristiansen		
	Under the hood of Yr		
0930-1100	Pragmatic Modelling	Population balance	Non-newtonian flows
	Chair: Jørn Kristiansen	Chair: Jannike Solsvik	Chair: Paal Skjetne
0930-1000	109: On pragmatism in industrial modelling.	10: CFD simulation of the droplet size	90: Front-tracking simulations of bubbles
	Part III: Application to operational drilling ,	distribution of liquid-liquid emulsions in stirred	rising in non-newtonian fluids , Battistella, van
1000 1020	72: CED modeling of dungmic emulsion	9: A multifluid PRE model for a slurpy hubble	21: Viscoalastic flow simulations in disordered
1000-1020	stability Patil Johansen	S. A multiplaid-PBE model for a starty bubble	porous media. De Kuipers, Peters & Padding
	stability , Fath, sonailsen	weight fractions and temperature, Vik,	porous mean, be, kaipers, recers er addnig
		Solsvik, Engh, Hillestad & Jakobsen	
1020-1040	127: Modelling of interaction between	3: Combined multifluid-population balance	69: Tire rubber extrudate swell simulation and
	turbines and terrain wakes using pragmatic	method for polydisperse multiphase flows ,	verification with experiments , Buist, van Dijk &
	approach, Røkenes, Panjwani, Lund, Samseth	Vikhansky	Mateboer
1040-1100	8: Recurrence CFD (rCFD) – Why don't run	12: Towards a CFD model for boiling flows:	102: A 2D sediment bed morphodynamics
	Scale resolved simulations in realtime?	Validation of QINUN predictions with	model for turbulent, non-Newtonian, particle-
		Marchisio Montova Baglietto	iouueu jiows, Busch, Khatibi, Johansen & Time
1100-1130	Break		
1130-1300	Breakup & Coalescence	Industrial applications	Euler-Lagrange
	Chair: Ivo Roghair	Chair: Yuqing Feng	Chair: Stefan Pirker
1130-1200	6: Experimental and numerical study on single	122: Experimental and CFD investigation of	13: Implementing the Kinetic Theory of
	droplet breakage in turbulent flow , Shi, Herø,	fractal distributor on a novel plate and frame	Granular Flows into the Lagrangian Dense
1005	Solsvik & Jakobsen	ion-exchanger , He, Kochergin, Li & Nandakumar	Discrete Phase Model , S.Cloete & Amini
1200-1220	78: Controlled coalescence with local front	41: Use of CFD as a design tool for a	80: Importance of the different fluid forces on
	reconstruction method , Rajkotwala et.dl.	Phospheric acid plant cooling pond , Davailles	particle dispersion in fluid phase resonance
1220-1240	39:Improved collision modelling for liquid	113: Urban Wind at the Gløshaugen Campus	91: Large scale modelling of bubble formation
1220 1240	metal droplets in a slag cleaning process;	Almeida, Simonsen & Sætran	and growth in a supersaturated liquid ,
	Yang, Wolters, Pischke, Soltner, Eckert & Fröhlich	· · · · · · · · · · · · · · · · · · ·	Battistella, Aelen, Roghair & van Sint Annaland
1240-1300	77: Modelling of bubble dynamics in slag	141: Numerical simulation on a high head	145: The dependence of the drag and lift of
	during its hot stage engineering , Wang, Cao,	Francis turbine, Tengs, Storli & Holst	non-spherical particles , Sanjevi & Padding
	Blanpain, Vanierschot & Guo		
1300-1400	Lunch	Lunch	Lunch
1400-1500	Keynote: Omar K. Matar / Damir Juric		
	challenges in the oil & gas industries		
1500-1630	Oil & Gas	DEM	CED codes
1500 1050	Chair: Dmitry Eskin	Chair: Alice Hager	Chair: Thomas Höhne
1500-1530	75: Direct numerical simulation of proppant	85: Adaptive coarse-graining for large-scale	139: Multiphase modelling by ANSYS and
	transport in a narrow channel for hydraulic	DEM simulations, Queteschiner, Lichtenegger,	recently implemented features;
	fracturing application , Maitri et.al.	Schneiderbauer & Pirker	A.Kvarnström
1530-1550	106: CFD erosion modelling of blind tees ,	79: A numerical approach to model aggregate	136: SOFT: a framework for semantic
	Sanchis, Skorgen	restructuring in shear flow using DEM in	interoperability of scientific software;
		Lattice-Boltzmann simulations , Saxena, Kroll-	Hagelien, Chesnokov, Johansen, Meese &
1550 1610	A2: Estimation of flow rates and parameters in	Rabotin & Sanders	LØVTall
1550-1010	two-phase stratified and slua flow by an	of a lab-scale pressurized fluidized hed using	relevant multiphase flows . Juric. Chergui, Shin.
	ensemble Kalman filter , Ferrari, Bonzanini,	a LES-DEM approach , Nigmetova, Dufresne,	Kahouadji, Craster & Matar
	Arioli, Poesio	Masi, Moureu, Fede & Simonin	
1610-1630	101: Multiphase Direct Numerical Simulations	130: On an efficient hybrid soft and hard	61: Development of gpu parallel multiphase
	(DNS) of oil-water flows through homogeneous	sphere collision integration scheme for DEM ,	flow solver for turbulent slurry flows in
	porous rocks, Patel, Kuipers, Peters	Buist, Seelen, Deen, Padding & Kuipers	cyclone , Mayank, Banerjee & Narasimha
1630-1700	Break	Вгеак	Break
1700-1830	Fluidized bed 1	Combustion	Immersed Boundary
1700 1720	Chair: Pascal Fede	Chair: Phil Schwarz	Chair: Bernhard Muller
1700-1730	with horizontally immersed membranes	and alternative carbon materials in the blast	Heat and Mass Transfer in Fluid-Solid
	Voncken, Roghair & van Sint Annaland	furnace raceway. Ölund	Systems . Lu. Peters & Kuipers
1730-1750	2: CLC process in a double looping fluidized	119: Combustion chamber scaling for energy	38: Immersed boundary method for the
	bed reactor with NI-based oxygen carriers ,	recovery from furnace process gas: waste to	compressible Navier-Stokes equations using
	Zhang, Chao & Jakobsen	value, Panjwani, Wittgens & Olsen	high order summation-by-parts difference
			operators , Khalili, M. E Larsson, M Müller, B
1750-1810	24: Extremely fast simulations of heat transfer	30: CFD modeling of a commerical-size circle-	110: A simulation concept for generic
	in jiulaizea beas , Lichtenegger & Pirker	arajt biomass gasifier , Liu, Cattolica, Seiser,	simulation of multi-material flow, using
1810-1920	137: The peculiar behaviour of elegated	70: Numerical study of coal particle	112: A cartesian cut-cell method, based on
1010-1030	narticles in fluidized bade: experiments versus	agification up to Reynolds numbers of 1000	formal volume guaraging of mass
	Durticles III IIuluizeu Deus, extremmentis versus		
	simulations, Mahajan, Nijssen, Kuipers &	Kriebitzsch & Richter	momentum equations . Dang, Johansen &

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### Wednesday May 31st

	Auditorium 1	Auditorium 2	Auditorium 3
0815-0830	Registration		
0830-0930	Keynote: Pascal Gardin		
	CFD as a tool to understand and optimize		
	metallurgical processes	- · · ·	
0930-1100	Metallurgy 1	Packed bed	Species & Interfaces
	Chair: Pascal Gardin	Chair: John Morud	Chair: Stein Tore Johansen
0930-1000	37: Experimental modelling of metallurgical	56: Numerical investigation of particle types	104: Multiscale approach to fully resolved
	processes , Gerbeth & Eckert	Influence on packed bed adsorber behaviour ,	boundary layers using adaptive grids , Panda,
1000 1020	21: Production of wall strasses in a steal	Haddadi, Jordan, Norouzi & Harasek	Peters, Baltussen & Kulpers
1000-1020	making ladle during graon gas purging	senaration processes Eggers Dewulf	surface active species transport - reaction in
	Mantrinragada & Sarkar	Baelmans & Vanierschot	welding processes Dorogan
1020-1040	54: State of the art: macroscopic modelling	50: Comparison of particle-resolved direct	83: Implementation, demonstration and
	approaches for the description of multiphysics	numerical simulation and 1D modelling of	validation of a user-defined wall function for
	phenomena within the electroslag remelting	catalytic reactions in a packed bed , Singhal,	direct precipitation fouling in Ansys Fluent ,
	process , Schubert,Rückert & Pfeifer	S.Cloete, Radl, Quinta-Ferreira & Amini	Johnsen, Pääkkönen, Johansen, Keiski & Wittgens
1040-1100	66: LES-VOF simulation of turbulent interfacial	67: A multi-domain 1D particle-reactor model	138: Adsorption-desorption modeling for a
	flow in the continuous casting mold .	for packed bed reactor applications . Tabib.	chemical reaction using Stochastic Rotation
	Saeedipour, Puttinger & Pirker	S.Cloete, Morud, Lysberg & Amini	Dynamics , Sengar, Padding, Kuipers, Santen
1100-1130	Break	Break	Break
1130-1300	Biomechanics & Industrial applications	Metallurgy 2	Fluidized bed 2
	Chair: Sigrid Kaarstad Dahl	Chair: Eirik Manger	Chair: Shahriar Amini
1130-1200	64: Oscillatory flow and mass transport in a	93: Numerical predictions of the shape and	123: Development of filtered particulate
	coronary artery, Gabriel, Ding, Gear & Feng	size of the raceway zone in a blast furnace ,	Eulerian modeling approach for the industrial
		Safronov, Richter & Meyer	prediction of bi-disperse gas-solid fluidized
			bed , Chevrier, Fede, Masi & Simonin
1200-1220	55: Patient specific numerical simulation of	17: CFD-DEM modelling of blast furnace	25: Effect of lift force on dense gas-fluidized
	flow in the upper airways for assessing the	tapping , Vångö & Lichtenegger	beds of non-spherical particles, Mema,
	effect of nasal surgery , Jordal, Johnsen, Dahl &		Mahajan, Fitzgerald, Kuipers & Padding
1220 1240	Muller	52: Multiphase flow modelling of furnase	40: Experimental and numerical investigation
1220-1240	dimensional transient two-fluid model for	tanholes Beynolds & Frwee	45. Experimental and numerical investigation
	stratified and slug flow simulations in nines	tapholes, heyholds & Erwee	Vang, Dadding & Kuipers
	Bonzanini, Picchi, Ferrari & Poesio		rang, radding & Rupers
1240-1300	86: Numerical evaluation of co-firina solid	53: Solidification modeling with user defined	95: Direct numerical simulation of the effective
	recovered fuel with petroleum coke in a	function in ANSYS Fluent , Eickhoff, Rückert &	drag in gas-liquid-solid systems , Baltussen,
	cement rotary kiln: Influence of fuel moisture ,	Pfeifer	Kuipers & Deen
	Isaac, Pedersen, Grévain, Jensen & Nielsen		
1300-1400	Lunch	Lunch	Lunch
1400-1500	Keynote: Rajat Mittal		
	Multiphysics Computational Models of		
	Cardiac Hemodynamics: from Fundamental		
	Questions to Clinical Applications		
1500-1630	Biomechanics	Metallurgy 3	Fluidized bed 3
	Chair: Rajat Mittal	Chair: Sabita Sarkar	Chair: Hugo Jakobsen
1500-1530	73: Investigating the numerical parameter	11: Modelling of chemical reactions in	92: Verification of filtered two fluid models for
	space for a stenosed patient-specific internal	metallurgical processes , Kinaci, Lichtenegger &	reactive gas-solid flows , J.H.Cloete, S. Cloete,
	carotia artery model , Mancini, Bergersen,	Schneiderbauer	Radi & Amini
1520 1550	22: A computational framework involving CED	14: Using CED analysis to ontimise ton	AA: High temperature fluidization - influence of
1220-1220	and data analytics for analyzing cartoid-artery	submerged lance geometries Gwynn-Jones	inter-narticle forces on fluidization behavior
	hifurcation disease Tabib Fonn & Rasheed	et al	Mihailovic Roghair & van Sint Annaland
1550-1610	125: Velocity profiles in a 2D model of the left	20: Numerical analysis of the temperature	34: A Lagrangian-Eulerian hybrid model for the
	ventricular outflow tract, pathological case	distribution in a martensic stainless steel strip	simulation of direct reduction of iron ore in
	study using PIV and CFD modeling , Leinan ,	during hardening , Pirouznia, Andersson,	fluidized beds , Schneiderbauer, Kinaci,
	Skjetne , Morud, Urheim & Dahl	Tilliander & Jönsson	Hauzenberger & Pirker
1610-1630	68: CFD simulations of turbulent flow in the	124: Validation of a rapid slag viscosity	48: A Two-Fluid Model study of hydrogen
	human upper airways , Aasgrav, Johnsen,	measurement by CFD, Vandensande, Nagels &	production via Water Gas Shift in fluidized bed
	Simonsen & Müller	Arnout	membrane reactors, Voncken, Roghair & van
			Sint Annaland
1630-1700	Coffee/Snacks	Coffee/Snacks	Coffee/Snacks

1900-2230 CONFERENCE DINNER AT CONFERENCE HOTEL

### BOOK OF ABSTRACTS FOR CFD2017

#### Thursday June 1st

	Auditorium 1	Auditorium 2	Auditorium 3
0830-0930	Keynote: Niels Deen		
	Modelling and intensifying bubble		
	columns across the scales		
0930-1100	Bubbly flows	Fundamental fluid dynamics	Metallurgy 4:
	Chair: Niels Deen	Chair: Ernst Meese	Chair: Gunter Gerbeth
0930-1000	131: Bubble generated turbulence in two fluid	108: A DNS study of droplet spreading and	129: Modelling and measurements in the
	simulation of bubbly flow , Schwarz, Feng & Witt	penetration on a porous medium , Das, Milacic,	aluminium Industry - Where are the obstacles?
		Patel, Deen & Kuipers	Manger
1000-1020	35: Modelling of fluid dynamics, mass transfer	22: Flow past a yawed cylinder of finite length	51: Granular flow described by fictitious fluids: a
	and chemical reaction in bubbly flows, Rzehak &	using a fictitious domain method , Pierson,	suitable methodology for process simulations,
1020 1040	A 5: Stochastic DSMC model for large scale dense	114: From linear to poplinear: Transient arowth	118: Cleaning of Polycyclic Aromatic
1020-1040	bubbly flows. Kamath, Padding, Buist &	in confined magnetohydrodynamic flows.	118. Cleaning of Polycyclic Aromatic
	Kuipers	Cassells, Vo, Pothérat & Sheard	Aydrocurbons (PAA) obtained from
1040 1100	116: On the surfacing mechanism of hubble	6E: A numerical ovaluation of the offect of	115: A multiccale numerical approach of the
1040-1100	plumes from subsea gas release. Olsen &	the eletro magnetic force on hubble flow	dripping slag in the coke bed zone of a pilot
	Skjetne	in aluminium smolting process. Fong	scale Si-Mn furnace , Letout, Ratvik, Tangstad
1100-1130	Break	Break	Break
1130-1300	Free surface flow	Population balance 2	Heat transfer
	Chair: Mark Sussman	Chair: Daniele Marchisio	Chair: Maike Baltussen
1130-1200	46: Influence of the Upstream Cylinder and	28: Numerical simulations of tubulent	7: CFD-simulation of boiling in a heated pipe
	Wave Breaking Point on the Breaking Wave	liquid-liquid dispersions with quadrature-	including flow pattern transitions using a multi-
	Forces on the Downstream Cylinder , Kamath,A.	based moment methods , Buffo, Li,	field concept, Höhne, Krepper & Lucas
	et.al .	Podgórska, Vanni & Marchisio	
1200-1220	84: Recent developments for the computation of	18: Simulation of dispersion of immiscible	23: The Pear-Shaped Fate of an Ice Melting
	the neccessary submergence of pump intakes	fluids in a turbulent couette flow ,	Front , Hewett, J.N. and Sellier
	with free surfaces, Bloemeling, F. and Lawall, R.	Vikhansky & Eskin	
1220-1240	126: Parallel multiphase flow software for	26: Simulation of aas-liquid flows in separators -	107: An Euler-Euler Model for Gas-Liquid Elows
1220 1240	solving the navier-stokes equations, Al-Rashed,	a Lagrangian approach , Morud, J.C. and Dahl,	in a Coil Wound Heat Exchanger, Acher, Knaup,
	F. S. and Shariff M.M.	S.K.	Braun & Zander
1240-1300	43: Unresolved CFD-DEM in environmental	76: CFD modelling to predict mass transfer in	103: Flow dynamics studies for flexible
	engineering: submarine slope stability and other	pulsed sieve plate extraction columns , Sen,	operation of continuous casters (flow flex cc),
	applications , Hager, A.et.al.	Singh, & Shenoy	Forslund, Barestrand, Ramirez Lopez, Jalali,
1300-1400	lunch	Lunch	
1400-1500	Keynote: Mark Sussman		
	A new paradigm for numerically		
	simulating multiscale phenomena using		
	the multimaterial moment of fluid method		
	and block structured adaptive mesh		
	refinement: applications to marine		
1500-1530	Summary / Coffee & snacks		

## **Conference sponsors:**







## UNDER THE HOOD OF YR

### Jørn KRISTIANSEN<sup>1</sup>

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Yr (www.yr.no), a collaboration between the Norwegian Meteorological Institute and NRK (The Norwegian Broadcasting Company), has advanced the dissemination of open weather information (Sivle et al. 2014s). Its impact since the start in 2007 is measurable: It is the world's 5th largest online weather service (largest outside USA); Peek value of about 9.5 million unique users per week; On the order of 100 million requests per day of weather data; Increased objective forecast skill; In Norway, Yr is synonymous to weather. A novelty is its point specific API. The short-term forecasts are updated four times per day from the regional numerical weather model AROME-MetCoOp (Müller et al. 2017), a configuration of HARMONIE-AROME<sup>1</sup> (Bengtsson et al. 2017), run in parallel on distributed high-performance computing facilities. MetCoOp is an operational collaboration between Swedish and Norwegian (and recently Finland) national meteorological institutes and is probably the first of its kind in the world. The forecasts are initialised (analysis) by using large amounts of observations to challenge and thereafter correct the previous forecast of the atmospheric state (e.g. Valkonen et al. 2017). From this analysis the weather is forecast (prognosis) by solving prognostic equations combining physics and dynamics on all spatial and temporal scales. The current model configuration is convection-allowing, i.e. explicitly representing physical phenomena down to and including deep convection. A timely weather forecast is unimaginable without high performance computers. To forecast the forecast uncertainty, AROME-MetCoOp is run as an ensemble of 10 almost identical forecasts but perturbed to represent the uncertainties in the analysis, model equations and lateral boundary conditions. This generates large amounts of data. Outside Norway the forecasts are based on the world-leading ECMWF model. Combining physics and statistics, the forecast data are then post-processed both in terms of correcting for local sources of error and product generation (Seierstad and Nipen, 2017). Good user-interfaces and feedback have been essential for advancing the forecast quality, data and products. The (almost) complete data set (real-time and archive) is made available on thredds.met.no which is built for an interoperable, distributed and metadata governed data distribution. It gives the opportunity for direct, real-time data streams into usersystems tailored to the user-needs. Yr has increased the effectiveness and automation of the weather service and is an example of modernization of the public sector in Norway. This again has increased the collaboration with various industries in different research projects, all supporting the development of the production chain for weather forecasting. One example is the collaboration with SINTEF on CFD, employing Simra to forecast turbulence at 20 Norwegian airports and over ocean

<sup>1</sup> HARMONIE-AROME is used for operational short range weather forecasts in Denmark, Estonia, Finland, Iceland, Ireland, Lithuania, Netherlands, Norway, Spain and Sweden. It is developed, maintained and validated as part of the shared ALADIN-HIRLAM system by a collaboration of 26 countries in Europe and Northern Africa on short range meso-scale NWP. HARMONIE-AROME is based on the model AROME-France developed within the ALADIN consortium.

(Süld et al. 2017; Rasheed et al. 2017). Future opportunities lies in combining the growing amount of user generated weather observations and information with the numerical weather models, e.g. machine learning and artificial intelligence, for mutual benefit between the national weather services and users of weather information, thereby improving their decision-making capabilities and creating novel new uses of weather data.

