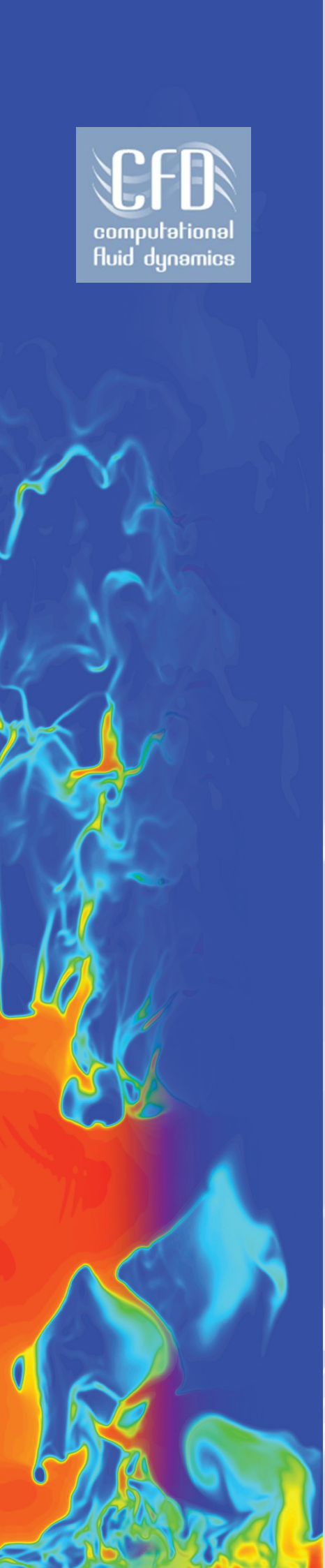

June 17- 19, Trondheim, Norway

CFD 2014

10th International Conference on

Computational Fluid Dynamics
in the Oil & Gas, Metallurgical and Process Industries

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of the 10th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries

SINTEF is pleased to host the 10th international conference in this series. The conference series was initiated by CSIRO and Phil Schwarz in 1997. So far the conference has been alternating between CSIRO in Melbourne and SINTEF in Trondheim. The conferences focuses on the application of CFD in the oil and gas industries, metal production, mineral processing, power generation, chemicals and other process industries. The conference is also known as CFD2014 for short.

This document contains the program and abstracts of the conference. It can be used as a guide for choosing sessions and presentations you like to attend. Note that the titles in the program on the next pages are active links to the belonging abstracts. The full papers are collected in the proceedings. The organizing committee would like to thank conference sponsors: FACE (the multiphase flow assurance centre), Total, ANSYS, CD-Adapco, Ascomp, Statoil and Elkem.

Stein Tore Johansen & Jan Erik Olsen

Monday June 16
1700-1800 Conference reception, RICA Nidelven

Tuesday June 17

	Auditorium A (Trondhjemsalen)	Auditorium B (Gråkallen/Lade)	Auditorium C (Strinda/Illsvika)
0800-0820	**Registration**		
0820-0840	**Opening**		
0840-0925	**Keynote: Phil Schwarz (CSIRO)** Complex multiphase flow applications of CFD - Experiences and Pragmatism		
0930-1100	**Session 1A: Pragmatic Modelling (Chair: Phil Schwarz)**	**Session 1B: Packed Beds (Chair: Gerald Pereira)**	**Session 1C: Casting & Solidification (Chair: Jan Erik Olsen)**
0930-1000	*On pragmatism in industrial modeling* , K.E. Trætli-Einarsrud, A. Solheim, S.T. Johansen & J. Zoric	*A two-fluid model coupled with porous medium description to predict liquid spreading in trickle-bed reactors,* Z.Solomenko, M.Fourati, Y.Haroun, F.Larachi, C.Boyer & F.Augier	*Prediction of mass transfer between liquid steel and slag at continuous casting mold* , P.Gardin, S.Gauthier & S.Vincent
1000-1020	*A six chemical species CFD model of alumina reduction in a Hall-Héroult cell* , P.J.Witt, Y.Q.Feng, G.A.Snook, I.Eick & M.Cooksey	*Local simulation of the effect of void fraction on the overall reaction rate in packed beds reactors* , M. Rolland	*Structure effect of turbo-swirl in an uphill teeming ingot casting process* , H. Bai, M. Ersson & P. Jönsson
1020-1040	*A pragmatic approach to CFD modelling of separation processes* , K.E.Trætli-Einarsrud, B.Panjwani & V.Pauchard	*Transport of the moments of the age distr. by CFD in fixed bed operation units,* L.Fangueiro Gomes, F.Augier, D.Leinekugel-le-Cocq, I.Vinkovic & S.Simoëns	*Modelling of tracer mixing in continuous casting tundishes* , C.Chen, A. Tilliander, L.T.I. Jonsson, G. Cheng & P. Jönsson
1040-1100	*Multi-scale process models to enable the embedding of CFD derived functions: Curtain drag in flighted rotary dryers,* A. Lee, M. Sheehan & P.A. Schneider	*A multi-scale model for oxygen carrier selection and reactor design applied to packed bed CLC* , M.Tabib, J.Morud, S.T.Johansen & S.Amini	*Num. investigation of the immersion quenching process for heat treated parts using an eulerian multi-fluid approach* , R.Kopun, D.Greif, Z.Kovacic & M.Suffa
1100-1130	**Break**		
1130-1300	**Session 2A: Pragmatic Modelling (Chair: Phil Schwarz)**	**Session 2B: Particles & DEM (Chair: Niels Deen)**	**Session 2C: High Temperature Processes (Chair: Peter Witt)**
1130-1200	*Pragmatic approach to efficient modeling of commercial MOVPE reactors* , H.Laux & J.Bassen	*DEM-CFD simulations and imaging experiments on charging of pneumatically conveyed powders* , M.W.Korevaar, J.T.Padding, J.Wang, M. De Wit, M.A.I.Schutyser, M.A.van der Hoef & J.A.M.Kuipers	*Multi-scale modeling of hydrocarbon injection into the blast furnace raceway* , C.Maier, C.Jordan, C.Feilmayr, C.Thaler & M.Harasek
1200-1220	*CFD in problem analysis and optimization – the importance of correct boundary conditions,* E.Manger	*Establishing predictive capability of DEM simulations: sliding and rolling friction coefficient of non-spherical particles,* L. Benvenuti, A. Aigner, D. Queteschiner, M. Combarros, S. Pirker & C. Kloss	*CFD modelling of a rotating arc plasma reactor* , S.G.Johnsen & A.J.Simonsen
1220-1240	*A combined multifluid-PBE model for a slurry bubble column reactor: application to the Fischer-Tropsch synthesis* , C.B.Vik, J.Solsvik & H.A.Jakobsen	*Understanding segregation in granular media,* G.G.Pereira, M.Sooriyabandara & P.W.Cleary	*Numerical investigation of syngas combustion in a HITAG system using CFD technique* s, M.Saffari Pour, P.Mellin, W.Yang & W. Blasiak
1240-1300	*Discussion on Pragmatic Modelling:* J.Zoric / S.T.Johansen	*Hard-sphere modelling of liquid bridge agglomeration* , B.V.Balakin, G.Shamsutdinova & P.Kosinksi	*CFD Simulation of a burner head in a secondary reformer for ammonia synthesis* , J.Bujalski & J.Dauparas
1300-1400	**Lunch**		
1400-1450	**Keynote: Fotis Sotiropoulos (University of Minnesota)** Immersed boundary methods for simulating flow-structure interaction in energy, environmental and cardiovascular problems		
1450-1620	**Session 3A: Fluidized Beds (Chair: Harald Laux)**	**Session 3B: Euler-Lagrangian Models (Chair: Stein Tore Johansen)**	**Session 3C: Combustion & Turbulence (Chair: Eirik Manger)**
1450-1520	*Num. investigation of the vertical plunging force of a spherical intruder into a prefluidized granular bed* , Y.Xu , J.T.Padding, M.A.van der Hoef & J.A.M.Kuiper	*Comparing Euler-Euler and Euler-Lagrange based modelling approaches for gas-particle flows* , M.Braun, M.Lambert, S.Ozarkar & J.Sanyal	*Multi-scale modelling of turbulent flows by embedded lattice-Boltzmann co-simulation* , S.Pirker, S.Puttinger, P.Seil, S.Schneiderbauer
1520-1540	*Operating experience with a high-temperature pseudo-2D fluidized bed reactor designed especially for detailed local data collection* , A.Zaabout, S.Cloete, S.T.Johansen, S.Amini	*Agglomeration study in the inlet section of a large scale spray dryer using stochastic Euler-Lagrange modelling* , S.K.Pawar, J.T.Padding, N.G.Deen, A.Jongsma, F.Innings & J.A.M.Kuipers	*Lifetime distributions of turbulent flow structures in chemical process equipment* , F.Ghasempour, R.Andersson, D.J.Bergstrom & B.Andersson
1540-1600	*Heat transfer in gas-solid fluidized bed through an integrated DIA/PIV/IR technique* , A.Patil, E.A.J.F.Peters & J.A.M.Kuipers	*State of the art in mapping schemes for dilute and dense Euler-Lagrange simulations* , S.Radl, B.Capa Gonzales, C.Goniva & S.Pirker	*Modeling of post combustion inside the off-gas duct system of the Ovako electric arc furnace* , N.Arzpeyma, M.Ersson & P.Jönsson
1600-1620	*Hybrid Eulerian-Lagrangian modelling of bi-disperse fluidized beds* , S.Schneiderbauer, S.Puttinger & S.Pirker	*Numerical simulation of ice accretion on vessels and structures due to sea spray* , M.Popescu & S.T.Johansen	*Modelling of the Ferrosilicon furnace: effect of boundary conditions and burst* , B.Panjwani & J.E.Olsen
1620-1650	**Break**		
1650-1800	**Sponsor presentations (Chair: Jan Erik Olsen)**	**Session 4B: Population Balance Methods (Chair: Kristian E. Trætli-Einarsrud)**	**Session 4C: Rotating Machinery (Chair: Fotis Sotiropoulos)**
1650-1720	CD-Adapco	*A study of breakage by single drop experiments* , J. Solsvik & H.A. Jakobsen	*CFD simulations of a Wankel pump with moving and static grids* , J. Y. C Leong, T. Ba, S. Y. M. Wan, Y. Zhao, C. W. Kang, W. L. Loh & A. T. B. Lim
1720-1740	ASCOMP	*Modelling of bubble size distr. by using homogeneous and inhomogeneous population balance approaches* , L.Deju, S. C. P.Cheung, G. H.Yeoh & J.Y.Tu	*CFD study of the Influence of pre-rotation of multiphase flow on pump performance* , M.P.Strongin
1740-1800	ANSYS	*Simulation of polydisperse gas-liquid systems with QBMM* , A.Buffo, D.L.Marchisio, M.Vanni, J.Hofinger & P.Renze	*Investigating CFD study of centrifugal compressor with vaneless diffusers* , N.Hasan
1800	**Close**		