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URL: <u>http://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=7636992&isnumber=4609444</u>

## CFD AS A TOOL TO UNDERSTAND AND OPTIMIZE METALLURGICAL PROCESSES

## Pascal GARDIN<sup>1\*</sup>

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Tremendous progress was realised in the last ten years to better understand and control the flow fields in the steelmaking reactors.

The purpose of this paper is to illustrate some of the problems associated with steelmaking processes when multiphase flows and multi-physics are involved. It shows the different models used for the simulations, the status of the validation as well as the perspectives when developments are still necessary.

In general, the studies aim either at acquiring knowledge to better understand the behaviour of steelmaking processes or at predicting the influence of an actuator before it is built. Two types of tools can then be used:

• experimental equipment that meets certain similarity criteria (but rarely all),

• predictive mathematical tools, which can take into account several physical mechanisms, but most of the time physical models must be validated.

Two processes are mainly discussed. The first one is the steel ladle, which is a key process for adjusting the liquid steel composition and eliminating the inclusions. Pneumatic stirring with argon bubble injection is the main contribution for steel movement. Different phases are simultaneously interacting: liquid steel, top slag layer, argon bubbles and inclusions. When composition adjustment should be performed, thermodynamics is considered and coupling with CFD for each cell of the mesh is realised.

The second process is the continuous casting machine, where the liquid steel is solidified. Once again it is a multiphase system, but solidified shell should be added. The key issues are the control of the solidification homogeneity and the limitation of the particle entrapment by the mushy shell. Different actuators are investigated by the CFD to "create" the good flow organisation inside the mould; main actuator is the shape of the submerged entry nozzle but more complex actuators could be tested, such as electromagnetic equipment.

For those two processes, a special emphasis to the validation of the mathematical models is given and perspectives for the further developments that should be performed are proposed.

# MODELLING AND INTENSIFYING BUBBLE COLUMNS ACROSS THE SCALES

### Niels G. DEEN \*

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In this keynote lecture I will discuss computational modelling of bubbly flows. One of the main issues of bubbly flows is the large separation of scales, i.e. systems often have the scale of O(m), whereas the flow in these systems is generated by bubbles of the size of O(mm). Modelling these systems poses a big challenge.

In the lecture I will give an overview of recent activities to close this gap.

This includes the modelling of reactive bubbly flows, and attempts to intensify bubbly flow reactors by improving the mass transfer. The latter is done by introducing a wire mesh in the bubbly flow that acts to cut large bubbles into smaller pieces.

A proof-of-principle of a micro-structured wire-mesh reactor is presented by means of lab-scale experimental data and macroscopic Euler-Lagrange numerical simulations. The latter make use of empirical closures for the bubble-wire interaction closures, which will be compared with DNS results.

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## A HIERARCHICAL BLOCK STRUCTURED SPACE-TIME SPECTRAL ELEMENT METHOD FOR SIMULATING COMPLEX MULTIPHASE FLOWS

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Progress in two projects will be presented.

For the first project, A new parallelized hierarchical space-time spectral element method has been developed for simulating multiphase compressible or incompressible flows in which the bulk regions of one or more of the fluids can be complex. Such flows occur in the study of ocean currents (Smith et al, 2014), atomization and spray in combustion engines (Li and Soteriou, 2016), and bubbly flows (Thomas et al, 2015). In previous work in simulating multiphase flows on a hierarchical block structured adaptive grid (Li and Soteriou, 2016; Jemison et al 2014), the level of efficiency of dynamic adaptive mesh refinement had to be decreased because the numerical solution on coarse levels was overly damped, resulting in incorrect feedback on multiphase interface(s), or retarding naturally occurring nonlinear flow phenomena. We shall present original work in which the solution in spectral elements spanning a single material is represented with space-time spectral accuracy (Minion 2004; Kadioglu et al 2008; Pei et al 2016). The discretization in multimaterial (>1 material) elements is the same as in our previous work (Jemison et al 2014). Our present hierarchical adaptive mesh strategy is to prescribe the highest order spectral elements on the coarse adaptive levels, and progressively reduce the order on finer levels. In the Figure below (coarsest level: 16<sup>th</sup> order; level 1: 8<sup>th</sup> order; level 2: 4<sup>th</sup> order; level 3: 2<sup>nd</sup> order), we show the simulation of bubble formation at a nozzle corresponding to the experiments of Helsby and Tuson (1955). The moment of fluid method

(Jemison et al 2014) captures the interface break up. A relatively easy to implement multigrid preconditioned BiCGSTAB (MGPBiCG) algorithm has been developed for the variable density projection equation on our new hierarchical adaptive spectral element grid. The efficiency of the MGPBiCG solver is comparable to that of the lower order MGPCG counterpart.

For the second project, a new algorithm for solving elliptic equations on (deforming) multimaterial regions (e.g. > 2 materials) has been developed. The material regions are represented sharply by the moment of fluid reconstructed interface. The moment of fluid method is amenable to representing thin filamentary materials. In previous work by Jemison et al (2015), a moment of fluid algorithm was developed for capturing deforming filaments in prescribed flows. In the present, a new algorithm has been developed for solving the heat equation in filamentary regions. The motivation for this work is the application to boiling problems with thin thermal layers and thin liquid films, and the application to predicting the initial stages in solidification (icing) problems (Vahab et al 2016).

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## 002: SIMULATION OF CHEMICAL LOOPING COMBUSTION IN A DOUBLE LOOPING FLUIDIZED BED REACTOR WITH CU-BASED OXYGEN CARRIERS

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## ABSTRACT

Chemical looping combustion (CLC) is an attractive technology that produces a pure CO2 stream and therefore the CO2 can be readily recovered by condensing water vapour. In order to understand the physical phenomena and to explore the chemical process performance of the CLC process, a CFD model has been developed. The model is implemented numerically in an in-house code including the kinetic theory of granular flow and reaction models. Methane is used as fuel and CuO is chosen as oxygen carrier. This process is configured with an air reactor and a fuel reactor. The two reactors are simulated by a sequential approach. The connection between the two reactors is realized through time-dependent inlet and outlet boundary conditions. The widely used drag models were selected to examine their effects on the flow behaviour. The results indicating that the cluster effect in the FR is higher than in the AR. The frequency factor in the reaction model was varied to fit with the experimental measurements. The predicted result with the frequency factor of  $1.35 \times 10^{-3}$  gives a reasonable prediction in comparison to the experimental data.

## 003: COMBINED MULTIFLUID-POPULATION BALANCE METHOD FOR POLYDISPERSE MULTIPHASE FLOWS

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## ABSTRACT

In the present work we analyse applicability of the adaptive multiple size-group (A-MuSiG) population balance method to modelling of multiphase flows. The dispersed phase is split into M size-groups, each one having its own mass- and momentum balance. An additional equation for the number density makes the method adaptive, that is, the groups sizes are not prescribed a priory, but calculated. A special attention is paid to the effect of the turbulent diffusion on size distribution. The method is implemented in the multiphase CFD code STAR-CCM+ of Siemens PLM Software.

## 006: EXPERIMENTAL AND NUMERICAL STUDY ON SINGLE DROPLET BREAKAGE IN TURBULENT FLOW

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### ABSTRACT

Droplet size distributions in liquid-liquid turbulent flow are determined by droplet breakage and coalescence. The current understanding of these processes are not sufficient. An experimental study on single droplet breakage in turbulent flow, where coalescence can be neglected, is presented in this paper to study the droplet breakage mechanism. A rectangular channel consisting of a pair of opposite steel walls having a series of stationary protuberances to enhance turbulence level, and a pair of opposite glass walls that are smooth to facilitate image capture of the droplet breakage process is used as the droplet breakage channel. The commercial CFD code FLUENT is utilised to simulate the continuous single-phase flow in the droplet breakage channel with interest particularly in the turbulent characteristics such as the turbulent kinetic energy and turbulent energy dissipation rate, as these parameters are closely related to the droplet breakage process. The large eddy simulation (LES) method was used to provide detailed features of the flow. Results from LES were also compared with those from a RANS model (SST k- $\omega$ ). The simulation results demonstrated that the turbulence level is enhanced across the pair of walls with protuberances. Some preliminary experimental results on droplet breakage are also presented.

## 007: CFD-SIMULATION OF BOILING IN A HEATED PIPE INCLUDING FLOW PATTERN TRANSITIONS USING A MULTI-FIELD CONCEPT

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### ABSTRACT

The paper presents the extension of the GENTOP model for phase transfer and discusses the submodels used. Boiling flow inside a wall heated vertical pipe is simulated by a multi-field CFD approach. Sub-cooled water enters the pipe from the lower end and heats up first in the near wall region leading to the generation of small bubbles. Further along the pipe larger and larger bubbles are generated by coalescence and evaporation. This leads to transitions of the two-phase flow patterns from bubbly to churn-turbulent and annular flow. The CFD simulation bases on the recently developed GEneralized TwO Phase flow (GENTOP) concept. It is a multi-field model using the Euler-Euler approach. It allows the consideration of different local flow morphologies including transitions between them. Small steam bubbles are handled as dispersed phases while the interface of large gas structures is statistically resolved. The GENTOP sub-models and the Wall Boiling Model need a constant improvement and separate, intensive validation effort using CFD grade experiments.

# 008: Recurrence CFD (rCFD) – Why don't run scale resolved simulations in realtime?

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Keywords: Multiple Time-scales, Large Eddy Simulations, Realtime Simulations

## ABSTRACT

Scale-resolved simulations or multiphase simulations require high spatial and time resolutions with associated high computational costs. Therefore, addressing long term processes is cumbersome if not hopeless.

Often unsteady processes can be characterized by recurring flow pattern. In this case the time-scales of flow dynamics and process operation can be separated. By means of recurrence CFD (rCFD) we compose a generic flow on the basis of recurrence statistics, which is then used to study e.g. turbulent mixing or heat transfer at very low computational costs.

In a first part we test rCFD with two multiphase configurations – heat transfer in a fluidized bed and a bubble driven loop reactor. In both cases we could speed-up simulations by <u>two</u> orders of magnitude while still operating on original spatial grid resolution. At the same time rCFD predictions agree very well with corresponding full CFD simulations.

In a second part we abstracted the concept of rCFD by focusing on recurring pattern of memory redistribution rather than focusing on recurring flow pattern. In a first example of single phase turbulent mixing, we could accelerate a Large Eddy Simulation on a 650k grid by <u>four</u> orders of magnitude, while still getting reasonable results at full resolution.

By means of rCFD classical CFD simulations can be transformed into realtime simulations.

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## 009: A MULTIFLUID-PBE MODEL FOR A SLURRY BUBBLE COLUMN WITH BUBBLE SIZE DEPENDENT VELOCITY, WEIGHT FRACTIONS AND TEMPERATURE

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### ABSTRACT

With kinetic gas theory as a starting point, equations of change for total mass, species mass, momentum and inner energy are developed for the dispersed gaseous phase and implemented to describe the Fischer-Tropsch synthesis carried out at industrial scale. The resultant model describes bubble velocity, composition and temperature in the gaseous phase as function of axial position and bubble size. The bubble size is found from the population balance equation (PBE) using a continuous mass density function which is calculated explicitly and used as basis for the gas-liquid transfer fluxes of species mass, momentum and heat. In the Fischer-Tropsch synthesis reactants are transported from inside gas bubbles through the gas-liquid interface into the liquid phase and subsequently into the catalyst pores to form hydrocarbon products at the active sites on the catalyst surface. Higher catalyst loading requires a higher mass transfer from the gas bubbles to the liquid phase and may cause the overall reaction to become mass transfer limited. In order to optimize reactor design, knowledge of the bubble size may thus be of importance. The liquid and solid phases are modelled using conventional continuum mechamics equations of change. The results of the simulations show that the weight percent of reactant varies by 20 percentage points from the smallest to the largest bubble size and thus a significant level of detail is added to the model when including bubble size in the mass fraction variable. For temperature the particle size dependency is negligible at the same conditions. It is noted that firm conclusions on the mass and heat transfer limitations can only be drawn when reliable estimates of the transfer coefficients are available.

## 010: CFD SIMULATION OF THE DROPLET SIZE DISTRIBUTION OF LIQUID-LIQUID EMULSIONS IN STIRRED TANK REACTORS

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## ABSTRACT

Predicting the drop size distribution (DSD) is essential in particulate flows such as emulsions as it affects mass transfer and heat transfer. In the current work we developed a novel numerical method to account for droplet breakup. The droplet breakup relies on an in-house developed correlation which depends on the local shear rate and some fluid properties. Commonly, a population balance equation (PBE) is employed to describe the breakup and coalescence of the droplets; however, such an approach does commonly not distinguish between different slip velocities of the smaller and larger droplets. Therefore, we propose a hybrid modelling strategy, which combines an Eulerian-Eulerian two-fluid model (TFM) and a Lagrangian discrete particle model (DPM), which is referred to as the Hybrid TFM-DPM model. This method enables the efficient evaluation of the poly-disperse liquid-liquid drag force form the local distribution of the different droplet diameters. The latter can be obtained by tracking statistically representative droplet trajectories for each droplet diameter class. Finally, we applied this novel approach to a liquid-liquid emulsion in a stirred tank presented. The results clearly show that the present method is able to predict the droplet size distribution for different rotational speeds of the stirrer.

## 011: MODELLING OF CHEMICAL REACTIONS IN METALLURGICAL PROCESSES

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## ABSTRACT

Iron-ore reduction has attracted much interest in the last three decades since it can be considered as a core process in steel industry. The iron-ore is reduced to iron with the use of blast furnace and fluidized bed technologies. To investigate the harsh conditions inside fluidized bed reactors, computational tools can be utilized. One such tool is the CFD-DEM method, in which the gas phase reactions and governing equations are calculated in the Eulerian (CFD) side, whereas the particle reactions and equation of motion are calculated in the Lagrangian (DEM) side. In this work, this method has been extended to cover the most common types of representation models for the reactions of solids submerged in fluids. These models are the Shrinking Particle Model (SPM) and the Unreacted Shrinking Core Model (USCM). With the use of the SPM, the implemented communication framework between the CFD and DEM sides have been verified by running some preliminary cases and comparing the species mass balances. In the modelling of iron-oxide reduction the SPM is insufficient to represent the different reaction steps, therefore a three-layered USCM is utilized. The implemented USCM is validated by running some preliminary cases.

## 012: TOWARDS A CFD MODEL FOR BOILING FLOWS: VALIDATION OF QMOM PREDICTIONS WITH TOPFLOW EXPERIMENTS

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## ABSTRACT

Boiling flows are very complex systems, usually confined in vertical pipes, where the liquid water moving upwards and the steam gas bubbles generated at the walls. The fluid dynamics of such systems is determined by the interplay of many different phenomena, including bubble nucleation, growth, condensation, coalescence, and breakage. For this reason, the development of a fully predictive computational fluid dynamics (CFD) model is very challenging, therefore we focus here only on some of the phenomena mentioned above (i.e. coalescence and breakage) by using population balance models (PBM). In this work, a coupled CFD-PBM model based on the two-fluid model and the quadrature method of moments (QMOM) was implemented in the open-source CFD code openFOAM. Simulation predictions obtained with this methodology are compared against the so-called TOPFLOWexperiments for the first time, where simpler air-water cold systems that mimic the complexity of real boiling flows were investigated. Comparison between the available experimental data and the results show that great care must be paid on some modeling details, such as the inlet bubble size distribution (BSD) at the sparger and the coalescence and breakage rates modeling.

## 013: IMPLEMENTING THE KINETIC THEORY OF GRANULAR FLOWS INTO THE LAGRANGIAN DENSE DISCRETE PHASE MODEL

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## ABSTRACT

The dense discrete phase model (DDPM) is a promising method for detailed simulation of fluidized bed reactors. It can resolve particle clusters on much coarser grids than the conventional two fluid model (TFM) and allows for a more natural inclusion of particle size distributions. However, the discrete nature of the DDPM presents challenges when implementing the kinetic theory of granular flows (KTGF), which is required for adequate predictions of fluidized bed behaviour. This paper outlines several methods for accomplishing this task. A good match with experimental and TFM data was achieved with different methods for implementing the KTGF, thus building confidence in the DDPM as a method for fluidized bed reactor modelling. It was also shown that the model completely fails in dilute riser flows when the KTGF is only partially implemented or neglected completely.

## 014: USING CFD ANALYSIS TO OPTIMISE TOP SUBMERGED LANCE FURNACE GEOMETRIES

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## ABSTRACT

The gas offtake design is an important aspect of the Top Submerged Lance (TSL) furnace technology. CFD modelling has been used to investigate the gas offtake geometry to better understand and address common industrial issues. The objective of the study was to understand how the shape of the offtake affected emissions from the roof ports, and influenced both the location of the post combustion reactions and the flow profile of the gas within the vessel and waste heat boiler (WHB). The conditions and gas species included in the modelling are based on typical large industrial copper smelters. Commercial software (ANSYS-FLUENT) has been used to investigate design variants by incorporating the effects of momentum, multi-component mixing, radiative and convective heat transfer, combustion reactions, and buoyancy. The learnings from the CFD modelling were integrated into the design of the new Novasmelt<sup>™</sup> TSL technology.

## 017: CFD-DEM MODELLING OF BLAST FURNACE TAPPING

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## ABSTRACT

The campaign length of a blast furnace is limited by the hearth inner lining lifetime. In order to maximize the campaign length and ensure a good draining of hot metal and slag, a good understanding of the flow in the hearth is essential. Challenges in modelling the flow involve several continuous phases (hot metal, slag and hot blast) as well as the presence of the deadman, a dense bed of coke particles. The shape and position of the deadman depend on the weight of the burden column above and the buoyancy forces from the liquids in the hearth. A numerical coupled CFD (Computational Fluid Dynamics) – DEM (Discrete Element Method) model was developed and implemented in CFDEMcoupling (Goniva et al., 2012), intended for future flow pattern investigation of the hearth during tapping. A VOF (Volume of Fluid) method is used to model the multiple continuous phases and DEM to model the discrete particles. The VOF and DEM models are coupled together in a 2-way manner, resulting in a complete 4-way coupled CFD-DEM model. We report the experimental validation of the model, performed on a small-scale particle filled tank. The tank was drained of water through the dense particle bed and the mass flow rate was measured. Difficulties in choosing a fine enough mesh for the VOF method to correctly resolve the interface and simultaneously ensure a stable and accurate void fraction calculation arose. Different methods was proposed to enable particle sizes in the same range of the CFD cells, involving alternative methods for mapping the void fraction field onto the CFD mesh, as well as smoothing of the void fraction. With the smoothing model of Radl et al. (2014), the simulation was stable and very good agreements were found with the experimental measurements.

## 018: SIMULATION OF DISPERSION OF IMMISCIBLE FLUIDS IN A TURBULENT COUETTE FLOW

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### ABSTRACT

Dispersion of immiscible fluids in a Couette device, in which the inner cylinder rotates whereas the outer one is immobile, is modelled. Two different modelling approaches are employed. The 1st approach is based on solving a one-dimensional Advection-Diffusion-Population Balance equation. An influence of upper and bottom Couette device covers (the so-called end effect) is ignored in this case. The Prandtl mixing length model of turbulence, employed for modelling of a Couette flow field, allows obtaining an analytical expression for calculation of the energy dissipation rate distribution across Couette device gap. Fixed Pivot method is employed for numerical solution of the population balance equation.

The 2nd approach is based on the CFD-population balance A-MuSiG method, recently implemented into the STAR-CCM+ code of Siemens PLM Software. The Reynolds stress turbulence model along with the Daly & Harlow transport model are employed for modelling two-dimensional axisymmetric flow field in a Couette device.

In the present work, modelling is limited to only droplet breakup; i.e., only non-coalescing droplets are considered. A modified droplet breakup model of Coulaloglou and Tavlarides (1977) is employed for all the computations.

Computed droplet size distributions are compared with those obtained in a laboratory Couette device of a relatively small height that is a cause of the significant end effect. Dispersion of water droplets in silicone oil is studied. Coalescence is suppressed by a surfactant. The experimental droplet size distributions are reasonably well fitted by both the models employed.

The most significant advantage of the 3-D computations over the 1-D modelling is accounting for the end effect, that in its turn affects both velocity and energy dissipation rate distributions over the Couette device gap. Also, to better fit the experimental data, a weak coalescence was formally introduced into the 3-D computational code.

## 020: NUMERICAL ANALYSIS OF THE TEMPERATURE DISTRIBUTION IN A MARTENSITIC STAINLESS STEEL STRIP DURING HARDENING

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### ABSTRACT

Due to the increasing demands on higher qualities of thin martensitic steel strips, a great attention needs to be paid to the dimension quality of the finished product within the hardening line. The temperature distribution within the strip during the process influences the flatness of the finished product. Therefore, a FEM model was developed based on physical theories. Specifically, the temperature for the section before martensitic transformation was predicted by using a steady state approach. In addition, the results of the numerical predictions were compared to measured temperature performed in industry by using infrared thermal imaging. The results showed that a significant temperature difference exists across the width of the strip. This difference was 41°C and 48°C at the position close to the bath interface according to the thermal imaging and modelling results, respectively. Furthermore, the temperature measurements showed that the temperature of the strip decreased by 245°C from the furnace temperature within the gas box beyond the hardening furnace. The measurements were performed at a position about 21mm away from the molten metal bath interface. Overall, the results of this study can be seen as initial fundamental knowledge of the modelling of the hardening process. Thereby, this knowledge can be used to modify the current hardening process as well as be used as input to study the stress in strip in future investigations.

## 021: VISCOELASTIC FLOW SIMULATIONS IN DISORDERED POROUS MEDIA

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## ABSTRACT

We investigate creeping flow of a viscoelastic fluid through a three dimensional random porous medium using computational fluid dynamics. The simulations are performed using a finite volume methodology with a staggered grid. The no slip boundary condition on the fluid-solid interface is implemented using a second order finite volume immersed boundary (FVM-IBM) methodology [1]. The viscoelastic fluid is modelled using a FENE-P type constitutive relation. The simulations reveal a transition of flow structure from a laminar Newtonian regime to a nonstationary non-Newtonian regime with increasing viscoelasticity. We find that the flow profiles are mainly governed by the porous microstructure. By choosing a proper length scale a universal curve for the flow transition can be obtained. A study of the flow topology shows how in such disordered porous media shear, extensional and rotational contributions to the flow evolve with increased viscoelasticity.

## 022: FLOW PAST A YAWED CYLINDER OF FINITE LENGTH USING A FICTITIOUS DOMAIN METHOD

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## ABSTRACT

In this work, the flow past a finite-end yawed cylinder is studied. This constitute a first step to understand the motion of freely moving particles. To this aim the Finite Volume / Fictitious Domain (FV/FD) method developed in the PeliGRIFF code (Wachs *et al.*, 2015) is intensively used. This method is validated using numerical results of the literature for a cylinder of finite length whose direction is parallel to the flow (Auguste, 2010). Efforts and vortex shedding frequencies are carefully analysed giving strong confidence in the numerical methodology. A detail study of the flow past a cylinder of aspect ratio L/D = 3 (where *D* is the diameter and *L* the length) at moderate Reynolds numbers ( $Re = rUD/\mu = 200$ ) is also carried out. The influence of the yaw angle (ranging from 0° to 90°) is identified both on the wake and on the hydrodynamic efforts. Three different regimes are successively encountered including standing-eddy pattern as unsteady vortex shedding. Otherwise the independence principle which states that the normal force on the cylinder only depends on the normal component of the velocity (Sears, 1948), is compared to the numerical simulations. Results indicate that the independence principle is inaccurate in this flow regime. A linear law obtained in the Stokes regime should be preferred.

## 023: THE PEAR-SHAPED FATE OF AN ICE MELTING FRONT

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## ABSTRACT

A fluid-structure interaction problem with the melting of water around a heated horizontal circular cylinder is analysed with numerical simulations. Dynamic meshing was used for evolving the flow domain in time as the melting front extended radially outward from the cylinder; a node shuffle algorithm was used to retain mesh quality across the significant mesh deformation. We simulated one case above the density inversion point of water and one case below, yielding pear-shaped melting fronts due to thermal plumes either rising or falling from the cylinder, respectively. Results were compared with previous experimental studies and the melting front profiles matched reasonably well and melting rates were in agreement. We confirm that natural convection plays a significant role in the transport of energy as the melt zone increases, and needs to be considered for accurately modelling phase change under these conditions.

# 024: EXTREMELY FAST SIMULATIONS OF HEAT TRANSFER IN FLUIDIZED BEDS

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## ABSTRACT

Besides their huge technological importance, fluidized beds have attracted a large amount of research because they are perfect playgrounds to investigate highly dynamic particulate flows. Their overall behavior is determined by short-lasting particle collisions and the interaction between solid and gas phase. Modern simulation techniques that combine computational fluid dynamics (CFD) and discrete element methods (DEM) are capable of describing their evolution and provide detailed information on what is happening on the particle scale. However, these approaches are limited by small time steps and large numerical costs, which inhibits the investigation of slower long-term processes like heat transfer or chemical conversion. In a recent study (Lichtenegger and Pirker, 2016), we have introduced recurrence CFD (rCFD) as a way to decouple fast from slow degrees of freedom in systems with recurring patterns: A conventional simulation is carried out to capture such coherent structures. Their re-appearance is characterized with recurrence plots that allow us to extrapolate their evolution far beyond the simulated time. On top of these predicted flow fields, any passive or weakly coupled process can then be investigated at fractions of the original computational costs. Here, we present the application of rCFD to heat transfer in a labscale fluidized bed. Initially hot particles are fluidized with cool air and their temperature evolution is recorded. In comparison to conventional CFD-DEM, we observe speed-up factors of about two orders of magnitude at very good accuracy with regard to recent measurements.

## 025: EFFECT OF LIFT FORCE ON DENSE GAS-FLUIDIZED BEDS OF NON-SPHERICAL PARTICLES

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## ABSTRACT

In industry we encounter many processes that rely on equipment in which particles are suspended by a gas flow, such as pneumatic conveyors, CFB gasifiers, combustors and fluidized bed reactors. In numerical models of these processes, particles have traditionally been represented as spheres, thus limiting complexities associated with drag or lift forces. However, spherical particles are not representative of the entities encountered in real systems. For example, non-spherical biomass particles of varying aspect ratios are used in the production of biomass fuels. Thus far literature is guite limited when it comes to hydrodynamic forces experienced by non-spherical particles under fluidized conditions. In fluidized beds, particles will experience varying lift force conditions dependent on the orientation of the particle relative to the direction of the flow. In this study, we investigate numerically the effect of different lift force coefficient correlations on fluidization of spherocylindrical particles. We employ correlations derived from previous simulations on non-spherical particles and aerofoil dynamics in simulations. We also look into the effect of the Di Felice approximation, in this case applied to take into account the effect of surrounding particles on the lift force. Particle interactions are modelled using the Open Source engine CFDEM, which uses the OpenFOAM computational fluid dynamics (CFD) solver to describe the fluid component and LIGGGHTS to implement discrete element method (DEM) calculations. We investigate the importance of lift forces on non-spherical particles under dense fluidised conditions and compare results to the case of spherical particles where lift forces are often neglected.

## 026: SIMULATION OF GAS-LIQUID FLOWS IN SEPARATORS. A LAGRANGIAN APPROACH

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## ABSTRACT

In order to simulate the separation efficiency of gas scrubbers, we have formulated and implemented a version of the Single-Particle Method. The method is suitable for CFD simulations of gas-droplet flows, and is based on using Lagrangian tracking of droplets. An implementation of the method has been made in a commercial CFD tool. The methodology and the CFD implementation have been validated against analytical results in the literature.

## 027: MODELLING AND NUMERICAL SIMULATION OF SURFACE ACTIVE SPECIES TRANSPORT - REACTION IN WELDING PROCESSES

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## ABSTRACT

This paper deals with the modelling of steel melting process during TIG welding operations on the nuclear power plants. The issue of the quality assurance of welding operations on some components is of great importance for the nuclear safety management. However, there are many parameters involved in the process which makes the uncertainty of the whole operation important. Moreover, some repair operations make impossible the quality control of the final weld bead. This is the case of one such a weld this study focus on. A way to ensure the quality of such weld beads could be based on the weld pool shape prediction by the numerical simulation. Thus, giving the operating parameters such as arc energy distribution, the flow simulation inside the weld pool could provide the information on the final weld pool dimensions. The model describing the metal flow during the welding process developed in this work is based on the classical MHD and the enthalpy equations. Yet, the flow in the weld pool is mainly governed by variable surface tension force, the phenomenon known as Marangoni effect. The surface tension variation is in this case highly dependent on the thermal and the surfactant concentration gradients. In order to better evaluate this force, in this work, we present a new formulation of transport-reaction equations for surfactant and relative species in the molten steel. Moreover, this model takes into account species chemical reaction and evaporation. This allows mass fractions and gradients computation at the weld pool surface, and by this mean a better prediction of the surface tension force in case of variable chemical composition. The results of the simulations are compared to experimental data on the weld pool dimensions.

## 028: NUMERICAL SIMULATIONS OF TURBULENT LIQUID-LIQUID DISPERSIONS WITH QUADRATURE-BASED MOMENT METHODS

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## ABSTRACT

The accurate description of droplet dynamics in turbulent liquidliquid dispersions is of great importance in many industrial applications, especially when the economy of the process is determined by the involved mass transfer and chemical reaction rates. In this respect, the proper estimation of the spatial and time evolution of the droplet polydispersity can offer a useful tool to the modeler to design and scale-up relevant processes. In the latest years, computational fluid dynamics (CFD) and population balance modeling (PBM) have been coupled into a single computational tool, paving the way to full-predictive macro-scale models that incorporate submodels for describing the rate of the relevant phenomena occurring at droplet-scale, such as coalescence, breakage, momentum and mass exchange with the continuous phase. In this work our recent advances on this topic are presented, with a particular attention to two distinct elements: 1) the choice of appropriate coalescence and breakage closures, pointing out the need to account for highorder turbulent phenomena, such as turbulent intermittency through the use of the so-called multifractal formalism; 2) the possibility to carry out simplified spatially homogeneous simulations when there is a clear separation of scales between coalescence/breakage and mixing. CFD simulations were carried out with our own implementation of the Quadrature Method of Moments (QMOM), combined with the two-fluid model, present in a solver of the open-source code OpenFOAM.

## 030: CFD MODELING OF A COMMERCIAL-SIZE CIRCLE-DRAFT BIOMASS GASIFIER

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## ABSTRACT

This work was focused on a commercial-size (2MWth.) circle-draft biomass gasifier. In this work a three-dimensional transient CFD (computational fluid dynamics) model was established to simulate the circle-draft biomass gasifier. The MP-PIC (multiphase particle-in-cell) method was applied to simulate multiphase reactive flows in the gasifier. In the MP-PIC method, the Navier-Stokes equation coupled with the large-eddy simulation (LES) was applied to describe the gas phase. The particulate phase was described in a Lagrangian way by computing the trajectories of parcels of particles solving Newtonian equations of motion for each parcel. The mass and energy transport equations were coupled with the momentum equation to simulate mass and energy transfer in the circle-draft gasifier. The heterogeneous solid-gas and homogeneous gas-phase reaction kinetics were integrated with the transport equations to simulate biomass drying, gasification, combustion, and other gas-phase reactions. The simulation results were compared with experimental data to validate the CFD model. The CFD model predicted gas species distribution, reaction zone temperatures, and producer gas composition in the circle-draft biomass gasifier.

## 031: Prediction of wall stresses in a steel making ladle during argon gas purging

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Keywords: Ladle furnace, Multiphase flows, Wall stresses, Stirred tanks.

## ABSTRACT

Ladle furnace is an important stage in secondary steel making, where the steel is further refined by removal of impurities and the composition is adjusted by addition of alloying elements. In this process, argon gas is injected into the ladle from the bottom to homogenize the bath in terms of composition as well as temperature and also to carry the impurities to the slag layer. However, agitation in the bath due to inert gas purging also generates stresses in the refractory wall which leads to wear of the refractory lining. There are only a few studies in the literature, that attempts to find the wall shear stress generated due to the hydrodynamic interactions in gas stirred systems. Furthermore, the dependence and distribution of these stresses on various parameters like gas flow rate, position and number of injectors, slag thickness etc. are not completely understood. The present work involves the study of stresses on the wall from hydrodynamic interactions of gas-liquid flow in a ladle geometry using computational fluid dynamic (CFD) approach. A transient, coupled level set- volume of fluid (CLSVOF) model is used to describe the flow dynamics of molten steel, argon gas and slag layer in an industrial scale steel making ladle. The effects of the above parameters on wall stresses of the ladle are studied. The localized regions along the refractory walls that are more susceptible to wear are also identified.

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## 032: A COMPUTATIONAL FRAMEWORK INVOLVING CFD AND DATA MINING TOOLS FOR ANALYZING DISEASE IN CAROTID ARTERY BIFURCATION

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## ABSTRACT

Cardiovascular diseases, like Carotid Artery Disease and Coronary Artery Disease (CAD) are associated with the narrowing of artery due to build-up of fatty substances and cholesterol deposits (called plaque). Carotid Artery Disease increases the chances of brain stroke. Hence, the main objective of this work is to apply computational tools to help differentiate between the healthy and unhealthy artery (with 25% stenosis) using a combination of Computational Fluid Dynamics (CFD) and data mining tools. In this work, first, the CFD has been qualitatively shown to provide similar results as the experimental Phase-Contrast Magnetic Resonance Imaging (PCMRI) technique. The CFD simulation shows that wall shear stress is an ideal parameter to identify the location of plaque formation and the existence of plaque conditions in the body (due to overall higher spatially averaged wall shear stress in the clogged case at all times in the cycle). Then data mining tools like Fast Fourier Transform (FFT) and Proper Orthogonal Decomposition (POD) have been used to unearth a pattern that can be useful for diagnosis. FFT shows that the flow constriction induced by plaque leads to lesser variation in magnitudes of energy of dominant frequencies at different locations like, wake region, mid-Internal Carotid Artery (mid-ICA) and mid-Common Carotid Artery (mid-CCA) regions, while for cleaner artery, there is more variation in the magnitude of energy of these dominant frequencies when measured at wake, mid ICA and mid CCA region. POD helps by confirming the location of regions with high energy in decomposed velocity modes for both the cases. More studies are required to develop a data mining based modern 21st century cardio-vascular patient care.

## 034: A LAGRANGIAN-EULERIAN HYBRID MODEL FOR THE SIMULATION OF DIRECT REDUCTION OF IRON ORE IN FLUIDIZED BEDS

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## ABSTRACT

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 iron can be reduced rapidly and efficiently from iron carrier materials using such. The primary energy sources and reducing agents are natural gas, coal, coke, pulverized coal, which are finally released as CO2 and in a lesser extent as H2O to the environment. Iron reduction consumes about 70% of the energy during steelmaking therefore offering potential in energy and CO2 savings. Due to the limited accessibility for measurements, simulation methods have become one of the most important tools for optimizing the iron making processes. While the two-fluid model (Schneiderbauer et al., 2012) would be a good candidate to attack the simulation of largescale multi-phase processes it lacks from a proper representation of the particle size distribution and the related physical phenomena. This, in turn, gives rise to particle-based approaches, such as the coupling between CFD and DEM methods, which can easily handle particle segregation, particle growth and particle mixing. Furthermore, chemical reactions can be evaluated per particle and it is not required to transfer these reactions to a continuum representation. However, CFD-DEM approaches require an appropriate coarse-graining to considerably reduce their computational demands. We, therefore, present a generalization of the Lagrangian-Eulerian hybrid model for the numerical assessment of reacting poly-disperse gas-solid flows (Schneiderbauer et al., 2016b) to fluidized beds used for iron ore reduction. The main idea of such a modeling strategy is to use a combination of a Lagrangian discrete phase model (DPM) and a coarse-grained two-fluid model (TFM) to take advantage of the benefits of those two different formulations. On the one hand, the DPM model unveils additional information such as the local particle size distribution, which is not covered by TFM. On the other hand, the TFM solution deflects the DPM trajectories due to the interparticle stresses. This hybrid approach further enables the efficient evaluation of the gassolid phase reduction of iron ore at a particle level using DPM. The predictive capability and numerical efficiency of this reactive hybrid modeling approach is demonstrated in the case of a lab-scale fluidized bed. The results show that the model is able to correctly predict fractional reduction of the iron ore. The results further give a closer insight about the temperatures and reaction gas consumption due to the reduction process.

## 035: MODELING OF FLUID DYNAMICS, MASS TRANSFER, AND CHEMICAL REACTION IN BUBBLY FLOWS

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### ABSTRACT

Mass transfer from gas bubbles to the surrounding liquid or vice versa is an important consideration in chemical engineering. Frequently such absorption or desorption processes are accompanied by a chemical reaction in the liquid phase. Compared with the fluid dynamics of bubbly flows, modeling and simulation of these processes is much less developed. The present work shows some recent advances made in validating closures for the Eulerian two-fluid framework of interpenetrating continua.
# 036: SHAPE FACTORS INCLUSION IN A ONE-DIMENSIONAL, TRANSIENT TWO-FLUID MODEL FOR STRATIFIED AND SLUG FLOW SIMULATIONS IN PIPES

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# ABSTRACT

In previous works, (Ferrari et al., 2017) have shown that a onedimensional, hyperbolic, transient five equations two-fluid model is able to numerically describe stratified, wavy, and slug flow in horizontal and near-horizontal pipes. Slug statistical characteristics, such as slug velocity, frequency, and length can be numerically predicted with results in good agreement with experimental data and well-known empirical relations. In this model some approximated and simplified assumptions are adopted to describe shear stresses at wall and at phase interface. In this paper, we focus on the possibility to account for the cross sectional flow by including the shape of the velocity profiles, inserting shape factors into the momentum balance equations. Velocity profiles are obtained by the pre-integrated model proposed by (Biberg, 2007) and they are computed at each time step and at each computational cell. Once that the velocity profiles are known, the obtained shape factors are inserted in the numerical resolution. In this way it is possible to recover part of the information lost due to the one-dimensional flow description. Velocity profiles computed in stratified conditions are compared against experimental profiles measured with PIV technique - see (Ayati et al., 2015), showing good agreement. Finally, first results in slug flow configuration are shown.

# 037: EXPERIMENTAL MODELLING OF METALLURGICAL PROCESSES

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#### ABSTRACT

Metallurgical processes often involve multi-phase flows of molten metals or molten slags. No doubt, CFD is a powerful tool to describe such flows, but for complex flow phenomena experimental data are needed for code validation. As for many melts such CFD grade data do not exist, liquid metal model experiments are more and more used in order to fill this gap. Several examples of it are described here.

# 038: IMMERSED BOUNDARY METHOD FOR THE COMPRESSIBLE NAVIER-STOKES EQUATIONS USING HIGH ORDER SUMMATION-BY-PARTS DIFFERENCE OPERATORS

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#### ABSTRACT

A ghost-point immersed boundary method is devised for the compressible Navier–Stokes equations by employing high order summation-by-parts (SBP) difference operators. The immersed boundaries are treated as sharp interfaces by enforcing the solid wall boundary conditions via flow variables at ghost points using bilinearly interpolated flow variables at mirror points. The approach is verified and validated for compressible flow past a circular cylinder at moderate Reynolds numbers.

# 039: IMPROVED COLLISION MODELLING FOR LIQUID METAL DROPLETS IN A COPPER SLAG CLEANING PROCESS

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#### ABSTRACT

Collision and coalescence among liquid metal droplets in a slag cleaning process enhanced by electromagnetic stirring were numerically studied. A hybrid collision algorithm was implemented to calculate the collision probability, which overcomes the mesh-dependency problem in a pure stochastic algorithm and is adaptive to both homogeneous and in-homogeneous cases. Theoretical analyses and numerical simulations based on the Volume-of-Fluid method were carried out in order to predict the result of droplet collisions, which are important for the copper slag cleaning process.. Based on the numerical results, a new regime map, which is specific to the liquid metal droplet collisions driven by shear slag flow at low capillary numbers, is provided.