Wednesday June 18

	Auditorium A (Trondhjemsalen)	Auditorium B (Gråkallen/Lade)	Auditorium C (Strinda/Illsvika)
0830-0925	**Keynote: William L. Oberkampf (William L Oberkampf Consulting)** Concepts and Practice of Verification, Validation, and Uncertainty Quantification		
0930-1100	**Session 5A: Pipe Flow (Chair: Sanjoy Banerjee)**	**Session 5B: Packed Beds & Permeability (Chair: Matthieu Rolland)**	**Session 5C: Metallurgy & Leaching (Chair: Pascal Gardin)**
0930-1000	*Forecasting turbulent drag reduction in a pipeline flow on the basis of Taylor-Couette device experimental data*, D.Eskin	*CFD simulations of flow in random packed beds of spheres and cylinders: analysis of the velocity field*, F.Dorai, M.Rolland, A.Wachs, M.Marcoux & E.Climent	*Modelling thermal effects in the molten iron bath of the HIsmelt reduction vessel*, P. Witt, Y.Q.Feng & M. P. Davis
1000-1020	*CFD modelling of gas entrainment at a propagating slug front,* J.Hua, J.Nordbø & M.Foss	*Pore-scale simulation of fluid flow in packed-bed reactors via rigid-body simulations and CFD*, G. Boccardo, L. Del Plato, D. Marchisio, F. Augier, Y. Haroun, D. Ferre & M. Icardi	*Design optimization of a metal tapping room for minimized dust emission*, B.Panjwani, B.Wittgens, S.T.Johansen & B.Ravary
1020-1040	*Computational modelling of subsea hydrates formation and associated risks and impact on flow assurance*, M.Labois, N.Pagan, D.Lakehal & C.Narayanan	*Automated workflow for spatially resolved fixed bed reactors with spherical and non-spherical particles*, T.Eppinger, N.Jurtz & R.Aglave	*Heap leaching simulation: beyond shrinking core models,* L.Cai, R.Ferrier, Q.Lin, P, Mostaghimi, J.G.Gorman & S.Neethling
1040-1100	*Pressure and temperature prediction in presence of hydrate*, N.Hasan	*Numerical model for flow in rocks composed of materials of different permeability,* R Li, S. Yang, J.Pan, G.G. Pereira, J. Taylor, B. Clennell & C. Zou	*Design and improvement of an industrial airlift reactor using computational fluid dynamics*, T.Song, K.Jiang, J.Zhou, D.Wang, N.Xu & Y.Feng
1100-1130	**Break**		
1130-1300	**Session 6A: Bubble & Droplet Dynamics (Chair: Antonio Buffo)**	**Session 6B: Fluidized Beds (Chair: Shahriar Amini)**	**Session 6C: Oil & Gas Applications (Chair: Martin Foss)**
1130-1200	*A critical comparison of surface tension models for the volume of fluid method*, M.W. Baltussen, J.A.M. Kuipers & N.G. Deen	*The parametric sensitivity of fluidized bed reactor simulations carried out in different flow regimes,* S.Cloete, J.H.Cloete, S.T.Johansen & S.Amini	*Cool down simulations of subsea equipment*, A. Jensen & S. Grafsrønningen
1200-1220	*Numerical simulation of the influence of bubble bursting on a molten iron surface*, Y.G.Xu, M.Ersson & P.G.Jönsson	*Bed expansion and pressure drop in a bubbling fluidized bed,* K.J.Mandich & R. J.Cattolica	*Predicting emulsion pressure drop in pipes through CFD multiphase rheology models*, N. J. Inkson, J. Plasencia & S. Lo
1220-1240	*An enhanced front tracking method featuring volume conservative remeshing and mass transfer*, I.Roghair, M.van Sint Annaland & J.A.M.Kuipers	*Validation of a CFD model for 3d cylindrical gas-solid fluidized beds*, V.Verma, J.T. Padding, N.G. Deen & J.A.M.Kuipers	*Transient modelling of relief lines for surface testing application*, B.Zielinska, F.Allouche, L.Fraser & N.Zafar
1240-1300	*Drop breakup modelling in turbulent flows*, B. Lalanne, S. Tanguy, J. Vejrazka, O. Masbernat & F. Risso	*Procedural method for simulating an industrial urea granulation process*, P.Lau & M.Kind	
1300-1400	**Lunch**		
1400-1450	**Keynote: Bernhard Müller (NTNU, Trondheim)** Mach-uniform methods for multiphase flow simulation.		
1450-1620	**Session 7A: Methods & Fundamentals (Chair: Bernhard Müller)**	**Session 7B: Fluidized Beds (Chair: Niels Deen)**	**Session 7C: Fluid Interfaces (Chair: Olivier Masbernat)**
1450-1520	*Towards a mechanistic model for subcooled flow boiling at low-pressure*, S.Vahaji , S.C.P.Cheung, G.H.Yeoh & J.Y.Tu	*DEM development of heat and mass transfer in a spout fluidized bed with liquid injection,* V.S. Sutkar, S.Taalman, N.G. Deen, V.Salikov, S.Antonyuk, S.Heinrich & J.A.M.Kuipers	*Lattice Boltzmann simulations applied to understanding stability of multiphase interfaces*, G.G.Pereira
1520-1540	*Enabling CFD codes to perform systematic parameter continuation and stability analysis for realistic applications*, N.Cheimarios, E.D.Koronaki, H.Laux & A.G.Boudouvis	*Simulation of rectangular fluidized bed with Geldart D particles,* M.P.Tandon & A.Karnik	*Orr-Sommerfeld stability analysis of two-fluid Couette flow with surfactant using Chebyshev collocation method*, V.Bojja & M.Fernandino
1540-1600	*Extending a serial 3D two-phase CFD code to parallel execution over MPI by using the PETSc library for domain decomposition*, Å.Ervik, S.T.Munkejord & B.Müller	*Hydrodynamic investigation into a novel IC-CLC reactor concept for power production with integrated CO2 capture*, A.Zaabout, S.Cloete & S.Amini	*Effect of compressibility in CFD simulations of an oscillating water column device*, A.Kamath, H.Bihs, J.E.Olsen, Ø.A.Arntsen
1600-1620	*Space-time hp-adaptive DG-FEM scheme for one-dimensional multiphase flow models*, J.S.B.van Zwieten, R.A.W.M.Henkes, D.R. van der Heul, P.I. Rosen Esquivel, B. Sanderse & C.Vuik	*CFD modelling of heat supply in fluidized bed fast pyrolysis of biomass*, P.Mellin, Y. Wu, E.Kantarelis & W.Yang	*CFD multiphase simulation of two-fluid sloshing with free surface motion using the level set method*, H.Bihs, A.Kamath & Ø.Arntsen
1620-1645	**Break/Close**		
1900	**Dinner (RICA Nidelven)**		

Thursday June 19

	Auditorium A (Trondhjemsalen)	Auditorium B (Gråkallen/Lade)	Auditorium C (Strinda/Illsvika)
0830-0925	**Keynote: Jiyuan Tu (RMIT University)** CFD Modelling of Bio-Fluids and Its Applications		
0930-1100	**Session 8A: Pipe Flow (Chair: Ernst Meese)**	**Session 8B: Discrete Particle Modelling (DPM/DBM) (Chair: Markus Braun)**	**Session 8C: Particles & Deposition (Chair: Jiyuan Tu)**
0930-1000	*CFD modelling of the two-phase flow of different mixtures in a closed system flow wheel* , J.F. Roca R, J.N.E. Carneiro, J.E.S. Oliveira, S. Mo, M. Fossen & S.T.Johansen	*Adding argon injection through the DPM +VOF technique to an advanced multi-physics and multiscale model for continuous casting of steel* , P.E.Ramirez Lopez, P.Jalali, U.Sjöström & C.Nilsson	*Analysis of particle deposition from turbulent liquid-flow onto smooth channel walls* , M.Dupuy, A.Xayasenh, E.Waz, P.Le Brun & H.Duval
1000-1020	*Modelling of particle transport and bed-formation in pipelines* , C. Narayanan, S. Gupta & D. Lakehal	*Governing physics of shallow and deep subsea gas release* , J.E.Olsen & P.Skjetne	*Modelling of pulverised fuel transport for industrial applications* , A.I.J.Love, D.Giddings & H.Power
1020-1040	*Quasi-3D modelling of two-phase flows in pipes* , A. Vichansky	*Modeling of bubbly flows with free surface using a hybrid volume of fluid and discrete bubble model approach* , D.Jain, J.A.M.Kuipers & N.G.Deen	*Numerical Study of the gas-particle flow in a conveying line: accounting for wall-friction and wall-roughness* , A.Soleimani, S.Schneiderbauer & S.Pirker
1040-1100	*Simulation of two-phase viscous oil flow* , S.T.Johansen, S.Mo, J.Kjølaas, C.Brekken & I.Eskerud Smith		*A study of simulation and experiment on airborne wear particles from wheel-rail contacts* , H.Liu, L.Jonsson & P.Jönsson
1100-1130	**Break**		
1130-1300	**Session 9A: Industrial Applications (Chair: Harald Laux)**	**Session 9B: Bubbly Flows (Chair: Ingo Eick)**	**Session 9C: Separation (Chair: Dmitri Eskin)**
1130-1200	*Fully coupled multiphase simulation of a bottom-spray wurster coater using a hybrid cpu/GPU CFD/DEM approach* , E. Siegmann, C. Radeke & J.G. Khinast	*A Baseline model for monodisperse bubbly flows* , R. Rzehak , E. Krepper, Th. Ziegenhein & D. Lucas	*CFD modeling of oil-water separation efficiency in three-phase separators* , L. Oshinowo, E. Elsaadawy and R. Vilagines
1200-1220	*Benchmark of multi-component diffusion models for simulation of MOVPE reactors* , J.Bassen & H.Laux	*Monodisperse bubbly flows with ANSYS CFX and OpenFOAM: a comparison,* S.H.L. Kriebitzsch, R. Rzehak & D. Lucas	*Towards simulating flotation with OpenFOAM* , G.Holzinger, G.Wierink & S.Pirker
1220-1240	*Effect of the wind turbine wake in large offshore wind farms* , M. Popescu, B.Panjwani, J.Samseth & E.Meese	*Experimental studies of bubbly flow in a micro-structured bubble column reactor using digital image analysis,* K. Thiruvalluvan Sujatha, J.A.M. Kuipers & N.G. Deen	Lagrangian and Eulerian simulations of inclusion behaviour in liquid metal processing, J.P. Bellot, V. Descotes & A. Jardy
1240-1300	*A modeling strategy for large-scale mechanical draught air-cooled systems* , C.J.Meyer & A.Zapke	*Two dimensional numerical simulation of bubble dynamics in a vertical Hele-Shaw cell* , X.Wang, B.Klaasen, B.Blanpain & F.Verhasghe	*Effect of geometric optimization of hydrocyclones* , N.Hasan
1300-1400	**Lunch**		
1400-1450	**Keynote: Sanjoy Banerjee (City College of New York)** What can DNS and LES do for us?		
1450-1515	**Closing/Awards**		
1515	**End**		

The organizing committee are grateful for the support from the conference sponsors: FACE (the multiphase flow assurance centre), Total, ANSYS, CD-Adapco, Ascomp, Statoil and Elkem.

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On Pragmatism in Industrial Modeling

Kristian ETIENNE TRÆTLI-EINARSRUD, Asbjørn SOLHEIM, Stein Tore JOHANSEN and Josip ZORIC
SINTEF Materials and Chemistry, 7465 Trondheim, NORWAY

Corresponding author's e-mail: Josip.Zoric@sintef.no

Keywords: Modeling, pragmatism, industry, process

ABSTRACT

Many natural or industrial processes are of extreme complexity, and where the time- and length scales range from atomistic level to years and kilometers. Often the processes or phenomena consist of multiple sub processes in which each comprises its own length and time scales. An example can be production of aluminum by the Hall-Heroult process, where process streams or raw materials, flow dynamics and segregation in silos, with time varying quality, the feeding and operational routines, the reduction cells with numerous sub processes, and the tapping process, all make up a complete process. In order to optimize such type of production with respect to economic and environmental parameters we will have to develop models which can give the overall picture and at the same time be accurate enough to support the optimization process. As there are many dynamic aspects of an industrial production, the ultimate need will be a model which can compute much faster than real time and which can be used to support operation and to develop new processes.
It has been stated at a previous CFD conference in Melbourne that no metallurgical process has hitherto been designed based on CFD. At the same time significant CFD work has been done on metallurgical processes. Keeping in mind the extreme complicity in a full process, and where CFD possibly could be used to optimize a single process step without seeing this as element in a larger system, the CFD alone may not be capable of driving technological-economical step changes. We will therefore have to investigate ways to model a process; ways which are simplified, but fast and sufficiently accurate to serve its purpose. These models should be based on physics, which is critical to ensure predictive power.

In this paper we discuss how this type of pragmatic industrial models can be developed. We will identify and discuss the tools needed for such an analyses, including the analyses process itself and the frameworks needed for such analyses. Key elements in our pragmatic modeling concepts are human knowledge, including capabilities to understand complex phenomena and how these can be modeled simplified but "good enough", systematic use of existing information, systematic analyses of what information (model results) is needed and at with which accuracy and speed the results must be produced. Another key element is the selection and collection of experiment data and the exploitation of data, organized and made accessible in the optimal manner to support the predictiveness of the pragmatism based model. The organization of all types of data is organized by a "bridge" (modeling middleware) between complex scientific (aspect/phenomenon oriented) physical models, simplified models and process data.
We believe that this type of pragmatic industrial models will enable a step change in both operation, operator training and process optimization, as well as design of new processes.
Finally, in a case study, we apply our pragmatic modeling concept to the aluminium production process and discuss the implications of our proposed concept.

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A SIX CHEMCIAL SPEICES CFD MODEL OF ALUMINA REDUCTION IN A HALL-HÉROULT CELL

Peter J. WITT[1], Yuqing FENG[1], Graeme A. SNOOK[2], Ingo EICK[3] and Mark COOKSEY[2]

[1] CSIRO Computational Informatics, Melbourne 3169, AUSTRALIA

[2] CSIRO Process Science and Engineering, Melbourne 3169, AUSTRALIA

[3] Hydro Aluminium AS, Neuss, GERMANY

Corresponding author's e-mail: peter.witt@csiro.au

Keywords: CFD, Process metallurgy, Alumina reduction, Hall-Héroult aluminium cell, Multiphase chemistry.

ABSTRACT

The industrial process for producing primary aluminium metal is the reduction of powdered alumina in a Hall-Héroult reduction cell. These cells operate at temperatures above 940 °C with a highly corrosive electrolyte making physical measurement of the process difficult or nearly impossible. Computational models of the electro-magnetic fields and heat transfer are widely used in industry to design cells. Only recently (Feng *et al.*, 2010, Witt *et al.*, 2012) have detailed computational models of the molten liquid-gas bath become available. Alumina distribution within the cells is important for cell efficiency and preventing anode effects. Using the bath flow information and an assumption of uniform reduction, a single scalar transport equation has been used to track the time variation of alumina within cells (Feng *et al.*, 2011).

In this work the previous single species model is extended to include six chemical species and four chemical reactions. The reaction pathway developed for the model is that solid alumina particles are fed to the bath surface, where they mix and submerge into the liquid bath, and then undergo dissolution from solid particles to the liquid species $Na_2Al_2O_2F_4$. Within the bath $Na_2Al_2O_2F_4$ reduces to $Na_2Al_2OF_6$, which is further reduced to carbon dioxide and AlF_3 at the anode surface. At the metal pad a cathodic reaction occurs with AlF_3 converting to aluminium metal. Species solubility rates are based on the work of Solheim *et al.* (1995).

A CFD model of a single anode in a bubbly cryolite bath was built based on a corner anode from an industrial cell. Steady state bath flows were calculated and used to transport the six chemical species in the new bath chemistry model. Results were obtained for 20,000 seconds of real time for species distributions in the ACD, change in mass of species in the bath with time, rates for the four reactions at locations in the bath and change in the species mass fraction with time at various locations during a feeding cycle.

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SOLHEIM, A. ROLSETH, S., SKYBAKMOEN, E. STØEN, L. STERTEN Å. and STØRE, T. (1995) "Liquidus Temperature and Alumina Solubility in the System Na3AlF6-AlF3-LiF-CaF2-MgF2", Light Metals 1995, 451-460

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10th International Conference on CFD in Oil & Gas, Metallurgical and Process Industries
SINTEF, Trondheim, Norway
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ABSTRACT NO. (Will be filled in by organizer)

MULTI-SCALE MODEL STRUCTURES TO FACILITATE THE EMBEDDING OF CFD DERIVED MATHEMATICAL FUNCTIONS: PSEUDO-PHYSICAL COMPARTMENT MODELLING OF FLIGHTED ROTARY DRYERS

Madoc SHEEHAN[1] , Andrew LEE[2], Phil SCHNEIDER[1]

[1] James Cook University, 4812 Townsville, AUSTRALIA

[2] University of Melbourne, 3010 Melbourne, AUSTRALIA

Corresponding author's e-mail: madoc.sheehan@jcu.edu.au

Keywords: CFD, compartment model, particle curtain, drag, multi-scale, averaging

ABSTRACT

Flighted rotary dryers are large industrial devices which are commonly used to dry mineral ores and mineral concentrates, as well as other valuable commodity products. They are high capital cost units as well as large consumers of energy. Solids movement and energy exchanges within these devices occurs via a range of complex mechanisms that involve rolling and bouncing in a dense bed of solids, as well as the falling through a cross-flowing gas stream in lean particle curtains. Although a fundamental approach is attractive, full CFD simulations of such devices would be prohibitively expensive. The complexity of such a model would preclude its use for design and control applications, which are the most prevalent concerns to industry. Pseudo-physical compartment modelling is a powerful alternative technique that can be used to reproduce, in a physically meaningful way, the important characteristics of dryers such as residence time distributions and loading states. This scalable modelling approach also provides a convenient multi-scale structure that facilitates the representation of a system (in this case a flighted rotary dryer) as a series of smaller, distinctive, interacting phases. It is these smaller phase structures that are suitable for modelling with either CFD or DEM type approaches. Averaging of the CFD results and formulation of correlations enables the embedding of CFD derived phase information within the broad process model. In this paper CFD simulations of gas induced drag on the curtain phase within a flighted rotary dryer are described. Integration of CFD results into a pseudo-physical compartment model for a flighted rotary dryer is also described. The methodology presented in this paper provides an example that could be adapted to enable the CFD modelling of evaporation, convection and radiation heat transfer in curtains to be accounted for. The effects of gas velocity on gas penetration distances into the falling curtains are presented. The use of the CFD simulations as a design tool to optimise flight spacing is also described.

SAMPLE RESULTS

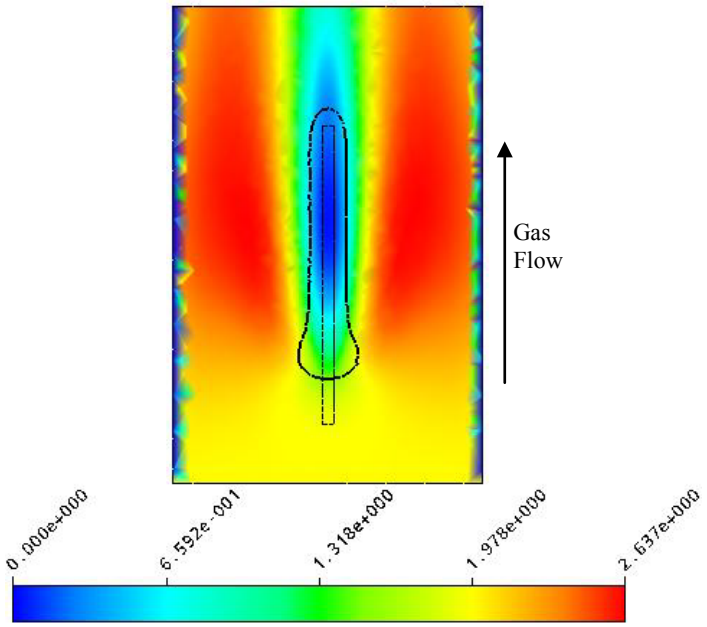

Figure 6.1. Horizontal gas velocity colour map at 1 m above tunnel floor (2 m/s initial gas velocity, 0.5 m inlet, 5.18 kg/m.s solids flow rate). Units are m/s.