# 040: INNOVATIVE COMPUTING FOR INDUSTRIALLY-RELEVANT MULTIPHASE FLOWS

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# ABSTRACT

The ability to predict the behaviour of multiphase flows accurately, reliably, and efficiently addresses a major challenge of global economic, scientific, and societal importance. These flows are central to virtually every processing and manufacturing technology. Significant advances have been made in the numerical methods to simulate these flows; examples of these include the use of Large Eddy Simulations to simulate turbulence, and interfacecapturing or tracking techniques to deal with the free surface. These codes have made progress in simulating the interaction of a turbulent flow field with an interface, however, there remains a large gap between what is achievable computationally and 'reallife' systems. We will present the latest on the modelling framework that we are currently developing within the Multi-scale Examination of MultiPHase physics in flowS (MEMPHIS) programme that will enable the use of numerical simulations as a reliable design tool. The framework features Front-Tracking/Level-Set hybrids, an Immersed Boundary approach to Fluid-Structure Interaction and sophisticated multi-scale, multi-physics models. The code we call BLUE is fully parallelised and can run on various platforms: from laptops to supercomputers (on over 250,000 cores). This allows the user the flexibility to choose between a quick 'answer' with a degree of uncertainty common to engineering applications or a high-fidelity solution, for targeted cases, that requires more time. BLUE also has builtin. user-friendly meshing capabilities that allow rapid construction of complex geometries. We present a number of simulations of problems of interest to process industries and biomedical applications, which include the design of container-filling processes, two-fluid mixing with a rotating impeller, high-speed atomization, microfluidic droplet encapsulation, falling film reactors featuring non-Newtonian fluids, and surfactant-driven non-isothermal flows.

# 041: USE OF CFD AS A DESIGN TOOL FOR A PHOSPHORIC ACID PLANT COOLING POND

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### ABSTRACT

Phosphate fertilizer plants are installations constantly evolving which make their design a challenging task. Phosphogypsum, a by-product of the manufacture of phosphoric acid, is piled up, forming stacks which may eventually alter the process efficiency as they encroach on process cooling ponds and locally modify the airflow fields. The easier access to high performance computing and the improvement of software capabilities allow to fully consider today the use of CFD within tight-schedule industrial projects, even the ones involving large-size geometry. As an example we describe how CFD can be efficiently used as a design tool for the revamping of a phosphate fertilizer complex. The use of recently emerged multi-software optimization tool is also explored as a way to enhance the engineering time dedicated to this problem.

# 042: ESTIMATION OF FLOW RATES AND PARAMETERS IN TWO-PHASE STRATIFIED AND SLUG FLOW BY AN ENSEMBLE KALMAN FILTER

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### ABSTRACT

Data assimilation methods were introduced to reduce production costs and to optimize processes in different industrial fields, such as oil & gas reservoir industry or transport of multiphase flows in pipelines. In flow assurance, these methods, called also soft-sensing techniques, allow to avoid the use of expensive and complex multiphase meters to measure some flow characteristics. Moreover, they allow the estimation of some flow parameters, whose actual values are unknown. Using these techniques, flow meters may be substituted by numerical simulations that solve a real-time dynamic model. Among data assimilation methods, sequential filtering techniques allow flow estimation using a mathematical recursive filter where the estimated state of the physical model is updated in real-time through a comparison with few available and easy to obtain measurements of the actual system. If an explicit matrix structure of the model is available, the Extended Kalman filter (EKF) can be used as a recursive filter; otherwise, in the case of a more complex physical model, the Ensemble Kalman filter (EnKF), that is a stochastic extension of the original Kalman filter, can be used in combination with a numerical code to estimate various pieces of information of a multiphase flow in pipe. Previous Authors (see Gryzlov et al. (2010)) used the Extended or the Ensemble Kalman filter in combination with the simplified one-dimensional nopressure wave and drift-flux models to estimate the inlet flow rate or some correlation parameters in liquid/gas twophase flow. In this work, the application of the Ensemble Kalman filter to the more complex Two-Fluid model for two-phase flow is investigated. The possibility to extend flow rate estimations to simulations where a flow regime transition from stratified to slug flow occurs, simulated with a one-dimensional slug capturing numerical code previously developed, is shown. The estimation of the pipe diameter by the real-time softsensing technique is performed in order to show the possibility of evaluating the presence of possible pipe restrictions or obstructions along the pipe due to wax deposition, solid phase scaling or other similar processes, without the use of ad-hoc physical model or invasive examination of the pipe. All the measurements used in this work for the soft-sensing process are obtained from previous numerical simulations of artificial actual systems kept as reference.

# 043: UNRESOLVED CFD-DEM IN ENVIRONMENTAL ENGINEERING: SUBMARINE SLOPE STABILITY AND OTHER APPLICATIONS

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#### ABSTRACT

When installing gravity foundations for offshore structures such as wind power stations or oil platforms, the seabed needs to be excavated for providing enough stability. To minimize the impact on the surrounding fauna and the installation costs, steep but stable slopes are desired. The work presented is done in a research project on the numerical investigation of the stability of submarine slopes, particularly under the impact of influences like material removal or wave-induced disturbances.

The method used in the current project is coupled CFD-DEM: while the dynamics of the fluid phase (water and in some cases water and air) are handled with computational fluid dynamics (CFD), the soil is modelled by spheres, whose motion is calculated with a discrete element method (DEM). Force models are used for considering the particles' effect on the fluid and vice versa, a void fraction field accounts for the volume of the particles on the CFD side. Due to the high number of particles in the domain only unresolved CFD-DEM (cf., e.g. Zhou (2010)) is suitable: in this case the particles are smaller than the cells of the CFD mesh.

In the presented work the investigations concentrated on the validation of the CFD-DEM models against small-scale experiments that were conducted by the authors. In a first step, the used materials were characterized and a lubrication force model was implemented. Furthermore, some basic investigations on the topic of dilatancy were carried out. Then an experimental setup and an according simulation were compared. In addition to that a three phase (air, water, particles) solver was used to depict the effect of surface waves onto the particle bed.

For the calculations CFDEM®coupling was used. CFDEM®coupling is an Open Source software for coupled CFD-DEM simulations. It uses the CFD framework of the Open Source CFD code OpenFOAM® and the DEM framework of the Open Source code LIGGGHTS®. Both CFDEM®coupling and LIGGGHTS® have been presented before (cf., e.g. Goniva et al. (2012), Kloss et al. (2012)), the used model equations were validated against analytical solutions and literature.

# 044: HIGH TEMPERATURE FLUIDIZATION – INFLUENCE OF INTER-PARTICLE FORCES ON FLUIDIZATION BEHAVIOR

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### ABSTRACT

Recent experiments have shown an influence of temperature on the minimum fluidization conditions in gas-solid fluidized beds, even when the gas phase density and viscosity were kept constant (Campos Velarde et al., 2016). Correlations that are available in the open literature, for predicting the minimum fluidization velocity and the bed voidage at minimum fluidization conditions at elevated temperatures, fail to describe their experimental data, in particular how the bed porosity at incipient fluidization conditions is changing with temperature.

It is hypothesized that at higher temperatures inter-particle forces play an important role in this phenomenon. Inter-particle forces, specifically van der Waals forces, are known to be important in the fluidization of very fine powders, and may incur detrimental effects on the process such as the formation of particle agglomerates or reduced particle mixing. However, the experimental results by Campos Velarde et al. (2016) have indicated that such forces may also become important during the fluidization of larger particles at increased temperatures. In this work, we characterize the effects of inter-particle forces using simulations with a Discrete Particle Model (DPM).

DPM is an Euler-Lagrange type model with a discrete description of the solids phase and a continuous description of the gas phase. The motion of each individual particle is tracked and described with Newton's second law, with van der Waals forces used to describe the inter-particle forces. Van der Waals forces are described with a Hamaker constant, which depends on the particle material and fluidization gas properties and may depend on temperature (Castellanos et al., 2003). Particle-particle interactions are dealt with using a soft-sphere collision model, which allows multiple simultaneous contacts between several pairs of particles. The gas phase is described with a set of volume-averaged Navier-Stokes equations, and full two-way coupling between the phases is implemented.

In this work we investigate the influence of the inter-particle forces (by variation of the Hamaker constant) on the minimum fluidization velocity (Umf) and the bed porosity at minimum fluidization ( $\varepsilon mf$ ), and relate the effects to the dominating phenomena prevailing at high-temperature fluidization.

# 045: STOCHASTIC DSMC MODEL FOR LARGE SCALE DENSE BUBBLY FLOWS

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### ABSTRACT

Bubble columns are widely used in the chemical industry because of their simple design and high efficiency. The scale-up of these kinds of columns is challenging and time-consuming. Since high throughput is targeted, they are operated in the heterogeneous bubbling regime where the flow is complex and turbulent. Large-scale bubble columns can in principle be simulated using continuum models (TFM/MFM) with closures from more detailed models such as Front Tracking (FT) or Volume of Fluid (VOF). Multi-fluid models are capable of predicting the flow field, but to accurately describe mass transfer rates, an accurate interfacial area of the bubbles is required as well as mass transfer coefficients for dense bubble swarms. This requires the MFM to be coupled with models that can predict bubble size distributions. The Discrete Bubble Model (DBM) can be scaled up but the bubble-bubble interactions make it computationally very intensive. Stochastic Direct Simulation Monte Carlo (DSMC) methods treat the bubbles in a discrete manner while more efficiently handling the collisions compared to the DBM. The DSMC model has earlier been used for very small particles in the size range of Angstroms to microns where the particles are purely inertial at high Stokes numbers. In the work of Pawar et al. (2014) this was used for micrometer sized particles/droplets where this method proved to be 60 to 70 times faster than more classical methods like the Discrete Particle Model (DPM). In this work the DSMC method has been extended to finite sized bubbles/particles in the order of millimeters. A 4-way coupling (liquidbubble-bubble) is achieved using the volume-averaged Navier Stokes equations. The model is verified first for monodisperse impinging particle streams without gas. Then the model is verified with the DBM of a 3D periodic bubble driven system. The collision frequencies are all within 10 percent accuracy and the speed up achieved per DEM time step is nearly 10 times compared to the DBM, which facilitates simulation of large systems.

# 046: INFLUENCE OF THE UPSTREAM CYLINDER AND WAVE BREAKING POINT ON THE BREAKING WAVE FORCES ON THE DOWNSTREAM CYLINDER

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# ABSTRACT

The interaction of breaking waves with marine structures involves complex free surface deformation and instantaneous loading on the structural members. A typical offshore platform or a coastal structure consists of several vertical and horizontal members exposed to breaking wave action. The breaking wave hydrodynamics and the effect of neighbouring cylinders on multiple cylinders placed in near vicinity is important due to force amplification or reduction resulting from interaction between the cylinders. The kinematics of breaking waves and the hydrodynamics of breaking wave interaction with a single vertical cylinder have been studied in detail in current literature. Studies have established that the location of a cylinder with respect to the wave breaking point has a major influence on the breaking wave forces on the cylinder. These studies have to be extended to investigate the hydrodynamics of cylinders placed close to each other to understand the modifications in the force regime due to the presence of neighbouring cylinders under a breaking wave regime. In this paper, the open-source Computational Fluid Dynamics (CFD) model REEF3D is used to simulate breaking wave interaction with a pair of tandem cylinders. The focus of the study is on the location of the wave breaking point with respect to the upstream cylinder and the consequences for the downstream cylinder. The free surface features associated with the incident breaking wave and the evolution of the free surface after interaction with the upstream cylinder are investigated. The overturning wave crest and the associated free surface deformation have a major influence on the wave that is then incident on the downstream cylinder. The development of a downstream iet behind the upstream cylinder leads to the negation of the shadowing effect on the downstream cylinder. This can lead to an unexpected higher force on the downstream cylinder. The evolution of this downstream jet and the extent of this phenomenon changes the character of the otherwise shadow region behind the upstream cylinder. A detailed understanding of this phenomenon can provide new insights into the wave hydrodynamics related to multiple cylinders placed in close vicinity under a breaking wave regime. The knowledge regarding force amplification or reduction on downstream cylinders will aid in designing a safer and reliable substructure for marine installations.

# 047: MASS TRANSFER PHENOMENA IN FLUIDIZED BEDS WITH HORIZONTALLY IMMERSED MEMBRANES

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#### ABSTRACT

Mass transfer phenomena in fluidized bed reactors with horizontally immersed membranes have been investigated using a verified and validated Two-Fluid Model. A binary hydrogennitrogen mixture was injected into the fluidized bed which was operated in the bubbling fluidization regime, and hydrogen was extracted via horizontally immersed membranes. The hydrogen flux is lowest on top of the membranes and highest at the bottom of the membranes. The main causes for the low flux on top of the membranes are densified zones and insufficient hydrogen replenishment due to the flow pattern of the gas. Gas pockets do not have a negative effect on the mass transfer towards the membranes. In systems with membrane tube banks, the membranes located at the walls perform worst, because solids mostly flow downwards near the walls of a fluidized bed, which causes gas back-mixing, which hinders hydrogen replenishment and thereby decreases the driving force for hydrogen transport. Removing the membranes vith inactive tubes has no significant effect on the system. The membrane tube banks also have a significant effect on the hydrodynamics.

# 048: A TWO-FLUID MODEL STUDY OF HYDROGEN PRODUCTION VIA WATER GAS SHIFT IN FLUIDIZED BED MEMBRANE REACTORS

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### ABSTRACT

Fluidized bed membrane reactors have been proposed as a promising reactor concept for the production of ultra-pure hydrogen via Water Gas Shift (WGS). High-flux thin-film dense palladium-based membranes are used to selectively extract hydrogen from the reaction medium, which shifts the thermodynamic equilibrium towards the products' side, increasing the conversion. A Two-Fluid Model (TFM) has been used to investigate the effect of hydrogen extraction via perm-selective membranes on the WGS reaction rates in the fluidized bed. A thorough TFM verification study was performed, which showed that the model is able to accurately predict the concentration profiles for various types of nth order and equilibrium chemical reactions. Also, the implementation of the WGS reaction rate in the TFM was checked. The results have shown a clear positive effect of the hydrogen permeation on the WGS reaction rates, both for vertically and horizontally immersed membranes. In systems with horizontally immersed membranes, gas pockets that contain a very small amount of catalyst develop underneath the membrane tube, resulting in reduced local reaction rates. Densified zones on top of the membrane tube show increased local reaction rates. Mass transfer limitations from the emulsion phase to the membrane surface is the most pronounced effect that reduces the overall reactor performance. The developed model allows further investigating different configurations and operation modes to further optimize the reactor's performance.

# 049: EXPERIMENTAL AND NUMERICAL INVESTIGATION OF A BUBBLING DENSE GAS-SOLID FLUIDIZED BED

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#### ABSTRACT

Eulerian models incorporating kinetic theory of granular flow (KTGF) are widely used to simulate gas-solids flow. The most widely used KTGF models have been derived for dilute flows of slightly inelastic, frictionless spheres. In reality, however, granular materials are mostly frictional. Attempts to quantify the friction effect have been somewhat limited. In this work, we focus on the validation of the KTGF model for rough spheres derived by Yang et al. (2016a, b) and the corresponding BCs from Yang et al. (2016c) for frictional walls. The present TFM simulations are validated by comparing with magnetic particle tracking (MPT) experimental data and results obtained from discrete particle model (DPM) simulations of a pseudo-2D bubbling fluidized bed. Numerical results are compared with respect to particle distribution, solids velocities, and energy balance in the bed. On comparison with a simple kinetic theory derived by Jenkins and Zhang (2002), we find that present model improves the predictions for particle axial velocity and flux upon simulation of inelastic rough particles. In conclusion, the current KTGF model obtains excellent agreement with experiment and discrete particle simulation for the time-averaged bed hydrodynamics.

# 050: COMPARISON OF PARTICLE-RESOLVED DIRECT NUMERICAL SIMULATION AND 1D MODELLING OF CATALYTIC REACTIONS IN A PACKED BED

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#### ABSTRACT

The work presents a comparison of catalytic gas-solid reactions in a packed bed as simulated on two widely different scales: direct numerical simulation (capable of accurately predicting transfer phenomena in and around a few particles) and 1D modelling (capable of engineering simulations of industrial scale reactors).

Particle-resolved direct numerical simulation (PR-DNS) is performed on a small geometry containing ~100 realistically packed monodisperse spherical particles generated via the discrete element method (DEM). These results are compared to a 1D packed bed reactor model using the effectiveness factor approach to account for intra-particle mass transfer and a suitable closure for gas-particle heat transfer.

The differences between the results from the two modelling approaches are quantified over a range of Thiele moduli, Prandtl numbers and reaction enthalpies. Results showed that existing 1D-model closures perform well for a simple first order catalytic reaction. Heat transfer completely dominates the overall reaction system when large reaction enthalpies are simulated, while mass transfer limitations dominate at low reaction enthalpies. Future work will extend this comparative approach to packings with more complex particle shapes and complex reactions.

# 051: GRANULAR FLOW DESCRIBED BY FICTITIOUS FLUIDS: A SUITABLE METHODOLOGY FOR PROCESS SIMULATIONS

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## ABSTRACT

The flow of granular materials is often present in metallurgical reactors. Metallurgical simulations are typically multidisci-plinary and the granular flow will often have a significant effect on the temperature distribution. The flow of bulk materials exhibits patterns that can be very different from fluid flows. Standard fluid flow methods are not applicable to describe such flows. For simple bulk flows with plug flow sections and mass flow hoppers, a reasonable flow field can, however, be computed with a standard CFD tool. The trick is to apply appropriate, non-standard, moving wall boundary conditions.

This simple approach does not work for complex flow cases, including sections with one or more free boundaries. For such cases, we apply the Discrete Element Method (DEM), which has emerged to be the preferred choice for simulation of granular flow. A suitable method has been developed to compute the volume averaged flow field by DEM and then import it into a code for multiphysics simulations.

To reduce the high computational cost of DEM simulations a hybrid approach is recommended. DEM simulations are then used for the complex flow regions while the simple model is used wherever applicable. In the multiphysics program the flow field is forced to be equal, or very close to, the DEM results by applying a suitable volume force.

# 052: MULTIPHASE FLUID FLOW MODELLING OF FURNACE TAPHOLES

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# ABSTRACT

Pyrometallurgical furnaces of many varieties make use of tapholes in order to facilitate the removal of molten process material from inside the vessel. Correct understanding and operation of the taphole is essential for optimal performance of such furnaces.

The present work makes use of computational fluid dynamics models generated using the OpenFOAM® framework in order to study flow behaviour in the taphole system. Single-phase large-eddy simulation models are used to quantify the discharge rate and laminar-turbulent transitions as a function of parameters such as height of material inside the furnace vessel, taphole geometry, and fluid properties. The results are used to inform boundary conditions in multiphase fluid flow models used for prediction of the qualitative behaviour of the free surface in the launder and tapping ladle for selected cases.

# 053: SOLIDIFICATION MODELING WITH USER DEFINED FUNCTION IN ANSYS FLUENT

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### ABSTRACT

The modelling of solidification processes in combination with fluid flow is one main application of ANSYS Fluent. The solid-ification is modelled with the enthalpy porosity technique. Therefor the fluid flow is damped like a flow through a porous media of dendrites. In case of materials with large solidification ranges, like the nickel based superalloy 718, the adjustment possibilities of ANSYS Fluent are often not adequate. The pro-gram postulates a linear dependency between liquid fraction and temperature. To improve the simulation, the solidification was implemented by a user defined function (UDF). The prin-cipal modelling of fluid flow is based on the theory of AN-SYS Fluent, but it is now possible to adjust the liquid fraction in fine temperature steps.

# 054: STATE OF THE ART: MACROSCOPIC MODELLING APPROACHES FOR THE DE-SCRIPTION OF MULTIPHYSICS PHENOMENA WITHIN THE ELECTROSLAG RE-MELTING PROCESS

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#### ABSTRACT

The electroslag remelting (ESR) process, which is used to pro-duce large ingots of high quality, bases on controlled solidifica-tion and chemical refinement mechanisms and is essential for the production of high quality steels and alloys designed for aer-onautical, reactor chemical or nuclear applications. Due to this, it is indispensable to enable many high technological applica-tions. Since the spreading of the industrial application of the ESR process in the 1960s, scientist and engineers worldwide are trying to deepen their understanding about this process to improve its flexibility, productivity and efficiency. Since the process conditions are very rough and measurements are quite costly, if possible at all, numerical simulation became the in-vestigation tool of choice. Over the time, the models became more detailed and more phenomena could be taken into ac-count. Today we are able to estimate electromagnetic fields, heat transfer, metallurgical flow and dendritic solidification in combination with each other within a macroscopic scale, based on actual physical models combined with the capabilities of nu-merical computing techniques. Out of this predictions about the influence of varied process control, or the occurring of mac-rosegregations and other defect types, became possible. In this paper state of the art, recent developments and critical aspects of the modelling of the ESR process will be shown. Common models, their strengths and weaknesses, as well as some possi-ble approaches to presently less considered phenomena will be presented.