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A two-fluid model coupled with porous medium description to predict liquid spreading in trickle bed reactors

Zlatko Solomenko[1], Yacine Haroun[1], Manel Fourati[1], Faïçal Larachi[2], Christophe Boyer[1], Frédéric Augier[1]

1: IFP Énergies nouvelles, Rond point de l'échangeur de Solaize, BP3, 69360, Solaize, France

2: Department of Chemical Engineering, Laval University, Quebec, QC, Canada, G1V 0A6

Corresponding author's e-mail: manel.fourati@ifpen.fr

Keywords: trickle-bed reactors, liquid spreading, capillary dispersion, mechanical dispersion, CFD, two-fluid model.

ABSTRACT

Trickle-bed reactors are widely used in refining industry, particularly in hydro-treatment processes, and continue to mobilize R&D efforts, especially with the growing constraints on sulphur level in diesel and gazoline[1,2]. In these reactors catalyst particles are packed to form a fixed bed where liquid and gas reactants flow downwards in cocurrent mode.

Liquid distribution in trickle bed reactors is a key hydrodynamic criterion for the reactor performance. A poor liquid distribution can basically result in poor utilization or precocious deactivation of the catalyst and may induce local hot spots and low reactor efficiency[1,2].
This makes it crucial to develop predictive models that allow solve for liquid distribution in order to assess proper design of the trickle-bed as well as other column internals such as distributors.
Many studies have, thus, focused on liquid spreading in trickle-bed reactors using both experimental and numerical approaches[1,3,4,5]. However, exhaustive numerical models that take into account all liquid dispersion mechanisms -mechanical and capillary[3,4]- remain scarce and not fully validated on the basis of experimental data.

In this paper, CFD is used to investigate liquid spreading in gas-liquid trickle-bed reactors using a two-fluid approach coupled with a porous medium description. Closure laws as regards porous resistances, gas-liquid interaction, capillary and mechanical dispersion are discussed and implemented as body source terms in momentum equations within ANSYS Fluent 14.5 environment.
Simulations were carried out for different catalyst sizes as well as liquid and gas flow rates with different bed porosities. Simulation results are then compared to experimental data obtained from literature and to a new set of experiments as well. A good agreement between simulation and experiments is obtained as regards liquid spreading and pressure drop from both qualitative and quantitative points of view. Moreover, simulations allowed capturing different liquid spreading behaviours depending on hydrodynamic and geometrical parameters. Finally, a discussion on the relative importance of dispersion mechanisms has been proposed.
This study has shown that CFD could be an accurate tool to predict gas-liquid distribution in trickle-bed reactors and help improve their design.

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SAMPLE RESULTS

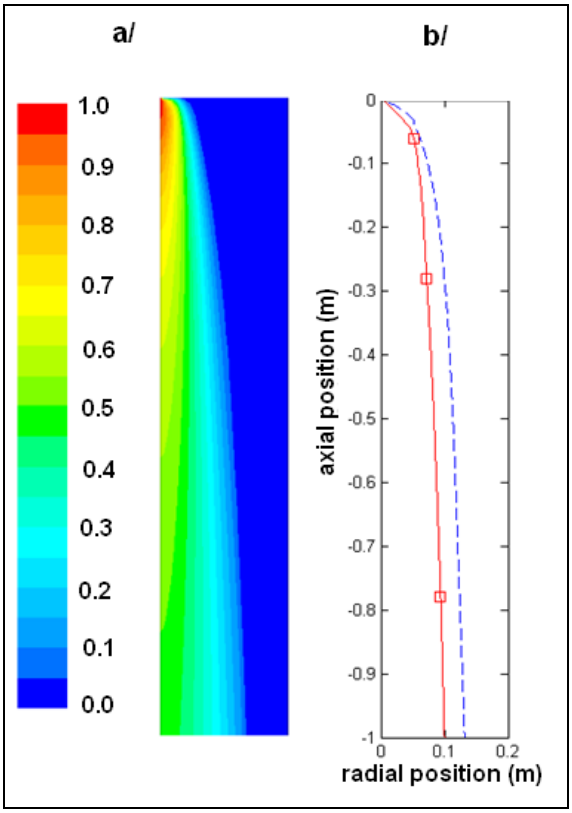

Figure 1: Simulation results on a 2D axisymmetric plane of the packed bed, a/ liquid saturation field, experimental (red) and numerical (blue) contours of liquid jet

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LOCAL SIMULATION OF THE EFFECT OF VOID FRACTION ON THE OVERALL REACTION RATE IN PACKED BEDS REACTORS

Matthieu ROLLAND[1]

[1] IFPEN, Process Intensification, 69360 Solaize, FRANCE

Corresponding author's e-mail: matthieu.rolland@ifpen.fr

Keywords: Chemical Reactors, Packed beds, Multiphase mass transfer

ABSTRACT

In lab-scale fixed bed reactors, void fraction is dependent on the solid loading procedure. Despite all precautions, it can never be exactly equal for two different reactors loaded with the same type of solids. The only practical criteria available to ensure that a reactor is correctly loaded is the repeatability of the packed bed height, and hence is based on the average void fraction. Little results support this empirical approach and we are interested in investigating the effect of void fraction on reactor overall reaction rate.

Direct numerical simulation of the coupled Navier-Stokes (laminar flow) and transport – diffusion equations is a very efficient tool to capture the effect of void fraction in single phase reactive flow as it allows a total control on geometry, fluid properties, fluid velocity and catalyst reaction rate. In our "reactive" experiments, a tracer present at the inlet is consumed by a first order surface reaction on the solid. Simulations of reactive flow were performed using Comsol Multiphysics for simple cubic (sc), body centred cubic (bcc), and face centred cubic (fcc) regular packings of identical spheres. To study the effect of void fraction, the lattice size was varied from 1.01 to 1.05 times the compact lattice size while keeping the sphere diameter constant. Other parameters are molecular diffusion (Dm: 10^{-10} to 10^{-5} m^2/s), inlet velocity (u: 10^{-5} to 10^{-2} m/s) and surface kinetic constant (k: 10^{-8} to 10^{-3} m/s).

In all cases (sc, bcc, fcc), the general trend is that increasing the lattice spacing leads to a lower overall reactor conversion: increasing the average flow path diameter slows the transverse transport from the main flow line to the catalyst surface. The magnitude of the effect of void fraction on reactor outlet mean concentration varies greatly depending on the parameters. It is strongly dependant on the ratio of the kinetic constant to the inlet velocity (k/u): for ratio k/u smaller than 10^{-3}, the void fraction has negligible effect (less than 1% difference on mean outlet concentration). On the other hand, mean outlet concentration could differ by more than 50% for k/u ratio larger than 0.1. In the simple cubic lattice, a local Peclet number in the range 10^{-2} to 10^{2} maximizes the effect of void fraction. In the other lattices, the effect of local Peclet number was not significant. As the sc lattice is the least tortuous, we propose that flow meandering improves transverse dispersion and limits the effect of flow path diameter increase.

We conclude from these results that, for a given reaction, the void fraction effect is minimal when the local velocity is larger than a critical velocity. When operating at constant contact time, this leads to long and narrow reactors. Tortuous packed beds are also probably less prone void fractions variations. It would be interesting to continue the work by simulations in random packings and also other type of catalyst shape like cylinders.

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TRANSPORT OF THE MOMENTS OF THE AGE DISTRIBUTION BY CFD IN FIXED BED OPERATION UNITS

Leonel Fangueiro Gomes[1] , Frédéric Augier[1*] , Damien Leinekugel-Le-Cocq[1] , Ivana Vinkovic[2] , Serge Simoëns[2]

[1] IFP Energies Nouvelles, BP3, 69360 Solaize, FRANCE

[2] Laboratory of Fluid Mechanics and Acoustics, CNRS UMR 5509, Ecole Centrale de Lyon, Ecully, FRANCE

Corresponding author's e-mail: leonel.fangueiro-gomes@ifpen.fr

Keywords: fixed beds, hydrodynamics, age distribution, separation.

ABSTRACT

Inside industrial fixed bed columns, as adsorption or trickle-bed units, the flow can deviate from the desired plug flow for different reasons. Depending on the operation units, flow discrepancies can be induced by near-wall channelling effect, macro scale objects within the packing such as pipes or beams, or free media chambers placed between the packed beds in the case of multi-bed operations. The case of Simulated Moving Bed (SMB) adsorption processes cumulate the difficulties listed above as their performances are very sensitive to axial dispersion, and their complex geometry can generate strong deviations from ideal plug flow.

To model hydrodynamics, three models with different levels of complexity can be considered. These models result from the modification of the laminar Navier-Stokes equations. The simplest is the Darcy's Law that describes the behaviour of a stationary and incompressible flow through the direct proportionality between the pressure gradient and the fluid velocity. To this, the Brinkman term can be added, to take into account the diffusion of the momentum due to viscosity effects. For high velocities, the inertial effects caused by the friction between the fluid and the bed particles need to be considered. To do this, the Forchheimer term must be added to the previous two. The transport of concentrations is calculated by a mass balance including advection and diffusion contributions, plus eventual source terms as reaction or phase exchange. To reproduce the dispersion caused by the packing, the diffusivity coefficient in the mass balance equation is generally assumed to be a diagonal tensor comprising axial and radial dispersion coefficients. These coefficients can both be calculated by assuming two Peclet numbers, one towards the fluid movement and another perpendicular to it.

The objective of this work is to validate the use of a CFD model used to solve momentum and concentration transport equations, in a specific geometry representative of industrial SMB adsorption columns. In this goal, the impact of several parameters is studied, as the effective viscosity in the Brinkman's term and the axial and radial Peclet numbers. The three hydrodynamic models previously described are compared to experimental results. In a mock-up representative of a slice of an industrial adsorption bed, tracer experiments are performed and compared with CFD simulations. The validation is partly based on the implementation of the spatial age distribution developed by Liu (2010), which is a powerful numerical approach used to predict the different moments of local age distributions inside stationary flows.

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SAMPLE RESULTS

In this work a laboratory scaled fixed bed was used. Pulse shape injections of a saline solution were delivered to the inlet water stream. The local residence time distribution (RTD) curves were locally obtained through 13 conductivity sensors, placed as shown in Figure 1.

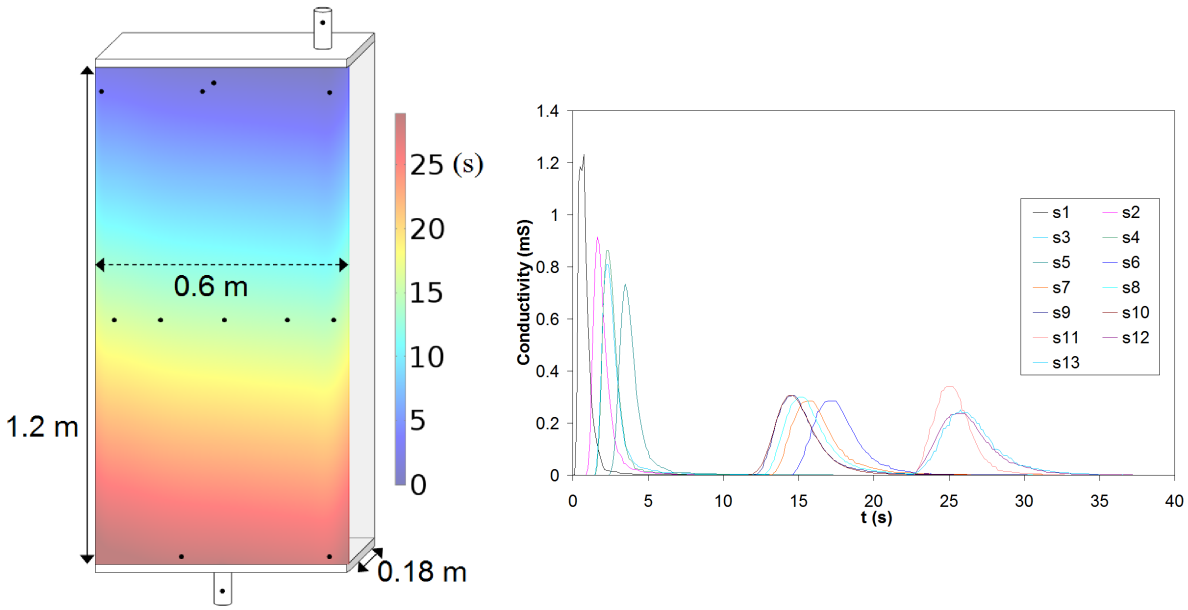

Figure 1: Schematic view of the laboratory unit with local mean age (s) obtained through CFD simulations and example of experimental RTD curves obtained.

This unit is packed with glass spheres with a diameter of 1 mm. The 13 sensors have a frequency of 8 Hz. The three hydrodynamic models previously described are shown below, in order of appearance, Darcy's Law (1), the Brinkman equations (2) and the Brinkman-Forchheimer model (3).

$$\rho(\vec{v}\cdot\nabla\vec{v}) = -\nabla p - \vec{v}\frac{\mu}{K} \tag{1}$$

$$\rho(\vec{v}\cdot\nabla\vec{v}) = -\nabla p - \vec{v}\frac{\mu}{K} + \mu_e\nabla^2\vec{v} \tag{2}$$

$$\rho(\vec{v}\cdot\nabla\vec{v}) = -\nabla p - \vec{v}\frac{\mu}{K} + \mu_e\nabla^2\vec{v} - \frac{\rho F|\vec{v}|\vec{v}}{\sqrt{K}} \tag{3}$$

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A MULTI-SCALE MODEL FOR OXYGEN CARRIER SELECTION AND REACTOR DESIGN APPLIED TO PACKED BED CHEMICAL LOOPING COMBUSTION

Mandar TABIB[1], John MORUD[2], Stein Tore JOHANSEN[1], Shahriar AMINI[1*]

[1] Flow Technology Department, SINTEF Materials and Chemistry, Trondheim, Norway.
[2]Chemical Engineering Department, SINTEF Materials and Chemistry, Trondheim, Norway

Corresponding author's e-mail: Shahriar.Amini@sintef.no

Keywords: Chemical looping combustion, Clean Energy, Catalyst design, Packed bed reactor, Multi-scale modelling, CO_2 capture, Discrete Element Modelling, CFD.

ABSTRACT

Proper selection of a catalyst shape (or a particle shape) can improve the performance of a gas-solid packed bed reactor. The particle shape affects the packing structure and the transport phenomena within the packed bed. This information is not available for many non-spherical particle shapes which limit reactor design options. To enable catalyst and reactor design, a 3D Computational Fluid Dynamics (CFD)-Discrete Element Method (DEM) model has been developed to resolve the flow around these particles and to obtain information on the transport phenomena (pressure drop correlation and heat/mass transfer coefficient). The DEM is used to obtain realistic packing structures for different particle shapes, and the CFD is conducted on these DEM generated packing structure. However, the 3D CFD-DEM model cannot be applied on the whole reactor as it is computationally prohibitive. Hence, a multi-scale modelling approach is developed, wherein correlations obtained by the 3D CFD-DEM model from a representative 3D volume of the packed bed is plugged into a 1D model for reactor design. Figure 1 represents this multi-scale modeling approach. The simple 1D particle-reactor model developed here is a combination of (1) a particle model for radial distribution of chemical species and temperature within a catalyst particle and (2) a 1D reactor model for mass and energy balance along the reactor. The 1D particle-reactor model is able to account for both intra-particle and inter-particle diffusional limitations. This multi-scale modelling approach has been applied to select an appropriate oxygen carrier shape for a Chemical Looping Combustion (CLC) packed bed reactor. This work compares the performance of different oxygen carrier shapes (fluted ring shape, cylindrical pellet shape and spherical shape) in terms of reactor operation. The simulations are used to recommend a pellet shape that offers least pressure drop, highest conversion and no fuel slip.

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SAMPLE RESULTS

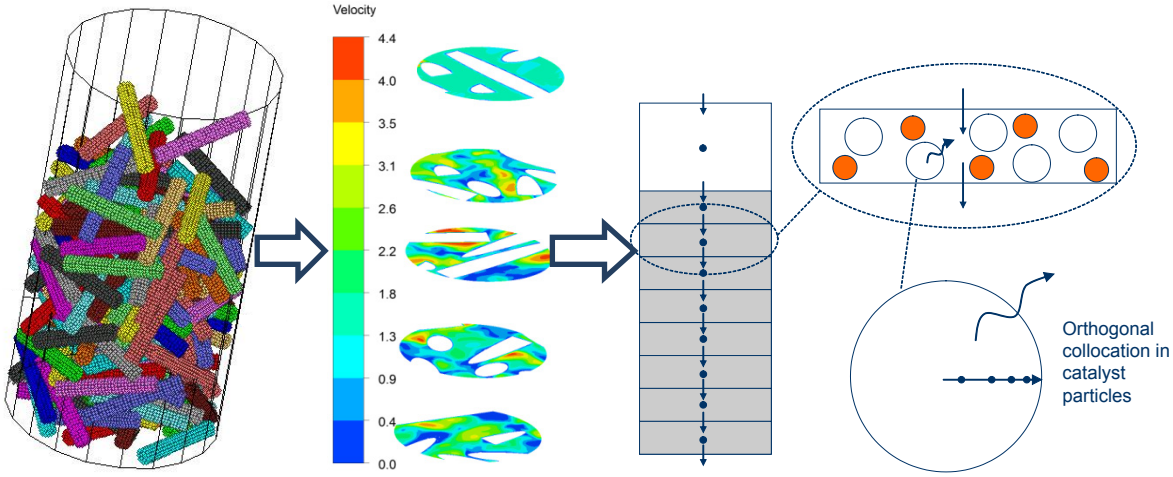

Figure 1. A schematic of the multi-scale model involving 3D CFD-DEM and 1D Particle-Reactor Model.

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PREDICTION OF MASS TRANSFER BETWEEN LIQUID STEEL AND SLAG AT CONTINUOUS CASTING MOLD

Pascal GARDIN[1*], Ségolène GAUTHIER[1], Stéphane VINCENT[2]
[1] ArcelorMittal Global R&D, 57283 Maizières-lès-Metz, FRANCE
[2] I2M, 33607 Pessac, FRANCE

Corresponding author's e-mail: pascal.gardin@arcelormittal.com

Keywords: Pragmatic industrial modelling, Multiphase Heat and Mass transfer, Metal Refining.

ABSTRACT

For the prediction of steel desulphurization and dephosphorization or the evolution of slag composition at continuous casting mold, mass transfer between two immiscible fluids in a turbulent situation should be calculated.

For this purpose, two possibilities are offered for the simulation. The first one consists in the calculation of the local chemical equilibrium with the simultaneous prediction of the species transport, but the cost is that very fine mesh should be used. The second is based on the assessment of the mass transfer coefficient from hydrodynamic calculations and further use of thermodynamic code fed with interface area and transfer coefficients. On a computing time point of view, this second method is more affordable for 3D configurations than the first one, but it is less accurate. Literature survey indicates that it is possible to obtain a realistic evaluation of the mass transfer coefficient from hydrodynamic calculations, under the condition of very precise description of the flow near the interface (see BANERJEE, 1990, 2004).

The paper explains the reasons for the different simplifications which were made to predict the mass transfer between liquid steel and slag, gives indication about the mesh refinement which is necessary to get the interfacial shear stress and mass transfer coefficient in an industrial configuration, and presents some results to get the evolution of the slag composition at continuous casting mold. Some preliminary validations are given, and several limitations of the method are illustrated. Perspectives and constraints to track real industrial interfaces are exposed.

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STRUCTURE EFFECT OF TURBOSWIRL IN UPHILL TEEMING PROCESS OF INGOT CASTING

Haitong BAI[1*] , Mikael ERSSON[1], Pär G. JÖNSSON[1]

[1] Division of Applied Process Metallurgy, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden

Corresponding author's e-mail: haitong@kth.se

Keywords: ingot casting; TurboSwirl; swirling flow; turbulence modeling; flaring angle.

ABSTRACT

It would be possible to produce steel with better surface quality in the uphill teeming process if a much more stable flow pattern could be obtained in the runners. Several technics have been utilized in the industry to try to obtain a stable flow of liquid steel. For instance, a swirl blade inserted in the horizontal or vertical runners could generate a swirling flow in order to make a lower hump height to avoid mold flux entrapment and improve the quality of the ingot products. In this research, a new novel swirling flow generation component, TuroSwirl, was introduced to improve the flow pattern. It has recently been demonstrated that the Turboswirl method could effectively decrease the risk of mold flux entrapment, lower the maximum wall shear stress, and decrease velocity fluctuations. The TurboSwirl was built at the elbow of the runners as a connection between the horizontal and vertical runners. It is located near the mold and it generates a tangential flow that can be used with an expanding nozzle in order to decrease the vertical flow velocity. This would enable a stable flow before the fluid enters the mold. However, high wall shear stresses appear on the walls due to fierce rotation in the TurboSwirl. In order to protect the refractory wall, some structural improvement were applied. It was found that by changing the flaring angle of the outlet, it was possible to get a lower tangential velocity and wall shear stress. Moreover, when the vertical runner was not placed on the centre of the TurboSwirl, a much more beneficial flow pattern was obtained. In addition, the swirling numbers of all the situation above were calculated to ensure that the swirling flow was strong enough to generate the liquid steel swirling in the TurboSwirl.