# 055: PATIENT SPECIFIC NUMERICAL SIMULATION OF FLOW IN THE HUMAN UPPER AIRWAYS FOR ASSESSING THE EFFECT OF NASAL SURGERY

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# ABSTRACT

The study is looking into the potential of using computational fluid dynamics (CFD) as a tool for predicting the outcome of surgery for alleviation of obstructive sleep apnea syndrome (OSAS). From pre- and post-operative computed tomography (CT) of an OSAS patient, the pre- and post-operative geometries of the patient's upper airways were generated. CFD simulations of laminar flow in the patient's upper airway show that after nasal surgery the mass flow is more evenly distributed between the two nasal cavities and the pressure drop over the nasal cavity has increased. The pressure change is contrary to clinical measurements that the CFD results have been compared with, and this is most likely related to the earlier steps of modelling – CT acquisition and geometry retrieval.

# 056: NUMERICAL INVESTIGATION OF PARTICLE TYPES INFLUENCE ON PACKED BED ADSORBER BEHAVIOUR

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# ABSTRACT

Packings are an inseparable part of Chemical Engineering processes like adsorption. Computational Fluid Dynamics (CFD) simulations on fully resolved packed beds can provide local flow information (e.g. wall effects and flow bypasses) which cannot be identified using —black boxl and/or one-dimensional modelling, which can have severe influence on the adsorption characteristics.

Creation of random packed beds is one of the main challenges in studying fully resolved packings; this can be covered using Discrete Element Methods (DEM). In this study the effect of using different types of particles on the fluid flow pattern in the packings was investigated. Three different types of particles (mono-disperse spheres, mono-disperse cylinders and poly-disperse cylinders) were packed into beds with identical dimensions (same height, same diameter) using custom DEM code and meshed using open source tools.

CFD simulations were performed using adsorpFoam, a newly developed solver for modelling adsorption, based on open source CFD code OpenFOAM®. In this stage of study particles were considered as non-reactive to investigate fluid flow only.

From simulated packings porosities as well as particle arrangements and positions have been analysed. Frequency and positions of high velocity spots were extracted. The residence time distributions were also analysed. Furthermore, experiments with the identical types of particles were performed to verify the validity of the packing structure and global simulation results. The pressure drops derived from simulations were compared to the measured values from the beds in the lab and also available correlations and a good agreement was observed.

# 057: CFD BASED STUDY OF DENSE MEDIUM DRUM SEPARATION PROCESSES

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### ABSTRACT

Dense Medium Drum (DMD) separation is applied particularly in the coal and recycling industries. Characteristic of the process is a separation based on density, driven by the buoyancy and gravitational forces acting on an object moving in a free surface flow. The fundamental phenomena occurring in a DMD have been widely investigated by (Napier-Munn, 1991). However, in contrary to other separation methods, such as the Dense Medium Cyclone which was investigated extensively by (Kuang et al., 2014) and others, no Computational Fluid Dynamics (CFD) studies have been conducted for the DMD separation. Even recent studies, like (Meyer and Craig, 2015), use first order models which need to be calibrated with performance data of the investigated drum. Hence, important parameters like the flow-velocity and the detailed design of the drum are only taken into account indirectly. This paper reports a detailed CFD analysis of the flow in a generic DMD separation process. The study comprises, a general understanding of the flow field and an analysis of the impact of different process parameters. Furthermore, the model predicts the actual separation performance of the DMD at different working points. To the authors' knowledge, this is the first study which conducts a CFD analysis of a DMD separation process. Therefore, findings concerning the flow field and its influence on the separation efficiency will be reported on. Moreover, the separation model can be used to derive the coefficients for highly used first order models without the need of experimental data. Like this, the early design phase of DMD separation processes can improve immensely.

# 058: DIRECT NUMERICAL SIMULATION OF COUPLED HEAT AND MASS TRANSFER IN FLUID-SOLID SYSTEMS

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### ABSTRACT

In this paper, an efficient ghost-cell based immersed boundary method is introduced to perform direct numerical simulation (DNS) of particulate flows. The fluid-solid coupling is achieved by implicit incorporation of the boundary conditions into the discretized momentum, thermal and species conservation equations of the fluid phase. Taking the advantage of a second order quadratic interpolation scheme, different boundary conditions could be realized consistently in our ghost-cell based immersed boundary method. The heat and mass transport in a fluid-particle system is coupled through the solid temperature, which offers a dynamic boundary condition for the fluid thermal equation.

# 061: DEVELOPMENT OF GPU PARALLEL MULTIPHASE FLOW SOLVER FOR TURBULENT SLURRY FLOWS IN CYCLONE

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### ABSTRACT

The development of GPU parallelized unstructured multiphase solver and its application in predicting turbulent swirling flow of slurries inside cyclones is presented. Algebraic slip mixture model (ASM) is modified with additional shear lift forces and slurry rheology is corrected with fines fraction. The modified ASM model coupled with LES is used to predict particle classification inside hydrocyclone. During hydrocyclone operation the residence time of the fluid is very small and hence there is insufficient time for the larger eddies to cascade into smaller eddies. LES can accurately resolve flow structures that are few times the Kolmogorov scale at an increased computational cost due to finer mesh requirement. Therefore, the solver has been parallelized using general purpose graphics processing units (GPGPUs). In the current solver, the Pressure Poisson equation has been parallelized with an algebraic multigrid solver on GPU architecture using CUDA programming language for unstructured grids. The single phase flow field predicted by LES shows good agreement with experimental results obtained from open literature. The turbulent flow fields, the size segregation and the particle efficiency curve obtained from multiphase simulations are presented. Additionally, computational speedup due to GPU parallelization is reported over its serial version of the solver.

# 064: OSCILLATORY FLOW AND MASS TRANSPORT IN A CORONARY ARTERY

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### ABSTRACT

Pulsatile flow is intrinsic to the cardiovascular system and is driven by the rhythmic beating of the heart. As a system for mass transport, the cardiovascular system hosts a variety of biochemical and cellular species whose transport is subjected to the corresponding flow oscillations. The influence is most prevalent near the heart and particularly within arteries, where pressure fluctuations are most significant. This makes modelling of long-term mass transport difficult to evaluate, since intermediate oscillations need to be explicitly resolved. By applying Reynolds averaging to the governing flow and mass transport equations on a representative period of oscillation, this problem may be alleviated. However, doing so introduces extra terms akin to the Reynolds stresses in the flow equations as well as perturbed-flux terms in the mass transport equations. These terms are investigated in the present study and their distributions assessed. A human right coronary artery is used as the subject geometry, wherein the oscillatory transport behaviour of blood flow and low density lipoprotein is studied.

# 065: A NUMERICAL EVALUATION OF THE EFFECT OF ELECTRO-MAGNETIC FORCE ON BUBBLE FLOW IN ALUMINIUM SMELTING PROCESS

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### ABSTRACT

This paper aims to investigate the effect of electromagnetic forces on bubble flow under an anode using a computational fluid dynamics (CFD) model with the volume-of-fluid (VOF) method to capture the gas-liquid interface. Current flow was solved simultaneously to determine the Lorentz forces. As an initial phase of investigation, the investigation was conducted using part of a single anode geometry as a test bed. The CFD model was run with a fixed bubble volume and two anode inclination angles. The effect of Lorentz forces was assessed in terms of bubble sliding velocities, bubble shapes and trajectories.

# 066: LES-VOF SIMULATION OF TURBULENT INTERFACIAL FLOW IN THE CONTINUOUS CASTING MOLD

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### ABSTRACT

Slag entrainment during continuous casting process is a multiscale problem strongly dependent on the molten metal flow in the mold. Large-scale flow structures in the mold interact with the slag layer at the top of the meniscus, and small-scale liquid structures in the form of slag droplets may be entrained into the solidifying metal. In this work a large eddy simulation - volume of fluid (LES-VOF) approach is applied to investigate the unsteady flow interaction with the metal-slag-air interface including the interface instability, deformation of the slag layer and its entrainment into the molten metal. A benchmark experiment was designed to investigate the flow field in the proximity of a liquid-liquid interface for validation purposes. The experiment uses water and paraffinum liquidum to model the combination of liquid steel and the slag layer. While the entrainment of oil droplets can be visualized via shadowgraphy the flow field was measured via particle image velocimetry PIV. In combination, these two methods allow a gualitative and guantitative comparison of the unsteady flow characteristics with the CFD results. The measurement data at different inflow conditions have been used to validate the simulation results. We compare the global flow characteristics and mean velocity of submerged entry nozzle jet upon injection to the mold. Furthermore, the statistics of turbulence including velocity fluctuations and turbulent kinetic energy are used to investigate the unsteady jet interaction with the slag layer as well as liquid-liquid interface dynamics. The comparison of CFD results and experimental data reveals fairly good agreement both quantitatively and qualitatively.

# 067: A MULTI-DOMAIN 1D PARTICLE-REACTOR MODEL FOR PACKED BED REACTOR APPLICATIONS

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#### ABSTRACT

A validated multi-domain 1D particle-reactor model has been developed to simulate packed bed reactor operation. Two main components of the model are: (1) a particle model for simulating the radial distribution of chemical species and temperature within the catalyst particles and (2) a 1D reactor model for solving mass and energy transport along the length of the reactor. The model captures the effect of intra-particle heat and mass transfer phenomena on the reactor performance. Its efficacy and usability is evaluated using a thorough verification and validation campaign. Validation has been carried out through comparisons to analytical solutions for: (a) the transient thermal response of the fixed bed to a step-change in inlet feed temperature and for (b) the maximum temperature rise during an exothermic oxidation process in a chemical looping combustion (CLC) operation. Further, its performance has been verified with two well-established solvers (a 1D Euler-Euler packed bed model developed in ANSYS FLUENT and a previously published 1D model) for simulating a realistic 500kW cyclic packed bed chemical looping combustion system involving dynamic fuel-air cycling. This successful verification demonstrates the ability of the model to simulate complex cyclic packed bed reactor processes involving stiff kinetics in an efficient manner. Further, significance of particle model is evaluated for mass transfer limiting condition and this reinforces the advantage of using the proposed 1D particle-reactor model in such cases.

### 068: CFD SIMULATIONS OF TURBULENT FLOW IN THE HUMAN UPPER AIRWAYS Elin AASGRAV<sub>1\*</sub>, Sverre G. JOHNSEN<sub>2</sub>, Are J. SIMONSEN<sub>2</sub>, Bernhard MÜLLER<sub>1</sub>

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# ABSTRACT

In this paper, investigations are conducted using Reynolds-averaged Navier-Stokes (RANS) turbulence models to investigate the importance of turbulence modelling for nasal inspiration at a constant flow rate of 250 ml/s. Four different, standard turbulence models are tested in a model geometry based on pre-operative CT images of a selected obstructive sleep-apnea syndrome (OSAS) patient. The results show only minor differences between them. Furthermore, the turbulence models do not give significantly different results than a laminar flow model. Thus, the main conclusion is that effects of turbulence are insignificant in CFD modelling of the airflow in the pre-operative model of the upper airways of the chosen patient.

# 069: TIRE RUBBER EXTRUDATE SWELL SIMULATION AND VERIFICATION WITH EXPERIMENTS

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#### ABSTRACT

Extrudate swell simulations and experiments have been performed with a viscoelastic tire rubber compound at high flow rates through a circular die. A 3-mode PTT model was fitted onto rheological data of the rubber. The PTT model covers the range of shear rates present in the simulation. Convergence of the simulation was achieved with some wall slippage. The simulated and experimental extrudate swell is in good agreement at 20 mm from the die exit for a wide range of flow rates.

# 070: NUMERICAL STUDY OF COAL PARTICLE GASIFICATION UP TO REYNOLDS NUMBERS OF 1000

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## ABSTRACT

The influence of turbulent structures on the gasification of coal particles, in particular on the char consumption and surface temperature, is studied . Existing submodels for char gasification are mainly based on results for laminar flow only, therefore the capability of these models to predict gasification at higher particle Revnolds numbers is evaluated using the simulation results. Two representative scenarios were studied: the gasification of a 2 mm particle at atmospheric pressure in a O2/CO2/H2O atmosphere at 2006 K and the gasification of a 263 µm particle at 30 bar in a different O2/CO2/H2O atmosphere at 1480 K. The simulation conditions were based on data obtained from the simulations of two different entrained-flow gasifiers. ANSYS Fluent™ was used to solve the Navier-Stokes equations for the flow field coupled with energy and species conservation equations. The model for the reaction system incorporates six gaseous chemical species H2, O2, CO, CO2, H2O, N2 and solid carbon. A semi-global reaction mechanism was applied for the homogeneous gasphase reactions and the water gas reaction, the Boudouard reaction and the oxidation of carbon to carbon monoxide were considered as heterogeneous gas-solid reactions. In the present work it is shown how the reaction zone is modified due to the change in wake structure, the impact of the turbulent effects on the overall carbon conversion rate are discussed, and hints how to adjust existing submodels to correctly predict char conversion at high particle Reynolds numbers are given.

# 072: CFD MODELING OF DYNAMIC EMULSION STABILITY

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#### ABSTRACT

Assuring transport and separation of oil and water crude emulsions is of significant importance to the oil and gas industries. The crude oil, due to its profuse chemical composition, has complex dispersion and emulsion flow behavior with water. As a result, of the interface chemistry, the bubbles and droplets may separate easily, or not separate at all, impacting flow regime, water holdup, pressure drop and separation efficiency during pipe transport. Using a recently developed new stirred tank characterization technique for emulsion stability droplet relaxation parameters can be studied. Multiple model oils and crude oils were characterized by this technique. This work discusses development of a pragmatic modeling method that can validate the experimental measurements. A time averaged velocity profile in a stirred tank is used to obtain a 1-D flux flow profile in the vertical direction. This 1-D flux profile is used as a simplified flow equation and scalar equations for droplet size and dispersed phase fraction is used for modeling the emulsion stability and relaxation. This method can help in fast simulation of emulsion stability that involves long time scales of coalesence and breakage evolution for crude oil and water.

# 073: INVESTIGATING THE NUMERICAL PARAMETER SPACE FOR A STENOSED PATIENT-SPECIFIC INTERNAL CAROTID ARTERY MODEL

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## ABSTRACT

Systemic risk factors are known to correlate with cardiovascular diseases, but e.g., atherosclerotic plagues are focally distributed and highlight the role of hemodynamically induced forces on vascular remodeling. Computational fluid dynamics (CFD) shows great promise for revealing mechanisms of atherosclerotic plague progression, but the utility of CFD depends on the robustness of the numerical methods. The aim of the study was to investigate the parameter space of the numerical solutions to understand the resulting flow effects in a stenosed patient-specific internal carotid artery model. Simulations were performed on meshes consisting of 2 to 50M-elements meshes with a kinetic energy preserving and minimally-dissipative solver, and time step size ranging from  $1 \cdot 10\%$ to  $5 \cdot 10$ ° seconds. The spatial refinement study revealed large differences in the instantaneous velocity fields, and the coarsest simulation did not provide any meaningful insight into the flow. That being said, the time-averaged results were in acceptable agreement for all spatial and temporal refinement levels. The variations in temporal resolution had minor effects, and the coarsest resolution was found to suffice. In conclusion, even for a highly accurate solver, a relatively high spatial resolution was needed to sufficiently resolve the flow, and we found the 22M-element mesh to offer an optimal balance between computational cost and time-averaged quantities.

# 075: DIRECT NUMERICAL SIMULATION OF PROPPANT TRANSPORT IN A NARROW CHANNEL FOR HYDRAULIC FRACTURING APPLICATION

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## ABSTRACT

An efficient and accurate model for the direct numerical simulations (DNS) of liquid-solid flows is presented in this work. In this numerical model, fluid-solid coupling is achieved by implementing the no-slip boundary condition at the particles' surfaces by using a second order ghost-cell immersed boundary method, allowing for a fixed Cartesian grid to be used for solving the fluid equations. The particle-particle and particle-wall interactions are implemented using the soft sphere collision model. Lubrication forces are included through a sub-grid scale model because of its range of influence on a scale smaller than the grid size. After the validation of the model, the transport of solid particles in a narrow channel is simulated to mimic the proppant transport in rock fractures in fracking process. The simulations are performed for solids volume fractions ranging from 1.7 to 20 % with the range of Reynolds and Archimedes number: 100-400 and 0-7848, respectively.

# 076: CFD MODELLING TO PREDICT MASS TRANSFER IN PULSED SIEVE PLATE EXTRACTION COLUMNS

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# ABSTRACT

A 2D CFD-PBM based numerical model to predict interphase mass transfer in a Pulsed Sieve Plate Column (PSPC) is reported. The model is based on Euler-Euler interpenetrating continuum approach. Drag law due to Schiller and Naumann is used to model the interphase momentum exchange term. Spatial and temporal variations of drop population are obtained by coupling Population Balance (PB) equations with flow equations. Suitable drop coalescence and breakage kernels are used in the PB equations. Species transport equation is solved in both phases to predict interphase mass. The developed model is validated against reported mass transfer experimental data in a 2 inch PSPC. Absolute average error in prediction is less than 5%. The validated model is used to understand the complex time periodic flow patterns inside the column.

# 077: MODELLING OF BUBBLE DYNAMICS IN SLAG DURING ITS HOT STAGE ENGINEERING

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#### ABSTRACT

Silica-rich additives are injected into the slag with N2/O2 as carrier gas to stabilize free lime in BOF (Basic Oxygen Furnace) steelmaking slag. In order to understand the mixing behaviour of the additives, bubble dynamics and momentum transfer are to be clarified at first. The objective of this work is to investigate the bubble breakup and the injected momentum transfer. To this purpose, a Volume of Fluid (VOF) two phase model was developed using ANSYS FLUENT software to study the dynamic breakup process of the gas phase and the velocity attenuation along the injected axis. Particle Image Velocimetry (PIV) measurements were used to validate the corresponding computational modelling. The validation between experimental measurements and computational modelling is reasonable in the turbulence model. Bubble breakup begins very quickly in the region near the inlet. The momentum contained in the gas phase is dissipated within a short distance from the inlet.
# 078: CONTROLLED COALESCENCE WITH LOCAL FRONT RECONSTRUCTION METHOD

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### ABSTRACT

The physics of droplet collisions involves a wide range of length scales. This poses a difficulty to accurately simulate such flows with traditional fixed grid methods due to their inability to resolve all scales with affordable number of computational grid cells. A solution is to couple a fixed grid method with simplified sub grid models that account for microscale effects. In this paper, we incorporate such framework in the Local Front Reconstruction Method (Shin et al., 2011). To validate the new method, simulations of (near) head on collision of two equal tetradecane droplets are carried out at different Weber numbers corresponding to different collision regimes. The results show a better agreement with experimental data compared to other fixed grid methods like Front Tracking (Pan et al., 2008) and Coupled Level Set and Volume of Fluid (CLSVOF) (Kwakkel et al., 2013), especially at high impact velocities.