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Modelling of Alloy Mixing in Continuous Casting Tundishes

Chao CHEN[1,2*] , Anders TILLIANDER[1], Lage T.I. JONSSON[1], Guoguang CHENG[2], and Pär G. JÖNSSON[1]

[1] KTH-Royal Institute of Technology, Division of Applied Process Metallurgy, Department of Material Science and Engineering, SE-100 44 Stockholm, SWEDEN

[2] University of Science and Technology Beijing, State Key Laboratory of Advanced Metallurgy, 100083 Beijing, P.R.CHINA

Corresponding author's e-mail: cchao@kth.se

Keywords: Mixing, Process Metallurgy, Tundish, Alloy mixing.

ABSTRACT

The mixing phenomena in tundishes has been widely studied during the last two decades. By using Residence Time Distribution (RTD) in water models and transient tracer concentration curves during ladle change, it has been possible to predict the inclusions floatation and the transient mixing length of slabs etc., respectively. However, a tundish can also be an alternative metallurgical reactor to achieve alloy mixing for steel grades such as REM alloyed steels were clogging occur.

A mathematical model of a tundish was developed to study the alloy mixing in tundishes. Compared to previous results of water modelling, the predicted KCL tracer concentration in the outlet matched well with the measurement results. With this verification, a model of the molten REM alloy injected into molten steel was established. The REM element concentration distribution as a function of injection time was calculated. Furthermore, when comparing the calculated results for different injection position, an optimized location was suggested.

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Numerical Investigation of the Immersion Quenching Process for Heat Treated Parts Using an Eulerian Multi-Fluid Approach

R. KOPUN[1] , D. GREIF[1], Z. KOVACIC[1], M. SUFFA[2*]

[1] AVL AST doo, Maribor, SLOVENIA

[2] AVL List GmbH, Graz, AUSTRIA

Corresponding author's e-mail: maik.suffa@avl.com

Keywords: Casting and solidification, Multiphase heat and mass transfer

ABSTRACT

This paper summarizes a computational methodology to predict by simulation the heat transfer between a heat-treated casted part and a quenchant (e.g. water). The numerical model implemented in the commercial Computational Fluid Dynamics (CFD) code AVL FIRE® v2013.1 accounts for the phase change within the quenchant due to the heat released from a heated casted part when submerged into the sub-cooled liquid by using an Eulerian multi-fluid modeling approach. Simulation results are presented and compared with measured data. Different solid part orientations were studied on a step-plate, a test piece with segments of varying thickness along its height, in respect to resulting solid temperatures and stresses. With the applied methodology the predicted temperature gradients in the solid material correlate very well with the provided experimental data. The paper will also provide examples for the industrialization of the method.

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Pragmatic Approach to Efficient Modeling of a Commercial MOVPE Reactor

Harald Laux, Hans Lindberg, Tobias Meyer & Adam Bauer

OSRAM Opto Semiconductors

Keywords: CFD, Simulation Tools, MOVPE, Aixtron G4

Metal-Organic Vapor Epitaxy (MOVPE) is a process widely used in the LED industry to deposit epitaxial films. For example, films based on nitride materials are processed mainly to blue to green LED chips which are the basis for illumination devices in industrial, automotive and solid state lighting today.

Often, an important requirement to an epitaxial film grown in a MOVPE reactor is homogeneity of film thickness and composition over the entire wafer. Film homogeneity is controllable by numerous reactor operation parameters, and there is a large parameter space in which optimization of the layer is carried out. In this large parameter space, the number of experiments to identify the optimal operational parameters is high.

Reactor scale simulation models in combination with film growth models have the potential to decrease experimental development time and costs. Such models can identify parameter settings which can serve as starting point for experimental optimization, thus, reducing the number of experiments necessary. This requires that simulations are robust and fast because many simulations are necessary to screen the parameter space. Moreover, it is important that such models predict film thickness and composition profiles with at least qualitative accuracy. Only then simulations can identify process parameters which provide levers to tune the experimental profiles.

A commercially available multi-physics CFD-ACE code is suitable for simulation of MOVPE reactor processes. In CFD codes everything from complex 3D models, including detailed geometry and fine meshes, can be combined with e.g. fluid flow, heat transfer, species transport, and gas and surface reaction models (film growth models). CFD models can be quite accurate but at the expense of long simulation times.

Another possible simulation model is a commercial software which is an engineering tool for epitaxial engineers not for simulation specialists. Its major advantage is its ease of use, robustness and short simulation times. Coarse meshes for predefined geometries of commercial reactors are hard-coded and cannot be edited by the user. The modeled reactor geometry comprises only the reactor chamber and not the full reactor. Besides the main process parameters, which the epitaxial engineer knows from his MOVPE tool, only temperature profiles need to be specified at the boundaries. This is the major drawback of the tool since the temperatures at the boundaries are not known experimentally and cannot be measured in an industrial setting. Thus, the thermal boundary condition can only be estimated and usually constant values are used. This can lead to problems with accuracy in the computed film thickness and composition profiles, while the average film growth rate and composition are mostly quite accurate.

Thus, there is the problem that simulations in the CFD code with higher accuracy are too time consuming while simulations with the tool are fast but do sometimes not provide the correct shape of the real growth profile. This, however, is the prerequisite for a successful simulation support for profile layer homogenization.

A possible way around this problem is developed in this work. The working hypothesis is that the accuracy of the profile prediction with the tool can be as good as with the CFD model when the thermal boundary conditions for the tool are known. Therefore, a CFD model is developed that allows calculation of those boundary conditions and then the corresponding temperature profiles are collected into a database which is coupled to the tool. In this way it is possible to supply the tool with accurate thermal boundary conditions. Finally, the coupling between tool and boundary condition database is fully automated allowing many simulations in a short time.

As a use case example the horizontal MOVPE reactor Aixtron G4 in a 6x6" configuration is studied. A quasi-3D axis-symmetric CFD model of the entire reactor is developed in the CFD software. In this model the boundaries are placed where the thermal boundary conditions are well known, e.g. the water cooled reactor lid. With this model the temperature profiles at the inside of the confining internal walls of the reaction chamber can be calculated. Still, the space spanned by the operation parameters is huge and the number of CFD model simulations should not be too large. Therefore it is shown that for this particular reactor type the large number of operation parameters can be reduced to four dimensionless parameters, i.e. the actual parameter space is spanned "only" by those four dimensionless parameters. Then it is shown that reaction and surface chemistry have a negligible effect on temperature profiles and, thus, can be omitted from the CFD model. Finally, the CFD model is trimmed for robustness and speed and a number of CFD model simulations are run to fill the profile database.

The coupling of database and tools is facilitated through a MATLAB tool. To this tool the same input parameters can be given as to the engineering tool. Based on the input parameters the tool calculates the dimensionless numbers, locates the position of the specified operation point in a triangulation of the parameter space given by the profiles in the database and interpolates the corresponding temperature profiles. Then a engineering tools script is automatically written and the corresponding engineering tool case can be started from the script. Thus, the epitaxial engineer would use the MATLAB tool to generate a number of scripts for the DOE runs planned and then be able to start all the planned runs from a script which automatically simulates the runs sequentially. Instead of having to set up and start, say, 20 simulations in the engineering tool, definition and start running of these cases are done from the MATLAB tool in a few minutes.

Examples from simulations with the thermal boundary conditions interpolated from the database and with standard constant temperature boundary conditions are shown and discussed.

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CFD IN PROBLEM ANALYSIS AND OPTIMISATION – THE IMPORTANCE OF CORRECT BOUNDARY CONDITIONS

Eirik MANGER[1]

[1] Acona Flow Technology, 3732 Skien, NORWAY

Corresponding author's e-mail: eirik.manger@acona.com

Keywords: CFD, Mixing, Process Industry

ABSTRACT

CFD has during the last decades developed and matured significantly, and is today an accepted tool within problem analysis and optimisation. There are lots of efforts spent in developing new and more accurate models handling e.g. turbulence and other complex physical phenomena. Still, superior models will only predict reliable estimates as long as the input provided by the user has equally good quality. In the authors opinion this might be an even larger source for erroneous simulation results than model accuracy.

This paper aims at demonstrating the importance of having correct boundary conditions as input to simulations. Two specific applications are studied. The model predictions are compared against measurements and findings in the real systems, and the validity of the models is discussed.

In the first application, gas mixing before two ammonia burners was investigated. Temperature measurements inside the burners, which are directly proportional to the ammonia concentration, showed that the gas mixing was insufficient before splitting the feed. A CFD simulation confirmed the mixing problem, and indicated that an extra static mixer would improve this. After rebuilding the situation did however not improve, but in some strange manner rather reversed. Different models were tested, without finding the cause of this change. Finally the response seen in the plant was traced back to a possibly faulty mixer element upstream the newly installed static mixer. During the next plant revamp, the element was inspected and found partly broken. After changing this, the mixing became sufficient – as predicted by the CFD simulation.

In the second application, local recirculation in a shell/tube gas condenser was studied. It was suspected that this phenomenon could be the reason for inlet corrosion. Local analysis using CFD indicated however that the inlet recirculation zone did not extended into the condensing zone, ruling out this as a possible cause. Different models and turbulence approaches were tested, all giving approximately similar answers. Taking the investigation one step further revealed that the inlet recirculation zone could become significantly longer if there is an angled inlet flow into the tubes. By extending the calculation domain further upstream, the CFD results showed that such conditions do occur, corresponding well with the area at which material wear was observed. Moreover the CFD model could be used to establish a new design which now seems to work well.

The two examples chosen illustrate clearly the importance of applying correct boundary conditions. Inappropriate input will lead to wring results – no matter how accurate the models are.