# 079: A NUMERICAL APPROACH TO MODEL AGGREGATE RESTRUCTURING IN SHEAR FLOW USING DEM IN LATTICE-BOLTZMANN SIMULATIONS

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### ABSTRACT

Aggregate shape and structure significantly impact rheological properties of fluids in many fields such as extractive metallurgy, oil field drilling and mineral processing. The morphology of the aggregates determines the porosity of solid structures and their dimensions, which in turn affects the solid-liquid and solid-solid interactions in the mixture, and hence the rheology of the system. Aggregates can undergo morphological changes induced by shear flow. The response of aggregate mixtures in terms of rheology as a function of their shear history has thus been studied in many fields (Coufort et al., 2005) with experimental approaches. Numerical investigations of aggregation dynamics and aggregate restructuration have also been conducted in low Reynolds conditions (Frungieri and Vanni, 2016), or using free draining approximation, in which the fluid particle interactions are exclusively through Stokesian drag (Eggersdorfer et al., 2010). In this study, a fully coupled Eulerian-Lagrangian approach is developed to evaluate the restructuring of aggregates in shear flows for low Reynolds numbers. In particular, a Discrete Element Method (DEM) is used for particle tracking, coupled with Lattice Boltzmann Method (LBM) for solving the liquid flow. An Immersed Boundary Method (IBM) is incorporated so that primary particle shapes and hydrodynamic interactions between particles are fully resolved (Niu et al., 2006). Selected particle-particle interaction models have been implemented in the DEM to represent the mechanical behaviour of aggregates. General attractive and repulsive force models, and the bending moment as described by Pantina and Furst (2005) have been included. Artificial aggregates were created and characterized using fractal dimension and radius of gyration. The evolution of these shape indicators over time has been studied while aggregates are subjected to a shear flow. Preliminary results obtained with fully coupled liquidsolid simulations were also compared with results based on the free draining approximation. In fully coupled simulations, significant perturbations in the flow field were observed due to the presence of particles, which leads to a significant difference in aggregate's restructuring. Different solid interaction contributions and their underlying impact on aggregate restructuring have been compared, at a given shear rate. While increasing shear or maximum cohesion forces lead to denser aggregates, effect of tangential forces on the aggregate's morphology appears to be more complex. Also, tangential forces were found to have a tendency to favor aggregate breakage.

### 080: IMPORTANCE OF THE DIFFERENT FLUID FORCES ON PARTICLE DISPERSION IN FLUID PHASE RESONANCE MIXERS

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### ABSTRACT

In Fluid Phase Resonance (FPR) mixers, a central pipe reaches into the liquid phase inside a mixing vessel. Thus two closed gas cushions are formed above the liquid – one inside the pipe and one above the liquid inside the vessel. A drive attached at the top of the pipe creates low frequency (typically in a range from 1 s-1 to 5 s-1) harmonical pressure oscillations in the gas cushion inside the pipe, which in turn induce a motion inside all the liquid in the vessel. This motion of the liquid is utilised for the purpose of mixing and dispersion of particles.

Simulations are performed for four different geometries of the central pipe's lower exit and for different particle Stokes numbers. Particle Stokes numbers are varied from 9.7·10-4 to 2.7 by changing the particle diameter and density. The flow field inside the vessel was simulated with a Volume-of-Fluid solver to capture the free surface and the influence of the gas cushions, which act like springs, until a quasi-steady state was reached. One of these simulations was verified with Laser Doppler Anemometry measurements. For each simulation, the flow fields of the last full oscillation period are stored. The particles are then repeatedly tracked through these flow fields for 15 oscillations with an Euler-Lagrange approach with one-way-coupling, so that there is no need to recalculate the flow fields. The particles are considered as point masses, which are exposed to added mass, buoyancy, drag, gravity, history, pressure gradient, rotational lift, and shear lift force. Hydrodynamic torque is also considered, as well as a Langevin model for turbulent dispersion and a wall collision model accounting for rotation.

Mixing quality and time are determined by means of correlation dimension and the 90% lifting criterion whereby one of the four pipe exit configurations was identified as the best one. For this configuration two more oscillation frequencies are also investigated. Increasing the frequency to the resonance frequency leads to a more intense mixing process. Increasing it further drastically reduces the fluid velocity and deteriorates the mixing properties.

Furthermore, the influence of the different forces on the particles is investigated. The often neglected added mass and history forces are quite relevant for all particles investigated, having always more than 10% of the drag force's magnitude, with maximum values of up to 142% for added mass and up to 66% for history force. Pressure gradient force is highly relevant for larger particles. The rotational lift force is important for large particles only. Finally, the shear lift force is highly important, especially for larger and denser particle, but negligible for small, light particles.

### 083: IMPLEMENTATION, DEMONSTRATION AND VALIDATION OF A USER-DEFINED WALL FUNCTION FOR DIRECT PRECIPITATION FOULING IN ANSYS FLUENT

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### ABSTRACT

In a previous paper (Johnsen et al., 2015) and presentation (Johnsen et al., 2016), we developed and demonstrated a generic modelling framework for the modelling of direct precipitation fouling from multi-component fluid mixtures that become super-saturated at the wall. The modelling concept involves the 1-dimensional transport of the fluid species through the turbulent boundary layer close to the wall. The governing equations include the Revnolds-averaged (RANS) advection-diffusion equations for each fluid species, and the axial momentum and energy equations for the fluid mixture. The driving force for the diffusive transport is the local gradient in the species' chemical potential. Adsorption mechanisms are not modelled per se, but the time-scale of adsorption is reflected in the choice of Dirichlet boundary conditions for the depositing species, at the fluid-solid interface. In this paper, the modelling framework is implemented as a userdefined function (UDF) for the CFD software ANSYS Fluent, to act as a wall boundary condition for mass-transfer to the wall. The subgrid, 1-dimensional formulation of the model reduces the computational cost associated with resolving the fine length-scales at which the boundary-layer mass transfer is determined, and allows for efficient modelling of industry-scale heat exchangers suffering from fouling. The current paper describes the modelling framework, and demonstrates and validates its applicability in a simplified 2D heat exchanger geometry (experimental and detailed CFD modelling data by Pääkkönen et al. (2012, 2016)). By tuning the diffusivity, only, good agreement with the experimental data and the detailed CFD model was obtained, in terms of area-averaged deposition rates.

# 084: RECENT DEVELOPMENTS FOR THE COMPUTATION OF THE NECESSARY SUB-MERGENCE OF PUMP INTAKES WITH FREE SURFACES

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### ABSTRACT

Swirling flow and gas entrainment induced by vortex formation at pump intakes are possible causes for pump failures and damages. Thus, the avoidance of hollow surface vortices is a safety-related issue for all plants which require a reliable pump operation.

The most efficient measure to avoid these problems is a sufficient submergence of the intake. An acceptable submergence can be determined by means of costly experiments, complex CFD calculations or special cor-relations. When using correlations their applicability for the specific case has to be taken into account carefully, because a universally applicable correlation is not avail-able yet. Hence, there is a present need for improved correlations or numerical methods which are capable to compute the necessary submergence.

Within the research alliance SAVE experiments and numerical simulations were performed to investigate the occurrence of surface vortices at industrial scales. Amongst others, the lengths of the gas cores of the sur-face vortices were measured with varying boundary conditions and the velocity fields were determined by means of PIV (Particle Image Velocimetry) measure-ments. These experiments were accompanied by CFD simulations, the results were compared with the experimental data. A methodology was developed based on single phase CFD simulations with ANSYS CFX in combination with the Burgers-Rott vortex model which can be used to compute the gas core length with very good accuracy. Additionally, two phase CFD simulations were performed which use a free surface model based on recent developments.

In order to develop an improved correlation for the computation of the necessary submergence, which con-siders in particular the circulation in the approaching flow, several parameter studies were performed. As a result of these studies two new theoretical approaches for the limiting cases of very small and very large circu-lation were developed which yield new correlations for the computation of the necessary submergence of pump intakes.

### 085: ADAPTIVE COARSE-GRAINING FOR LARGE-SCALE DEM SIMULATIONS

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### ABSTRACT

The large time and length scales and, not least, the vast number of particles involved in industrial-scale simulations inflate the computational costs of the Discrete Element Method (DEM) excessively. Coarse grain models can help to lower the computational demands significantly. However, for effects that intrinsically depend on particle size, coarse grain models fail to correctly predict the behaviour of the granular system. To solve this problem we have developed a new technique based on the efficient combination of fine-scale and coarse grain DEM models. The method is designed to capture the details of the granular system in spatially confined sub-regions while keeping the computational benefits of the coarse grain model where a lower resolution is sufficient. To this end, our method establishes two-way coupling between resolved and coarse grain parts of the system by volumetric passing of boundary conditions. Even more, multiple levels of coarse-graining may be combined to achieve an optimal balance between accuracy and speedup. This approach enables us to reach large time and length scales while retaining specifics of crucial regions. Furthermore, the presented model can be extended to coupled CFD-DEM simulations, where the resolution of the CFD mesh may be changed adaptively as well.

# 086: NUMERICAL EVALUATION OF CO-FIRING SOLID RECOVERED FUEL WITH PETROLEUM COKE IN A CEMENT ROTARY KILN - EFFECT OF FUEL MOISTURE

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### ABSTRACT

This paper presents a numerical simulation model for co-combustion of coarse Solid Recovered Fuel (SRF) with pulverised petroleum coke in a rotary kiln producing cement clinker. The objective is to derive a reliable modelling methodology for design and optimisation of a kiln burner and for the control of the co-combustion process. In this simulation model both the solid fuels are treated as dispersed phases using the Lagrangian method. Two separate shape factors are used to account for the thermodynamic and aerodynamic behaviour of the coarse irregular-shaped SRF particles. Both the fuels undergo similar combustion process - heating, drying, devolatilisation followed by volatile and char combustion. Using such a numerical model the influence of fuel moisture on ignition, flame intensity, fuel burnout and heat output is evaluated. Further insight into the behaviour of SRF particles and the flame characteristics are obtained from video images of the combustion process recorded at a cement plant.

### 090: FRONT-TRACKING SIMULATIONS OF BUBBLES RISING IN NON-NEWTONIAN FLUIDS

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### ABSTRACT

In the wide and complex field of multiphase flows, bubbly flows with non-Newtonian liquids are encountered in several important applications, such as in polymer solutions or fermentation broths. Despite the widespread application of non-Newtonian liquids, most of the models and closures used in industry are valid for Newtonian fluids only, if not even restricted to air-water systems. However, it is well known that the non-Newtonian rheology significantly influences the liquid and bubble behaviour. CFD represents a great tool to study such complex systems in more detail and gain useful insights on the dynamics of gas-liquid (and possibly solid) systems with the ultimate aim to help the development or the design of industrial reactors. In this study, a DNS Front Tracking (FT) method is applied to study the rise of bubbles in different power-law fluids. Detailed information is obtained regarding the flow of single or multiple bubbles, especially concerning the viscosity profile around single rising bubbles, their shapes and their rising velocity. To describe the bubble rise velocity in less detailed model, a closure for the drag force is needed. With the use of Front Tracking, an existing drag correlation, which was derived for Newtonian fluids, is adapted and improved to non-Newtonian rheologies. When the effect of the viscosity changes are limited, such as for not extreme exponents (0.5 < n < 1.5), the correlation can predict reasonably well the drag coefficient for power-law fluids.

# 091: LARGE SCALE MODELLING OF BUBBLE FORMATION AND GROWTH IN A SUPERSATURATED LIQUID

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### ABSTRACT

Bubble formation due to supersaturation or superheating plays an important role in many different areas from boiling flows to reactions producing gases, such as in electrolytic processes or fermentation. The predominant mechanism for bubble formation is heterogeneous nucleation and, while it has been studied on the microscale, the effect of bubble nucleation on the large-scale performance of bubble column reactors is still scarcely investigated. This work presents a modelling and simulation study on phase transition in bubble column reactors on the meso-scale using a discrete bubble model (DBM). The Discrete Bubble Model is an Euler-Lagrange model which tracks each bubble individually. The model has been extended to include the formation of bubbles due to the presence of supersaturation. With this model, phase transition from liquid to gas in a supersaturated liquid has been studied for two cases: bubble formation on a solid surface and in a liquid bulk. The second case shows a larger number of bubbles formed, with a bigger size. The concentration front presents differences, as in the first case it shifts from a lower concentration at the bottom to the opposite. To conclude, a starting point for simulations of phase transition due to supersaturation has been given in this work, showing that the choice of the mechanisms of bubble formation highly influence bubble densities, sizes and movements in the considered liquid.

### 092: VERIFICATION OF FILTERED TWO FLUID MODELS FOR REACTIVE GAS-SOLID FLOWS

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### ABSTRACT

CFD simulations of fluidized bed reactors are generally limited to the laboratory scale because of the fine grid sizes that are required to resolve complex particle clustering phenomena. The filtered Two Fluid Model (fTFM) approach has recently emerged as a promising method for allowing reasonable predictions of large-scale fluidized beds. This paper presents a verification study of new two-marker fTFM closures. In general, the fTFMs matched well to the resolved simulations. It was shown that the two-marker models significantly increased the predicted degree of phase segregation (resolved in coarse grid simulations), and hence have superior capabilities compared to simpler one-marker models. Also, the two-marker model predicted a more dynamic transient flow behaviour. However, further work is recommended to extend the present study over a wider range of flow conditions.

# 093: NUMERICAL PREDICTIONS OF THE SHAPE AND SIZE OF THE RACEWAY ZONE IN A BLAST FURNACE

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### ABSTRACT

A 3D transient numerical model has been developed to predict the shape and size of the raceway zone created by the force of the blast air injected through the tuyeres in the coke bed of a blast furnace. The model is based on the solution of conservation equations of both gas and solid phases as interpenetrating continua on an Eulerian-Eulerian frame of reference. A modified k-e model has been adopted for gas phase turbulence including gas– coke turbulent interaction. The solid phase is characterized by the solid pressure, bulk viscosity and shear viscosity, which are evaluated by applying kinetic theory to granular flows. The influences of the air blast velocity, granular properties of the coke phase, and tuyere diameter on the shape and size of the raceway zone have been predicted by numerical simulations and described using semi-empirical relations. The effect of the cohesive zone on the raceway geometry is also taken into account. The trends of the derived results are compared with experimental data reported by various researchers with reasonable agreement.

### 095: DIRECT NUMERICAL SIMULATION OF THE EFFECTIVE DRAG IN GAS-LIQUID-SOLID SYSTEMS

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### ABSTRACT

Due to the increase in the oil prices and the depletion of the oil reserves, Fischer-Tropsch processes for the production of synthetic fuels, methanol synthesis and other gas-to-liquid processes are rapidly gaining interest. These reactions are commonly performed in slurry bubble columns, i.e. three-phase gas-liquid-solid reactors. Although slurry bubble columns are already widely used, challenging scale-up and operational issues are encountered when these reactors are used for the Fisher-Tropsch process. To improve the fundamental understanding of these complex reactors, this work focuses on the effective drag acting on particles and bubbles in dense flows, using Direct Numerical Simulations. We combined the Front Tracking method of Roghair et al. (2013b) and the second order implicit Immersed Boundary method that is able to simulate dense three phase flows and quantify the effects. For a system consisting of 2 mm bubbles and 1 mm particles, effective drag closures are developed for both the bubbles and the particles at several phase volume fractions. In future research, the developed methodology will be applied to study the effect of the bubble and particle size and their ratio as well as heat and mass transfer.

# 096: Three-dimensional numerical simulation of a lab-scale pressurized fluidized bed using a LES-DEM approach

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Keywords: Gas-particle flow, Dense fluidized bed, Euler-Lagrange approach, LES-DEM

### ABSTRACT

Gas-solid fluidized beds are used in a wide range of industrial applications and their modeling remains challenging because of their large-scale geometry compared to the characteristic length scales of the fluid and particles. The mathematical modeling and numerical simulation of such industrial fluidized beds are mostly performed with two fluid continuum model using the Kinetic Theory of Granular Flows (KTGF) that requires many hypotheses, in particular, on the modeling of particle-particle and particle-wall collisions. To validate these assumptions from macroscopic scale and to gain insight in the local and instantaneous behavior of such complex flows, a mesoscopic investigation may therefore be retained as an alternative. Numerical simulations at mesoscopic scale make it possible to analyze the effect of many complex phenomena occurring in dense fluidized beds like friction and rotation.

In this work, three-dimensional (3D) numerical simulations of a lab-scale pressurized fluidized bed are performed using an Euler-Lagrange approach. The gas phase is modeled solving the low-Mach variable density Navier-Stokes equations in a LES framework (Moureau et al., 2011a), and the solid phase is tracked by the Discrete Element Method (DEM). The implemented approach allows detailed investigation of the effects of i) fluid-particle drag force and particle-particle soft sphere collision model, ii) particle-wall collisions, accounting for dynamic friction, and iii) multiple particle-particle contacts for collisions occurring in dense regime.

The 3D unsteady numerical simulations are realized in the frame of the flat frictional wall assumption for the particle boundary conditions and for different particle-particle and particle-wall restitution coefficient values in order to analyze their influence on the dynamic behavior of the fluidized bed. Results from Euler-Lagrange numerical simulations are compared with the predictions obtained using a two-fluid continuum approach (Fede et al., 2016). Furthermore, time-averaged quantities are computed and numerical predictions are compared with available experimental measurements, obtained from Positron Emission Particle Tracking for the same pressurized bed configuration (Ingram et al., 2007a). In this context, the effect of wall roughness on the particle boundary conditions is found to be of a great interest and is under development in the numerical tool. The following step should be to analyze the effect of the rotation and of the friction on the particle statistics and on the dynamic behavior of the fluidized bed.

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# 100: MODELLING COMBUSTION OF PULVERIZED COAL AND ALTERNATIVE CARBON MATERIALS IN THE BLAST FURNACE RACEWAY

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### ABSTRACT

The impact of injection lance design and injection materials on the combustion conditions inside the raceway of the blast furnace has been investigated. Operational injection tests in LKAB's Experimental blast furnace have been conducted and data describing particle dispersion and temperatures at the tuyere was gathered. A three-dimensional, multiphase numerical model of pulverized material injection (pulverized coal and alternative carbon materials) was developed in order to increase the understanding of raceway conditions in terms of combustion efficiency and reaction rates. In total two different injection lances and two alternative carbon materials in varying blend ratios with pulverized coal were investigated in the numerical study. Simulation results agreed quite well to the experimental data. Furthermore, simulation results agree with published findings regarding the general effect of material properties of pulverized coal on combustion efficiency.

### 101: MULTIPHASE DIRECT NUMERICAL SIMULATIONS (DNS) OF OIL-WATER FLOWS THROUGH HOMOGENEOUS POROUS ROCKS

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### ABSTRACT

Water flooding is commonly used to recover oil from porous rocks using pressurized water. Present study focuses on fully resolved pore-scale level multiphase Direct Numerical Simulations (DNS) of oil-water flows through homogeneous porous rocks. A second order accurate implicit Immersed Boundary Method (IBM) is used to resolve fluid-solid interactions on a non-body fitted Cartesian computational grid. Dynamic evolution of the fluid-fluid interface is tracked by a mass conservative sharp interface Volume of Fluid (VOF) method. The IBM and VOF method are coupled by a prescribed contact angle boundary condition at the fluid-fluidsolid contact line. Our method has been extensively validated especially for the test cases involving oil-water flows. Simulations of water flooding process through periodic homogeneous configurations of spheres are performed based on typical pore-scale capillary and Reynolds numbers. Effect of wettability on the mobility of oil through oil-wet and neutrally-wet rocks has been quantified as well.

### 102: A 2D SEDIMENT BED MORPHODYNAMICS MODEL FOR TURBULENT, NON-NEWTONIAN, PARTICLE-LOADED FLOWS

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### ABSTRACT

In petroleum drilling, cuttings transport problems, i.e. an accumulation of drilled of solids in the wellbore, are a major contributor to well downtime and have therefore been extensively researched over the years, both experimentally and through simulation. In recent years, Computational Fluid Dynamics (CFD) has been used intensively due to increasing available computational power. Here, the problem of cuttings transport is typically investigated as a laminar/turbulent, potentially non-Newtonian (purely shear-thinning) multiphase problem. Typically, an Eulerian-Eulerian two-fluid model concept is utilized, where the particle phase is treated as a second continuous phase. Optionally, a granular flow model, based on the Kinetic Theory of Granular Flow (KTGF), may be used to account for the dense granular flow properties of cuttings forming a sediment bed. One issue of the state of the art CFD approach as described above is the proper resolution of the bed interface, as this may not be accurately resolved in an industrial-relevant CFD simulation.

In this paper, an alternative approach is taken based on modeling concepts used in environmental sediment transport research (rivers, deserts). Instead of including the sediment bed in the computational domain, the latter is limited to the part of the domain filled with the particle-loaded continuous fluid phase. Consequently, the bed interface becomes a deformable domain boundary, which is updated based on the solution of an additional scalar transport equation for the bed height, which is based on the so-called Exner equation (Exner, 1925), a mass conservation equation accounting for convection, and additionally deposition and erosion in the bed load layer. These convective fluxes are modeled with closures relating these fluxes to flow quantities.