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A COMBINED MULTIFLUID-PBE MODEL FOR SLURRY BUBBLE COLUMN REACTOR: APPLICATION TO THE FISCHER-TROPSCH SYNTHESIS

C. B. VIK[1*] , J. SOLSVIK[1], H. A. JAKOBSEN[1]

[1] NTNU Department of Chemical Engineering, 7491 Trondheim, NORWAY

Corresponding author's e-mail: camilla.berge.vik@ntnu.no

Keywords: Clean energy, industrial reactive flows, population balance equation, Fischer-Tropsch synthesis, slurry bubble column, least-squares method

ABSTRACT

Forecasts about decreasing fossil liquid fuel sources have induced increasing interest in synthesized liquid fuels, among them second generation biofuels. Such a liquid fuel may be produced through the Fischer-Tropsch synthesis. A particular reactor choice for this liquid reaction is the slurry bubble column, with reactants injected in the gas phase and the catalyst present along with the liquid products in the slurry.

In order for the reactions to occur, the reactants must be transferred from the dispersed gas phase via the liquid phase to the catalyst surface. The interfacial heat and mass transfer fluxes are given by the product of the transfer coefficients, the contact area per unit volume and the driving force. The contact area is determined by the bubble size distribution. Along the reactor length, bubble-bubble interactions and fluid-bubble interactions will give rise to bubble breakage and coalescence phenomena, affecting the bubble size distribution in the reactor. This size distribution will influence the reaction rate as larger bubbles have a smaller contact area per volume, and the contrary for smaller bubbles. The bubble size distribution can be modeled through the population balance equation (PBE).

The research group at NTNU has developed a novel modeling framework formulating a combined multifluid-PBE model explicitly in terms of a mass density function and solved by the least squares spectral method for cold flow, see e.g. Dorao et al (2006), Zhu et al (2009), Nayak et al (2011), Solsvik et al (2013). Recent work on modelling the Fischer-Tropsch synthesis by Sehabiague (2013) accounts for two classes of bubble sizes, whereas current work allows for a distribution of bubbles.

This work aims at a model combining chemical reaction, flow regime and the population balance to model the production of liquid fuels from biomass. The gas phase will be modelled using the population balance equation. Standard cross-sectional averaged multifluid equations (mass, species mass, momentum) will be applied for the pseudo-homogeneous slurry phase. The momentum equations will be solved in order to describe the flow.

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SAMPLE RESULTS

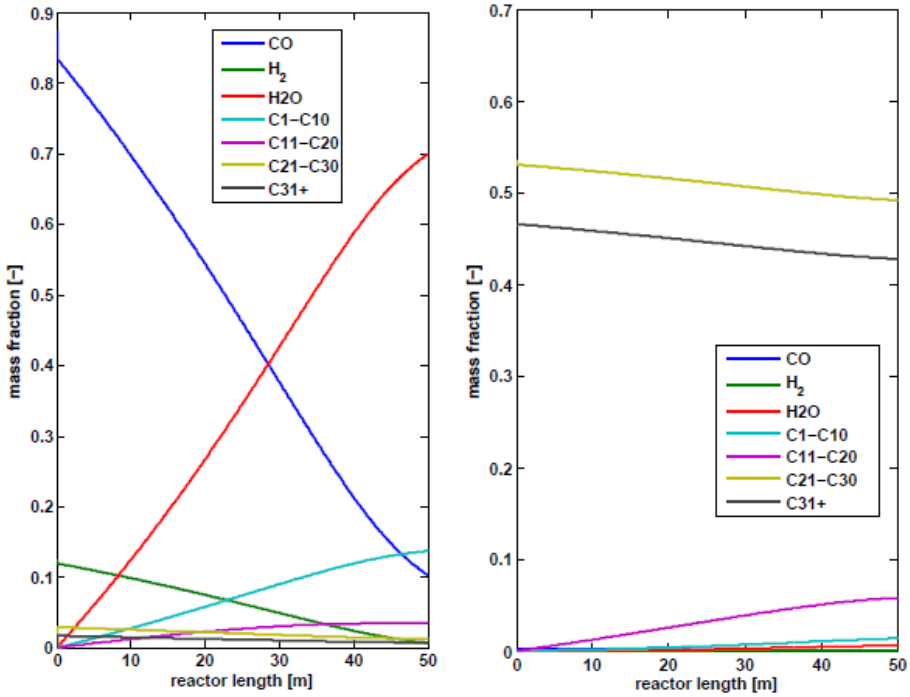

Figure 1: Outlet mass fractions for gas phase (left) and liquid phase (right) for reactants (CO and H_2), products (hydrocarbons of various lengths, lumped into four groups) and by-product (H_2O).

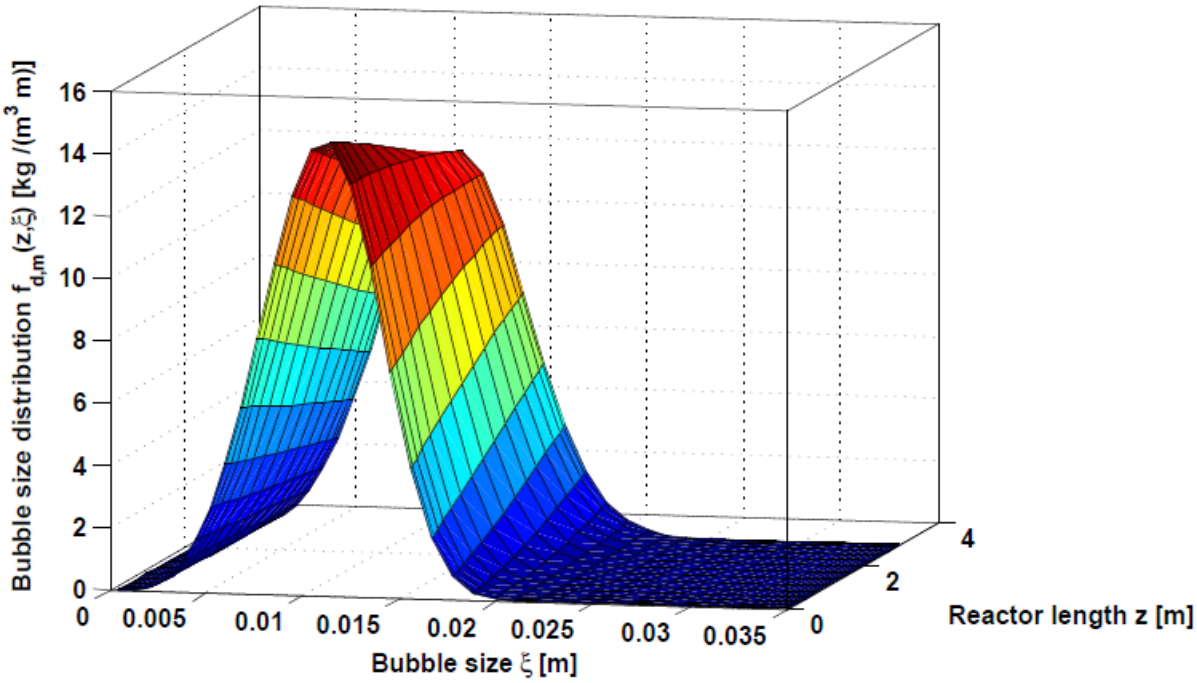

Figure 2: Bubble size distribution at various reactor lengths.

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DEM-CFD simulations and PIV/PTV experiments on charging of pneumatically conveyed powders

Martin W. Korevaar[1], Johan T. Padding[1*], Martin A. van der Hoef[2], Hans A.M. Kuipers[1]

[1] SINTEF Materials and Chemistry, 7465 Trondheim, NORWAY

[1] Eindhoven University of Technology, Department of Chemical Engineering and Chemistry, 5632 WD Eindhoven, THE NETHERLANDS

[2] Twente University, Department of Physics, 7500 AE Enschede, THE NETHERLANDS

Corresponding author's e-mail: J.T.Padding@tue.nl

Keywords: Tribo-electrification (contact charging); Fluid Structure interaction; Granular flows; experimental validation studies; Separation; Meshless methods (DEM-CFD); PIV/PTV

ABSTRACT

As the world population increases, the demand for food increases as well. This urges the production of (enriched) food to become more energy efficient in order to have a sustainable situation. A possible approach is to switch to separation techniques that do not require water. One such a method is tribo-electric separation where the driving force for separation is the different polarity and/or magnitude acquired by different fractions due to contact charging (also known as tribo-electric charging or tribo-electrification). Contact charging occurs always when objects (of different material) touch; the magnitude and polarity is a property of the combination of the two touching materials. Consequently, the method is suitable to separate mixtures in which the components have sufficiently different charging characteristics.

Many configurations are possible to utilize contact charging to charge powders. Here we investigate pneumatic conveying of powder through a metal duct; while traveling through the duct, particles will hit the walls and acquire charge.

To gain more understanding in the system, an experimental set-up of such a conveying system was developed by J.Wang and M. Schutyser at WUR, The Netherlands. In this system, the cumulative acquired charge of the particles can be measured and the particles are optically accessible. This enables measurement of the particle distribution in the duct using high speed camera's and Digital Image Analysis (DIA). Furthermore, Particle Image Velocimetry (PIV) and Particle Tracking Velocimetry (PTV) measurements are performed to gain information on the particles' velocity distribution.

The particles' behaviour in the duct is also investigated using DEM-CFD to gain a more detailed understanding. To that end, our in-house DEM-CFD code is extended with a model of contact charging of the particles, as well as with the electrostatic interactions between both particle-particle and particle-wall.

Under the prerequisite that the interaction between wall and charged particles is treated correctly, it is shown that the DEM-CFD model is a valuable tool; it gives more detailed information than possible by experiments. Furthermore, it is able to describe some of the trends correctly and is thus able to reveal some of the limits in which the charging of the powder is effective.

SAMPLE RESULTS

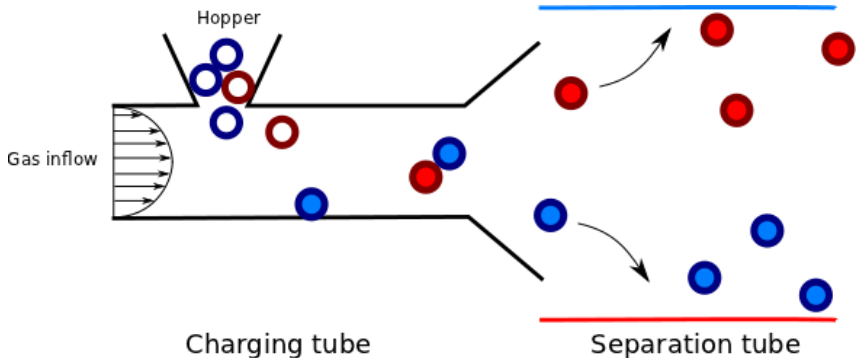

Figure 1: Schematic diagram of experimental set-up.