As a first step, a 2D model was implemented in ANSYS Fluent R17.2 using Fluent's dynamic mesh capabilities and User-Defined Function (UDF) interfaces. The model accounts for local bed slope, hindered settling, and non-Newtonian, shear-thinning viscosity of the fluid phase as well as turbulence. Model results are benchmarked with experimental data for five different operating points. Most probably due to the utilized unsteady Reynolds-Averaging framework (URANS), the model is not capable of predicting flow-induced dunes; however, it does predict bed deformation as a consequence of for instance non-equilibrium boundary conditions. Other model issues such as e.g. non-Newtonian formulations of the closures are identified and discussed.

# 103: FLOW DYNAMICS STUDIES FOR FLEXIBLE OPERATION OF CONTINUOUS CASTERS (FLOW FLEX CC)

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### ABSTRACT

Flow dynamics of liquid steel within the Continuous Casting (CC) mould are critical for process stability and the quality of final products. An "optimal" flow provides enough circulation of the metal to avoid freezing, but it is stable enough to avoid defects during solidification. This requires a trade-off between speed and stability that is difficult to achieve for the variety of conditions faced by the Scandinavian steel industry (e.g. small orders with high variability in size and steel grades). This is difficult to address with typical CFD models used by the industry and suppliers for design of flow control devices (nozzle, stoppers, etc.), since flow optimization requires a better understanding of the level instabilities inside the mould (i.e. free surface) and its highly turbulent behaviour. Consequently, CC requires advanced multiphase models as well as accurate turbulent and time scales resolution.

The investigation presented uses a multiphase approach (Volume of Fluid, VOF + Discrete Phase Modelling, DPM) to solve the molten steel and argon injection within the mould combined with Large Eddy Simulation (LES) to improve the resolution of turbulent scales compared to typical 2-equation models. CFD simulations were successfully validated with results from a Continuous Casting Simulator using a low melting point alloy. Then, these tools were used to design and test different SEN types for various mould sizes in order to optimize their flow pattern and performance in the mould. The project included a comprehensive set of plant trials at an industrial caster to validate/calibrate model predictions, test nozzle resistance and explore process improvement opportunities.

# 104: MULTISCALE APPROACH TO FULLY RESOLVED BOUNDARY LAYERS USING ADAPTIVE GRIDS

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### ABSTRACT

Bubbly flows are omnipresent in most industrial processes. Often the intended use of such processes is to facilitate efficient mass and heat transfer for reactive flows. Mass and heat transfer coupled with fluid flow in gas-liquid systems gives rise to multiscale transport phenomena. Because of large Schmidt and (possibly) Prandtl numbers in the liquid phase the concentration and temperature boundary layers are much thinner than the momentum boundary layers. When using fully resolved CFD modeling on an uniform grid, these small scales would demand an overall refinement which requires an immense computational effort. Here, however, a hybrid mesh approach is used which couples a fixed Cartesian grid for the hydrodynamics and a tree structure based mesh, which can be adaptively refined for heat and mass transfer. Tree based adaptive refinements commonly suffer from low order accurate numerical schemes. A higher order finite volume scheme on a parallel tree data structure for solving the convection-diffusion equation has been implemented using an implicit formulation. The resulting set of linear algebraic equation are then solved with AMG class of matrix solvers. This approach presents a solution to resolve the fine boundary layers of scalar transport for realistic range of Schmidt and Prandtl numbers. The present study will demonstrate the robustness of this framework to capture sharp boundary layers in fairly simple analytical flow fields. A detailed comparison is performed with overall refined simulations on multi core parallel architectures.

### **106: CFD EROSION MODELING OF BLIND TEES**

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### ABSTRACT

In subsea components such as Production Trees (XT) where the production flow path is machined out of steel blocks, the flow changes direction abruptly at blind tees or sharp elbows, causing increased erosion risks compared to a piping design. The risk of erosion is largely controlled by the depth of the cavity inside a flow-turning element, which may vary between zero for a sharp elbow and more than one time the Inner Diameter (ID) for a full blind tee. In this paper, a comparison between the erosion response of three different flowturning elements is performed by using Computational Fluid Dynamics (CFD) with transient particle tracking: a blind tee with a deep cavity, a blind tee with a shallow cavity (depth < 1ID) and a sharp elbow. The DNVGL-RP-O501 (2015) erosion response model is implemented in the simulations with a modification to the angle function which aims at filtering out erosion results due to impacts at low angle. The transient formulation causes the sand particles to be dispersed naturally by the flow field, yielding time-averaged realistic erosion results without any need for area-averaging or numerical dispersion schemes. The CFD model is successfully benchmarked against the DNVGLRP- O501 (2015) guidelines for standard piping components such as bends. The simulation results reveal that the shallow cavity blind tee creates a very high risk of erosion inside the cavity which is not predicted by the guidelines, with peak erosion rates one order of magnitude higher than for a sharp elbow. This is observed both for a gas and liquid production case, and a physical explanation for this behaviour is provided based on an analysis of the transient flow and sand particle dynamics. Although further numerical sensitivities and experimental evidence are required to confirm this result, it is advised to avoid blind tees with a shallow cavity (less than one time the inner diameter of the flow path) for designing subsea production systems where sand production can be expected.

# 107: AN EULER-EULER MODEL FOR GAS-LIQUID FLOWS IN A COIL WOUND HEAT EXCHANGER

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### ABSTRACT

Coil-wound heat exchangers (CWHE) are commonly adapted in process engineering for the efficient transfer of heat between fluids which feature wide temperature and pressure ranges. The field of application for this apparatus ranges from heating or cooling of single-phase flows, over the evaporation or condensation of fluids, to the utilization as isothermal reactor. Due to their large specific heat transfer area accompanied by a compact design, coil-wound heat exchangers are widely used in various process plants (e.g., LNG plants). Depending on the application, twophase flows may occur at both, the tube- as well as the shellside of the apparatus. For the design of a CWHE, the fluid and thermodynamic processes in the unit are commonly represented by a system of one-dimensional correlations. This approach implies uniform thermohydraulic conditions on horizontal cutting planes of the exchanger. Fluid and thermodynamic effects in the apparatus which result in radial parameter variations are inaccessible to these conventional design tools. To this end, a multidimensional CFD model has been established to enhance the representation of fluid and thermodynamic phenomena in CWHE design. The shellside of the CWHE and all tube-side sections are each numerically represented by separate domains which are coupled by source terms to account for the thermodynamic interaction between tube- and shell-side. In each flow region, the hydraulic effect of the tube bundle is modeled as a porous medium with corresponding fluid dynamic characteristics. The gas-liquid dynamics in each flow region is modeled based on an Euler-Euler approach. Unlike classical Euler-Euler models, local phase fractions and fluid properties are calculated from species relations as well as pressure and temperature fields. This model framework is augmented by locally evaluated correlations for pressure drop and heat transfer to account for apparatus internals and thermal coupling. The models for gasliquid interaction forces are derived from standard correlations and augmented by findings from detailed CFD studies. Remaining parameters are specified by a parameterization study based on experimental findings.

# 108: A DNS STUDY OF DROPLET SPREADING AND PENETRATION ON A POROUS MEDIUM

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### ABSTRACT

We have investigated the dynamics of droplet spreading and liquid penetration at the surface of a porous medium at zero-gravity condition. A coupled IBM-VOF finite volume code has been used to perform pore-scale level fully resolved numerical simulations. The geometrical details of the solid porous matrix are resolved by a sharp interface immersed boundary method (IBM) on a Cartesian grid, whereas the motion of the gas-liquid interface is tracked by a mass conservative volume of fluid (VOF) method. At small scales, the contact line dynamics mainly govern the spreading and capillary penetration. In the present case, the motion of the gas-liquid interface at the immersed boundary is modeled by imposing the contact angle as a boundary condition at the threephase contact line. All the simulations are performed using a model porous structure that is approximated by a 3D cubic scaffold with cylindrical struts. The porosity (e) of the porous structure is varied from e = 0 (flat plate) to e = 0.65 and the equilibrium contact angle Q is varied from Q = 30X (hydrophilic) to Q = 135X(hydrophobic). The effect of porosity and contact angle on the transient evolution of penetration and spreading have been presented and compared with classical models.

### **109: ON PRAGMATISM IN INDUSTRIAL MODELING**

### PART III: APPLICATION TO OPERATIONAL DRILLING

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### ABSTRACT

In this paper, we will apply the concepts of pragmatic industrial modelling to the development of a real time drilling support tool. We develop requirements to such a modelling tool, regarding both input and output, model response times, and accuracy requirement.

The selected application will next be the subject to more theoretical discussions on analyses, standards, technologies, design of the database, and the interface for the modelling framework

On the selected pragmatic modelling case, we evaluate the proposed solutions and outline requirements for the realization of the described tool. We give a proposal of the architecture for such a system, and examples of analysis / modelling workflows, presented in pseudo-code.

We summarize the findings and discuss how this specific "pragmatism in industrial modelling" case should be concluded and prepared for further software/hardware implementation, reuse, sharing, and collaboration. Partial standardization of work processes (illustrated as workflows in pseudocode), data, and metadata is a necessity for building more consistent and informative industrial models. It will answer to customer needs for relevant results, actual accuracy, and delivery speed, and will definitely pave a way towards a tool, which can enable an automated drilling process.

# 110: A SIMULATION CONCEPT FOR GENERIC SIMULATION OF MULTI-MATERIAL FLOW USING STAGGERED CARTESIAN GRIDS

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### ABSTRACT

Simulation of multiphase flows is generally treated by various classes of Eulerian methods, Lagrangian methods, and various combinations of these. In the SIMCOFLOW initiative, we have set out to develop a framework for simulation of multi-material flows, using a Eulerian description. A fundamental part is the application of Cartesian grids with cut cells, and with a staggered representation of the grid for velocities and scalars. The model equations are derived based on formal volume and ensemble averaging (Quintard and Whitaker, 1995), (Gray and Lee, 1977) and (Cushman, 1982). Solid walls or moving solid materials are treated in the same manner as any flowing material (fluid, deforming material). The interface is characterized by a level set or by a 3D surface. In grid cells that are cut by a large-scale interface, the stress acting at the cut surface can be computed based on the level set or volume fractions. The exchange of mass, energy, and momentum between continuous fluids (note: walls are also considered a continuous fluid) can be estimated using wall functions in the case of coarse grids. The methods applied to the flow in a general geometry are closely related to the FAVOR method (Hirt and Sicilian, 1985) and the LS-STAG method (Cheny and Botella, 2010). In this paper, we discuss the derivation of the equations and the numerical solution strategy needed to handle such complex physics within the framework of finite volume methods. We further discuss briefly the ongoing developments such as adaptive gridding and the computational framework. The results of this work will end up as open source software.

# 112: A CARTESIAN CUT-CELL METHOD, BASED ON FORMAL VOLUME AVERAGING OF MASS, MOMENTUM EQUATIONS

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### ABSTRACT

Simulation of multiphase flows are generally treated by various classes of Eulerian methods, Lagrangian methods and various combinations of these. In the SIMCOFLOW initiative we have set out to develop a framework for simulation of multi-material flows, using an Eulerian description. A fundamental part is the application of Cartesian grids with cut cells, and with a staggered representation of the grid for velocities and scalars. The model equations are derived based on formal volume and ensemble averaging (Gray and Lee, 1977; Quintard and Whitaker, 1995; Cushman, 1982). Solid walls or moving solid materials are treated in the same manner as any flowing material (fluid, deforming material). The interface is characterized by a level set or by a 3D surface. In grid cells which are cut with a large scale interface the stress acting at the cut surface can be computed based on the level set or volume fractions. The exchange of mass, energy and momentum between continuous fluids (note: walls are also considered a continuous fluid) can be estimated by wall functions in the case of coarse grids. The methods applied to the flow in a general geometry is closely related to the FAVOR method (Hirt and Sicilian, 1985), the LSSTAG method (Cheny and Botella, 2010) and the cut-cell method of (Kirkpatrick et al., 2003). In this paper we present the derived equations and applications of the method to a single phase two-dimensional flow, and where solid walls are treated as a non-moving secondary phase. Simulations are performed for flow over a cylinder in crossflow. Simulation results are compared with experiments from literature. The results are discussed and critical issues are pointed out.

## 113: Urban Wind at the Gløshaugen Campus

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Keywords: CFD, Wind Energy, Urban wind

### ABSTRACT

In recent years, due to increase in urbanization and industrialization, energy demand has risen around the world [1,2] Therefore, and in order to develop the renewable energy resources, wind energy stands as a major energy resource when it comes to energy production. In this respect, Urban Wind, i.e. utilization of the local wind resource where the energy demand actually is located, has been projected as a strong alternative as its is clean, affordable, safe and available in the long term. To gain knowledge about the methodology and the energy potential for Urban Wind energy production, a small wind farm is to be installed on the Gløshaugen, NTNU Trondheim, campus area. The current work describes the process of identifying and determining the optimal location for wind power generation at Gløshaugen. A digital model of the whole campus area and close surroundings (Figure 1) was established and imported into a CFD code for flow analysis. Experimental data for the wind conditions at a local site at the campus, gathered through a 4 months experimental campaign (an extension of this campaign is underway)[3], was used to define the most probable wind characteristics (Figure 2). From this, the most promising case studies were analysed with CFD giving the flow field for the whole campus area. The calculations were validated through comparison with experimental data. Finally, the computed flow field formed the basis for the optimization of energy output returning the most promising location and main turbine design parameters.

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Figure 1: Gløshaugen Campus 3D model



Figure 2: Wind Direction Probability

### 114: FROM LINEAR TO NONLINEAR: TRANSIENT GROWTH IN CONFINED MAGNETOHYDRODYNAMIC FLOWS

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### ABSTRACT

The underlying flow mechanisms for the destabilisation of an electrically conducting fluid under the influence of a transverse magnetic field in a square duct are investigated. Such flows are applicable to metallurgical processes where magnetic fields are used to dampen disturbances to increase homogeneity in material production, in addition to cooling blankets of nuclear fusion reactors, where flow disturbances can aid in improving convective heat

transfer. A preliminary investigation into optimal linear growths at Hartmann numbers 10 <Ha

<1000 and Reynolds number Re = 5000 identifies two regimes for the scaling of optimal

linear growths; when perturbation structures are dominated by three-dimensional variation in the vertical side-wall boundary layers, and for when quasi-two-dimensional (Q2D) disturbances are prevalent. Through comparison with existing literature, the Q2D model of Sommeria & Moreau (1982) is shown to be an excellent predictor of fundamental growth mechanisms for Ha > 150. A two-step method incorporating the seeding of an unperturbed base flow with optimal linear perturbations in a high magnetic field strength regime shows that no increase in energy amplification can be achieved via initial seeding energies in the range  $10^{-6} < \text{Ep} \ <10^{-2}$ . The dominant dissipative mechanisms for these different seeding energies are also analysed, where it is shown that strong magnetic damping does not always necessitate the smoothing of the velocity field towards pure anisotropy, which has potentially useful applications for aiding convective heat transfer in magnetically damped flows.

# 115: A MULTISCALE NUMERICAL APPROACH OF THE DRIPPING SLAG IN THE COKE BED ZONE OF A PILOT SCALE SI-MN FURNACE

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### ABSTRACT

The Si-Mn alloy process production in submerged arc furnaces (SAF) is investigated. The aim of the studies currently in progress is an enhancement of the knowledge about the key reactions and the mass transport phenomenon related to the metal production. Some small scale experiments on raw materials and bigger pilot scale experiments are done to understand local kinetic and its extension to real condition production furnaces. As it is impossible to observe what is happening in the core of the furnace during operation, excavation of the pilot scale furnace are realised after operations. Based on bibliographical description of similar processes, observations and species analyses after excavation, a numerical simulation is currently in development to test the hypothesis formulated about the internal behaviour of the furnace. As it is difficult to model the complex entire furnace, the work presented here is focusing on what are the phenomenas inside the coke bed, in the dripping zone where the slags flow around the carbon particles before reaching the bottom of the furnace. The thrickling of the slags across the coke bed can be evaluated by a simulation of the droplets finding their path by gravity through the packing of carbon particles. This study has to be very local in space and time, but can give some useful informations such as velocities and drag force. At a larger scale (ie furnace scale), the coke bed particles are modelled by a granular phase in an eulerian-eulerian representation where the slag phase flow interact in the same way as in the local study. The slag is found to flow across the coke bed under the form of droplets of a maximum diameter of 10mm. The apparent velocity of the fluid is about 0,12 m/s. However the residence time of the droplets is longer due to the liquid trapped along the coke bed.

# 116: ON THE SURFACING MECHANISM OF BUBBLE PLUMES FROM SUBSEA GAS RELEASE

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### ABSTRACT

A subsea release of gas poses a risk to humans and assets at the surface. Assessing this risk requires knowledge on how much gas reaches the surface and how it is distributed at the surface. This can be estimated by various modelling techniques, e.g. CFD. Reported surfacing flux can then be fed into a CFD model for atmospheric dispersion calculations. This paper briefly discusses how the surface flux can be calculated by CFD, but primarily focuses on the surfacing characteristics and discusses how the surface flux can be reported and issues related to this.

### 118: CLEANING OF POLYCYCLIC AROMATIC HYDROCARBONS (PAH) OBTAINED FROM FERROALLOYS PLANT

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### ABSTRACT

Polycyclic Aromatic hydrocarbons (PAHs) are organic compounds consisting of only hydrogen and aromatic carbon rings. PAHs are neutral, non-polar molecules that are produced due to incomplete combustion of organic matter. These compounds are carcinogenic and interact with biological nucleophiles to inhibit the normal metabolic functions of the cells. In Norway, the most important sources of PAH pollution are considered to be metallurgical industries, offshore oil industries, transport and wood burning. Stricter governmental regulations regarding emissions to the outer and internal environment combined with increased awareness of the potential health effects have motivated Norwegian metal industries to increase their efforts to reduce emissions considerably. One of the objective of the ongoing industry and Norwegian research council supported "SCORE" project at SINTEF is to remove PAH from a hot gas stream through controlled combustion of the PAH inside a dedicated combustion chamber. The sizing and configuration of the combustion chamber depends on the properties of the bulk gas stream and the properties of the PAH itself. In order to achieve efficient and complete combustion of the PAH, the residence time and temperature need to be optimized. In the present study, the oxidation of pure PAH and PAH mixed with process gas is modelled using a Perfectly Stirred Reactor (PSR) concept. PSR concept was useful for understanding the influence of residence time and temperature on the oxidation of PAH to CO2 and water. Furthermore, a computationally fast approach based on Chemical Reactor Network (CRN) is proposed for understanding the oxidation of PAH inside complex geometries. The Chemical Reactor Network (CRN) yields a detailed composition regarding species and temperature in the combustion chamber.

### 119: COMBUSTION CHAMBER SCALING FOR ENERGY RECOVERY FROM FURNACE PROCESS GAS: WASTE TO VALUE

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### ABSTRACT

One of the byproducts during the metal reduction process is energy rich off-gas of which the energy is normally not used. In the present paper, a novel concept for energy recovery from process gas is discussed. The concept is founded on the idea of introducing a combustion chamber in the off-gas section, which will provide an additional degree of freedom for optimizing energy recovery and minimizing Polycyclic Aromatic Hydrocarbon (PAH) and NOx concentrations. Design and operation of the combustion chamber depend on many parameters, including the total power capacity of the combustion chamber, residence time for combusting the complex PAH. The design criteria for the combustion chamber have been identified and discussed. The scaling of the combustion chamber based on proposed design criteria is presented. Engineering methods and Computational Fluid Dynamics (CFD) has been utilized extensively for scaling the combustion chamber. The results from our CFD simulations of the flow in the combustion chamber, exploring different off-gas fuel compositions, are presented. In brief, the paper covers all aspects which influences the scaling of the combustion chamber, including insulation thickness, choice of insulating material, heat transfer through extended surfaces, multi-staging and secondary air injection.

### 122: EXPERIMENTAL AND CFD INVESTIGATIONS OF FRACTAL DISTRIBUTOR ON A NOVEL PLATE AND FRAME ION-EXCHANGER

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### ABSTRACT

Conventional pressure based flow distributors face challenges in the form of operational limits as their low outlet density and non-uniform flow distribution path, often act as bottleneck in the overall chemical equipment efficiency. Recently, a new distributor design inspired by the concept of fractal shows promising performance over a wide range of applications and operating conditions. The inherent scaling symmetry from such fractal distributors allows identical hydraulic flow path length to all outlets as well as much higher outlet density. In this study, we have designed a novel 12" by 12" plate and frame type ion-exchanger called "Fractal Pack" and tested it in pilot scale adopting fractal distributors with 256 outlets under operating flow rates ranging from  $6.31 \times 10^{-5}$  m3/s to  $2.52 \times 10^{-4}$ m3/s. For comparison, ion-exchanger with 16 distributor outlets has also been assembled to mimic the performance of conventional pressure-based design. Both residence time distribution test and CFD investigations have been conducted. From CFD results, at highest flow rate, we found the overall pressure drop for ion-exchanger with 16 outlets is about 6 times larger than with fractal distributor and 78% of its pressure drop is caused by sudden expansion and contraction at 16 outlets. In addition, a key index, degree of heterogeneity which measures the percentage of mal-distribution zones inside resin, has been defined to quantify flow distribution inside resin. The distributor equipped with 16 outlets shows 4 times more mal-distribution zones than 256 outlets at highest flow rate. This work demonstrates that fractal distributors can reliably provide superior performance over conventional distributors in a compact design framework; by introduction of symmetry, fractal distributors can aid process intensifications for many chemical processes that are plagued by heterogeneities and poor process efficiencies. The work also demonstrates how CFD can assist in avoiding ad-hoc design decision on dimensions and systematically explore the design space for optimum design decisions, using optimization criteria like coefficient of variation, degree of dispersion or heterogeneity.

## 123: Development of Filtered Particulate Eulerian Modeling Approach for the Industrial Prediction of Bi-Disperse Gas-Solid Fluidized Bed

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**Keywords:** gas-solid flow, circulating fluidized bed, polydisperse mixture, filtered approach, subgrid model, particle-particle collision.

### ABSTRACT

Due to computational resource limitation, Eulerian gas-solid fluidized bed simulations of industrial processes are usually performed with mesh sizes much larger than the smallest meso-scale structure size. Thus, these effective simulations do not fully account for the particle segregation effect (cluster or bubbles formation) and neglecting these structures generally leads to poor prediction of bed hydrodynamic [1]. According to previous numerical studies, this effect seems to be very effective in bi-solid mixture with large inertia difference between the solid species.

Following Igci et al. [2], filtered approach may be developed where the unknown terms accounting for the influence of unresolved structures, called sub-grid contributions, have to be modelled in terms of the computed (filtered) variables. In the work presented here, the development of such modelling approach is based on a priori analysis of 3D periodic circulating bi-disperse gas-solid fluidized bed simulations using computational grids cell size of a few particle diameters [3]. Using the 3D N-Euler multiphase code NEPTUNE\_CFD, separate transport equations are computed for the number density, velocity and random kinetic energy of the two solid species, coupled by collisions terms developed in the frame of kinetic theory of granular media supplemented by interstitial gas effect. The mesh-independent results obtained are filtered using volume average to analyse the effect of the subgrid scales on the terms of the momentum and the particle kinetic agitation equations. Thanks to those results, closure models are developed for the subgrid fluid-particle and particle-particle interactions terms in bi-disperse gas-solid fluidized beds. Those closure models include parameters which may depend on the particle and gas properties and are dynamically adjusted using a multi-level filtering procedure [3, 4]. Several monodisperse and bi-disperse fully resolved simulations have been performed and enable to test the models for a wide range of diameter and density.

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Figure 1: Resolved and subgrid (SGS) contributions in the momentum equation of the *p*-particles. Data extracted from a bidisperse numerical simulation of *p*-particles ( $d_p = 75 \ \mu m$  and  $\alpha_p = 5\%$ ) and *q*-particles ( $\alpha_q = \alpha_p$  and  $d_q = 2d_p$ ). Drag: gas-particle momentum exchange, press: gas pressure particle volume fraction correlation and part-part: inter-particle momentum exchange.



Figure 2: Resolved and subgrid (SGS) contributions in the kinetic agitation equation of *p*-particles. Data extracted from a bidisperse numerical simulation of *p*-particles ( $d_p = 75 \ \mu m$  and  $\alpha_p = 5\%$ ) and *q*-particles ( $\alpha_q = \alpha_p$  and  $d_q = 2d_p$ ).  $\Pi_p$ : production by velocity gradient,  $\epsilon_{pg}$ : transfer between gas and particles, coll: sum of all collision terms.



Figure 3: Resolved and subgrid (SGS) contributions in the kinetic agitation equation of *p*-particles. Data extracted from a bidisperse numerical simulation of *p*-particles ( $d_p = 75 \ \mu m$  and  $\alpha_p = 5\%$ ) and *q*-particles ( $\alpha_q = \alpha_p$  and  $d_q = 2d_p$ ).  $P_{pq}$ : production by slip velocity between solid phases,  $T_p$ : transfer between particles,  $\epsilon_{pq}$ : dissipation due to inelastic collisions.

### 124: VALIDATION OF A RAPID SLAG VISCOSITY MEASUREMENT BY CFD

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### ABSTRACT

Slag viscosity is an important property in daily process practice, as well as for modelling flows in metallurgical processes accurately. Measuring slag viscosities is a challenging task, and usually requires a specific high-temperature furnace set-up, which needs to be gas tight and still allow for e.g. torque measurements on a well-aligned rotating viscometer spindle. The inclined plane technique is an alternative, requiring little time and no complex instruments. A slag sample, heated in a crucible or from an industrial furnace, is poured onto an inclined steel plate, and runs down while solidifying, to form a ribbon of a certain length. The ribbon length has been experimentally proven to be correlated rather accurately to the high temperature viscosity. However, as the viscosity increases sharply during cooling, the ribbon length should also depend on the temperature dependence of the viscosity. To study these effects, a CFD model has been built in this project. This model also allows to understand the effect of slag weight, steel plate thickness, temperature, and inclination, which could influence the results. The model is based on a VOF description for the slag surface and uses accurate heat capacity and viscosity functions based on thermodynamic calculations. This approach allows to increase the reliability of the fast slag viscosity measurement.
### 125: VELOCITY PROFILES IN A 2D MODEL OF THE LEFT VENTRICULAR OUTFLOW TRACT, PATHOLOGICAL CASE STUDY USING PIV AND CFD MODELING

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### ABSTRACT

In the current study, we present an experimental (in vitro) 2D flow model for studying blood flow in the human left ventricular outflow tract (LVOT) and the first part of the aorta using particle image velocimetry (PIV) and computational fluid dynamics (CFD). Two cardiac pathologies were investigated in this study; 1) anterior mitral leaflet (AML) billowing, and 2) asymmetric septal hypertrophy (ASH). Each of these conditions has the potential to alter the normal direction of the flow entering the aortic valve apparatus from the LVOT and therefore place an abnormal stress distribution on the aortic valve leaflets. We found good agreement between the PIV results and the CFD calculations. The largest discrepancy between the experimental data and the numerical results was found in the recirculation zone adjacent to the left coronary leaflet. The main limitations in the current study when evaluating the clinical significance of the results are the choice of a 2D geometry with stiff and stationary walls. Keeping this in mind, our results show that AML billowing and ASH bulging alone does not alter the flow field in the LVOT dramatically. However, when the two conditions combine, we see a significant flow separation and re-circulation zone forming at the left coronary leaflet, covering half of the aortic outflow tract at peak systole.

### 126: PARALLEL MULTIPHASE FLOW SOFTWARE FOR SOLVING THE NAVIER-STOKES EQUATIONS

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### ABSTRACT

A code based on finite element method was built and applied on the variable density incompressible Navier-Stokes equations for accurately simulating immiscible two phase flows. The algorithm simulates the interface between the two liquid phases with high accuracy; it utilizes both the level-set method with a third order strong stability property Runge-Kutta (SSPRK) time integrator and a secondorder projection method for the momentum equation. The solver developed is based on deal.II, an open source framework code. Numerical assessments on the transport and momentum equations are presented to verify the code accuracy. Nonconforming manufactured solutions are shown to produce the expected convergence rate of the used numerical schemes. Simulation of classical Rayleigh-Taylor instability was carried out and shown to match those in the published work.

### 127: MODELLING OF INTERACTION BETWEEN TURBINES AND TERRAIN WAKES USING PRAGMATIC APPROACH

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### ABSTRACT

Kongsberg Digital (KDI) is currently developing a decision support system for wind farms (Kongsberg EmPower). The objectives of Kongsberg EmPower are to optimize the total power production from a wind farm, forecast the power production and monitor the performance and condition of the wind turbines. Power production from a wind farm depends on the flow field around the wind turbine, which is highly influenced by the interaction between turbine and terrain wakes. Furthermore, increased turbulence due to wake-wake interaction increases structural and fatigue loads on the wind turbine blades, leading to higher operational and maintenance (O&M) cost. An improved understanding on the wake-wake interaction is extremely important for optimizing the power production and for reducing the O&M cost. Performing extensive velocities measurements for an entire wind farm is time consuming and expensive. The traditional approach within wind research and industry has been to use full CFD models when complex flow phenomena have to be taken into consideration, but this is computationally demanding. On the other hand, simple engineering models are unable to capture the interaction of flow over complex terrain and wind turbine wakes. KDI and SINTEF are running a project to develop a fast response simulator with simplified representations of terrain effects and turbine wakes. In the proposed approach a pragmatic model for turbines and terrain wakes interaction is presented. Complex flow over a terrain is estimated with mass consistent model and wake from wind turbine is computed using well established wake models i.e. Jensen and Ainslie model. The pragmatic model for coupling the interaction between turbine wakes and terrain approach is presented. The results obtained from the mass consistent approach are verified with CFD using OpenFoam.

## 129: MODELLING AND MEASUREMENTS IN THE ALUMINIUM INDUSTRY - WHERE ARE THE OBSTACLES?

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### ABSTRACT

In this paper the necessity of obtaining experimental data with good enough quality for model verification is addressed. Relevant examples from the aluminium industry are shown to illustrate some cases where measurements and model results work hand in hand on identifying bottlenecks and improving the situation. Moreover, measurements and their interpretation are briefly touched upon, trying to enlighten a few of the challenges on data collection in industrial environments and comparison with models.

Realising that measurements only uncovers parts of the real picture, an approach to estimate data interpretation errors is briefly outlined. A good model can and should rule out erroneous measurements – with the right use it can even give some guidelines on where to get good measurements.

### **130: NOVEL EFFICIENT HYBRID-DEM COLLISION INTEGRATION SCHEME**

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### ABSTRACT

A hybrid collision integration scheme is introduced, benefiting from the efficient handling of binary collisions in the hard sphere scheme and the robust time scaling of the soft sphere scheme. In typical dynamic dense granular flow, simulated with the soft sphere scheme, the amount of collisions involving more than two particles are limited, and necessarily so because of loss of energy decay otherwise. Because most collisions are binary, these collisions can be handled within one time step without the necessary numerical integration as needed in a soft sphere method. The remainder of the collisions can still be handled with the classical soft sphere scheme. In this work the hybrid collisions integration scheme is shortly described and tested with a bounding box problem. The hybrid scheme is capable of solving the same problem as a classic soft sphere scheme but is roughly one order of magnitude faster.

## 131: BUBBLE GENERATED TURBULENCE IN TWO FLUID SIMULATION OF BUBBLY FLOW

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### ABSTRACT

Bubbly flows are central to many processes in the minerals extraction and metal production industries, mainly because they enhance heat and mass transfer rates. These transfer rates depend on the turbulence level in the multiphase flow. Bubbles rising in a liquid give rise to an additional component of turbulence in the continuous phase, known as bubble-induced turbulence. Various models have been proposed in the literature to account for this mechanism in two-fluid Reynolds-averaged (RANS) simulations of bubbly flow, but there is considerable uncertainty about the form of terms that should be added to account for the effect, and even the flow physics underlying the phenomenon is poorly understood. Simulations are carried out of flow around a simplified bubble arrangement in order to clarify this flow physics, to allow a consistent definition of bubble-induced turbulence, and to point the way to a reliable determination of the source terms. It is argued that a component of the fluctuations due to flow around bubbles should not be considered to be turbulence since the energy of these fluctuations is actually recoverable. This fact seriously complicates efforts to obtain bubbleinduced turbulence from experimental velocity measurements or direct numerical simulations. Simulations of flow around a bubble using the SST turbulence model allow the prediction of the source of actual bubble-induced turbulence for a single isolated rather than the pseudo-turbulence related to bubble motion. The source of actual turbulence for an isolated bubble of diameter 5 mm with a mobile interface is predicted to be very small, while for an immobile interface, a finite source is distributed in the wake of the bubble. The source of "bubble-induced" turbulence for a bubble swarm is a more complex issue, but the present simulations can give insights and point the way forward to a more complete formulation.

## 136: SOFT: A FRAMEWORK FOR SEMANTIC INTEROPERABILITY OF SCIENTIFIC SOFTWARE

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### ABSTRACT

In this paper we present our strategy and implementation of a datacentric modelling framework (SOFT, SINTEF Open Framework and Tools) with focus on information interchange in throughprocess and multiscale applications. SOFT needs to accommodate for a inhomogeneous set of in-house open source and proprietary simulators, often written in different programming languages, and storing data in different formats. The complexity and diversity of such a system requires that we have formal schemas and structures of metadata that allow for information interpretation regardless of the original storage formats, which application produced the data, and which application processes the data. We propose a standard for data exchange, separately describing metadata specific to different knowledge domains, SOFT, via a mechanism of plugins, offers the possibility to utilize different tools for storage of such data and metadata. Further, SOFT facilitates scientific software development by clear separation of numerical routines and platform-dependent input, output, and analysis routines. Automated testing and simulation data analysis are also achieved in SOFT via external plugins and interfaces to scripted languages such as Python and Javascript. The framework has been developed and tested within such flow modelling projects as LedaFlow, NanoSim and SimcoFlow.

### 137: THE PECULIAR BEHAVIOR OF ELONGATED PARTICLES IN FLUIDIZED BEDS : EXPERIMENTS VERSUS SIMULATIONS

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### ABSTRACT

Gas-solid fluidized beds are widely used in industry. Numerous experimental, theoretical and numerical studies have been done to better understand the complex behaviour of fluidized phase. Almost all of these studies have been done on spherical particles. However, in industry granules are largely non-spherical in nature. Understanding of shape effects of such particles under fluidized conditions is severely lacking in literature. In this work, fluidized bed of rod-like particles is studied through experiments (PIV, PTV and DIA) and CFD-DEM simulations. Global bed dynamics are investigated by measuring pressure drop, bed height, solid circulation velocity and mass flux in the bed. Particle orientation is investigated for wall-proximity effects and also at different inlet gas flowrates. Experimental findings are compared with simulations for all the above parameters and also for effect of different particle co-ordination number. The importance of hydrodynamic torque in CFD-DEM simulations is also demonstrated.

# **138:** Adsorption-desorption modeling for a chemical reaction using Stochastic Rotation Dynamics

Sengar, A., Padding, J. T. Kuipers, J. A. M. Santen, Rutger A. van

Combining fluid mechanics with reactive systems at a mesoscale level is important to study coupled reaction-diffusion-convection problems where any of the processes can play a part in determining yield of the product. Stochastic rotation dynamics (SRD), a mesoscale coarse grained technique has been used to study the particle-particle interaction in the bulk and connection to the surface reactive system is achieved by expanding upon Langmuir Hinshelwood reaction model kinetics. Evolution of the reaction leads to a multi-component mixture inside the bulk of the system, where hydrodynamic interactions of participating species lead to Maxwell-Stefan-like diffusion in the bulk. We look at the spatial and temporal concentration profiles of reactant across the model reactor developed and study them as a function of Damkohler number, Da. We end the discussion by commenting on the yield of product species generated and looking at the future prospective of including a flow to complete the reaction-diffusion-convection system.

### 141: Numerical simulation on a high head Francis turbine

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Keywords: CFD, RSI, Hydro turbine, Francis99, Validation

### ABSTRACT

In the last decades, there have been several turbine failures in high head power plants in Norway. Worryingly, many of these turbines have been brand new. The main problem is fatigue and crack formation. The fatigue stems from a fluctuating pressure field in the turbine runner, which is inevitable in turbines with rotor and stator components. A solid understanding of this rotor-stator interaction (RSI), as well as the structural response is key to a good turbine design.

This article will compare numerical simulations in ANSYS CFX with experimental results. The Francis99 model turbine at the Norwegian University of Science and Technology has been used as validation case. The main focus is the RSI effects, and fluctuating pressure components in the runner, as well as global parameters as head and torque. The full 360° turbine runner, full spiral casing and draft tube is modelled.

The results show that global parameters are solved satisfactory. The error is of the order of 1% in head, torque and static pressure values. A spectral analysis of the pressure in a runner channel reveals that the frequencies are perfectly predicted, but the pressure amplitudes are slightly underestimated. Furthermore, Fourier-based models have been implemented in an attempt to reduce the simulation time, without affecting the accuracy. The Fourier coefficients from the decomposed pressure signal could further be imposed on a structural analysis to obtain the actual stresses and strains in the runner.

### 145: THE DEPENDENCE OF ORIENTATION ON THE DRAG AND LIFT OF NON-SPHERICAL PARTICLES

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Keywords: Non-spherical particles, Particles in fluids.

### ABSTRACT

The flow around different prolate (needle-like) and oblate (disc-like) spheroids is studied using a multi-relaxation-time lattice Boltzmann method. We compute the mean drag coefficient  $C_{D,\varphi}$  at different incident angles  $\varphi$  for a wide range of Reynolds numbers (*Re*). We show that the sine-squared drag law as  $C_{D,\varphi} = C_{D,\varphi=0^{\circ}} + (C_{D,\varphi=90^{\circ}} - C_{D,\varphi=0^{\circ}})\sin^2\varphi$  holds up to large Reynolds numbers, *Re*=2000. Further, we explore the physical origin behind the sine-squared law, and reveal that, surprisingly, this does not occur due to linearity of flow fields as is the case of Stokes flow. Instead, it occurs due to an interesting pattern of pressure distribution contributing to the drag at higher *Re* for different incident angles. The present results demonstrate that it is possible to perform just two simulations at  $\varphi = 0^{\circ}$  and  $\varphi = 90^{\circ}$  for a given *Re* and obtain particle-shape-specific  $C_D$  at arbitrary incident angles.

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### SAMPLE RESULTS



**Figure 1:** (*a*) The normalized drag coefficient  $(C_{D,\varphi} - C_{D,\varphi=0^{\circ}})/(C_{D,\varphi=90^{\circ}} - C_{D,\varphi=0^{\circ}})$  plotted against the incident angle  $\varphi$ . The solid line indicates  $\sin^2 \varphi$ . Data include (a) a prolate spheroid (+) and (b) an oblate spheroid (×), both of aspect ratio 5/2, both for *Re*=0.1, 10, 100, 1000 and 2000, and (c) a prolate spheroid of aspect ratio 4 ( $\Delta$ ) for *Re*=2000. (*b*) The difference between the normalized drag coefficient and  $\sin^2 \varphi$ .



**Figure 2**: The normalized lift coefficient  $C_{L,\varphi}/(C_{D,\varphi=90^{\circ}} - C_{D,\varphi=0^{\circ}})$  plotted against the incident angle  $\varphi$ . The solid line indicates  $\sin \varphi \cos \varphi$ . (*a*) Prolate spheroid of aspect ratio 5/2 for *Re*=0.1, 10, 100, 1000 and 2000 (+); prolate spheroid of aspect ratio 4 at *Re*=2000 ( $\Delta$ ); (*b*) oblate spheroid of aspect ratio 5/2 for *Re*=0.1, 10, 100, 1000 and 2000 (×); oblate spheroid of aspect ratio 4 at *Re*=100 ( $\bigtriangledown$ ). It should be noted that the oblate spheroids are experiencing stronger deviations compared with prolate spheroids.