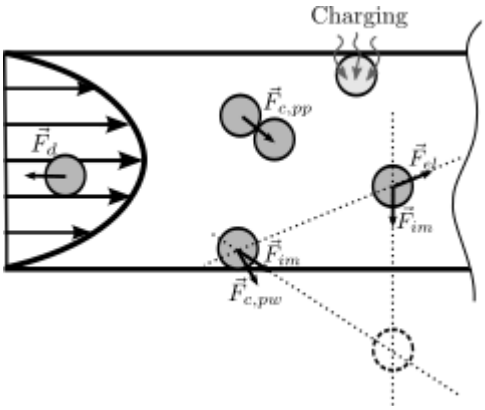

Figure 2: Overview of forces acting on the particles in DEM-CFD.

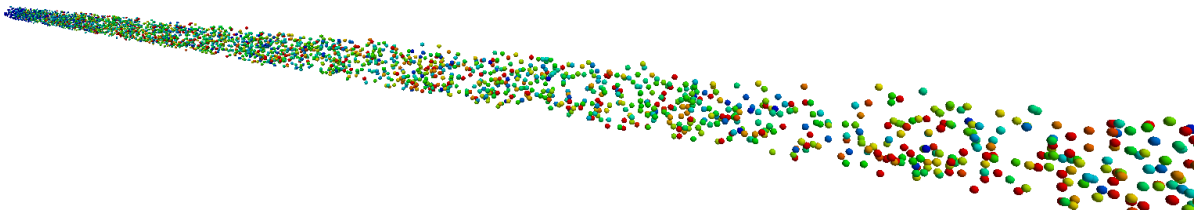

Figure 3: Results from the DEM-CFD simulations showing how the charge increases (from blue through green to red) when particles travel through the duct (from left to right).

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ESTABLISHING PREDICTIVE CAPABILITY OF DEM SIMULATIONS: SLIDING AND ROLLING FRICTION COEFFICIENT OF NON-SPHERICAL PARTICLES

Luca BENVENUTI[1], Andreas AIGNER[1], Daniel QUETESCHINER[12], Mar COMBARROS[3], Stefan PIRKER[1], Christoph KLOSS[12]

[1] JKU Department of Particulate Flow Modelling, 4040 Linz, Austria

[2] DCS Computing GmbH, 4040 Linz, Austria

[3] TUBS Institut für Partikeltechnik, 38104 Braunschweig, Germany

luca.benvenuti@jku.at

Keywords: Meshless methods (DEM), Rheology, experimental validation studies, process industries, process metallurgy, LIGGGHTS, Material characterization

ABSTRACT

Discrete Element Method (DEM) simulations are widely used to understand particle behavior in process, metallurgy and a variety of other industries. Among the key parameters, defining accurately the inter-particle friction parameters is very relevant to perform simulations of medium to dense granular flows.
The open-source DEM code LIGGGHTS (Kloss et al., 2012), along with the simplified Jenike shear cell tester (SJSCT) simulation (Aigner et al., 2013), has been proven able to define the coefficient of sliding friction for coarse round particles.
To model non-spherical particles with spherical elements, we use an elasto-plastic-spring-dashpot model (EPSD2)(Ai et al., 2011; Wensrich and Katterfeld, 2012). The overall model consists of Coulomb's law and the EPSD2 model, and thus requires the determination of the sliding and rolling friction coefficients to be used as parameters, obtained by fitting numerical simulations to experimental measurements.
The bulk solids were characterized through the Schulze ring shear cell tester (SRSCT)(Schulze, 2007) and the SJSCT, particularly, we assessed the pre-shear internal friction angle (PSIFA). The PSIFAs obtained through the SRSCT and the SJSCT revealed almost coincident values (less than 1% difference), and therefore we could validate the latter experimental device.
The DEM coefficients of friction of coal (0-3.15 mm) and silibeads (2 mm) calculated by numerical simulations revealed very good agreement with previous published reports as well as in-house experiments. Especially the DEM parameters were used in static angle of repose (AOR) simulations, and then compared to AOR experiments. In the light of the data we obtained, we can state that the SJSCT experimental and simulation setup was able to define the DEM parameters for the tested materials.

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PRELIMINARY RESULTS

The preliminary results obtained through the SRSCT and the SJSCT can be observed in Table 1. It is also possible to compare them with the first data given from the numerical setup.

	mean ϕe-SRSCT [°]	median ϕe-SRSCT [°]	mean ϕe-preshear-SRSCT [°]	median ϕe-preshear-SRSCT [°]
coal	46.37	45.00	40.88	40.41
iron ore	46.26	46.00	41.67	41.10
limestone	47.20	46.10	41.97	41.53
silibeads	23.03	21.60	21.38	20.19
sinter fine	48.47	47.00	41.49	40.97

	mean tan(ϕe-SRSCT) [-]	mean tan(ϕe-preshear-SRSCT) [-]	Mean tan(ϕe-SJSCT) [-] – 561 Pa	Mean tan(ϕe-PMSCT) [-] – 1026 Pa
coal	1.05	0.87	0.98	0.85
iron ore	1.04	0.89		
limestone	1.08	0.90	1.24	1.10
silibeads	0.43	0.39	0.38	0.34
sinter fine	1.13	0.88		

	Mean tan(ϕe-SJSCT) [-] – 1588 Pa	Mean tan(ϕe-SJSCT) [-] – all	Mean tan(ϕe-DEM) [-] – 5kPa	Mean tan(ϕe-DEM) [-] – 10kPa
coal	0.72	0.85	0.87	0.75
iron ore				
limestone	0.92	1.08		
silibeads	0.30	0.34	0.43	0.41
sinter fine				

	Mean angle of repose - exp [°]	Mean angle of repose - DEM [°]	DEM sliding friction coeff. [-]	DEM rolling friction coeff [-]
coal	58.68	50.30	0.80	1.40
iron ore				
limestone	44.85			
silibeads	21.09	21.80	0.08	0.02
sinter fine				

Table 1: Preliminary experimental and numerical results' comparison table.

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UNDERSTANDING SEGREGATION IN GRANULAR MEDIA

Gerald G PEREIRA[1] Mahasen SOORIYABANDARA[1], Paul W CLEARY[1]
[1] CSIRO Computational Informatics, Clayton, 3166, AUSTRALIA

Corresponding author's e-mail: Gerald.Pereira@csiro.au

Keywords: Granular flows, meshless methods, mixing, segregation

ABSTRACT

Segregation and mixing in granular media is significantly important in a variety of industries ranging from pharmaceuticals and food processing to mining and metallurgy. Segregation of granular media occurs when discrete particles of different size, shape, density, or some other fundamental particle property are forced to flow together. Various fundamental physical mechanisms such as percolation cause one particle type (for example in percolation it is the smaller particles) to segregate from the remainder of the particles. As yet, this is not clearly understood and a fundamental device for studying segregation is a rotating tumbler roughly half filled with a granular material. In this study we investigate segregation in granular mixtures in a rotating tumbler where the mixture's particles differ in size, density and/or shape. We use Discrete Element Method (DEM) as well as fundamental, continuum type models to explain the variety of segregation patterns which evolve. We particularly focus on the dynamics of segregation and its relationship to the underlying segregation mechanisms.

10th International Conference on CFD in Oil & Gas, Metallurgical and Process Industries
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HARD-SPHERE MODELLING OF LIQUID BRIDGE AGGLOMERATION

Boris V. BALAKIN[1], Guzel SHAMSUTDINOVA[2], Pawel KOSINSKI[3]

[1] Bergen University College, Department of Mechanical– and Marine Engineering, 5020 Bergen, NORWAY

[2] Far Eastern Federal University, Vladivostok, RUSSIAN FEDERATION

[3] University of Bergen, Department of Physics and Technology, 5020 Bergen, NORWAY

Corresponding author's e-mail: Boris.Balakin@hib.no

Keywords: pragmatic modelling, Lagrangian methods, new techniques, multiphase pipeline transport

ABSTRACT

Agglomeration of particles by liquid flocculants is often met in petroleum industry and therefore the importance of its numerical reproduction is indubitable. The most accurate approach to multiphase flow modelling is of the Euler-Lagrange type (see e.g. Crowe et al., 2011) where the motion of a separate particle or a droplet is resolved individually. Nevertheless, an industrial scale system contains billions of dispersed objects and it often requires extensive computational costs to be investigated numerically. The situation is even more complicated by the need to account for inter-particle interactions, which, in case of liquid bridge agglomeration, involve capillary and lubrication forces. These forces are the drivers of agglomeration that act within nano– or micro-layer of flocculant. The so-called distinct element approach (DEM) is capable for the precise integration of the aforementioned forces during the entire collision, i.e. the dynamics of interparticle motion is resolved at nanoscale. The spatial and temporal resolution required by DEM models is, however, high so that the technique is hardly applicable to industrial scales. Therefore the present research proposes an alternative and pragmatic way to model interparticle collisions within Eulerian-Lagrangian approach. The model implies an analytic pre-solution of the dynamics of collision in a way that it is capable for prediction of either the velocities of particles after collision in presence of the liquid bridge or particle agglomeration. This strategy is generally inspired by the well-known hard-sphere technique (e.g. Crowe et al., 2011), which is based on the estimation of the particle velocity after collision using solely analytic relations. The hard-sphere model was further updated in this research: we took into account the amount of relative momentum conserved by the bridge applying the expressions derived in our recent work (Balakin et al., 2013). In the present paper we report results of the modelling of liquid bridge agglomeration of 200-μm solid spheres in a Couette flow of viscous oil. The simulation results focus on spatial positions and velocities of resulting agglomerates together with the pressure and velocity fields of the carrier phase. The general description of the agglomeration process is highlighted in terms of the history of the mean particle size, agglomeration efficiency and particle size distribution. The simulation results are validated against analytics. The computational time spent for our simulations is approximately 3 times lower than for the equivalent DEM-simulation performed by the CFD commercial software STAR-CCM+ provided by cd-Adapco. This illustrates the efficiency of the technique used in this research.

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SAMPLE RESULTS

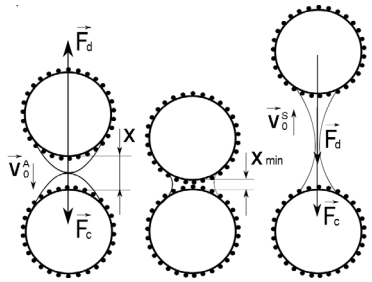

Figure 1: Schematic representation of an inter-particle collision with liquid bridge.

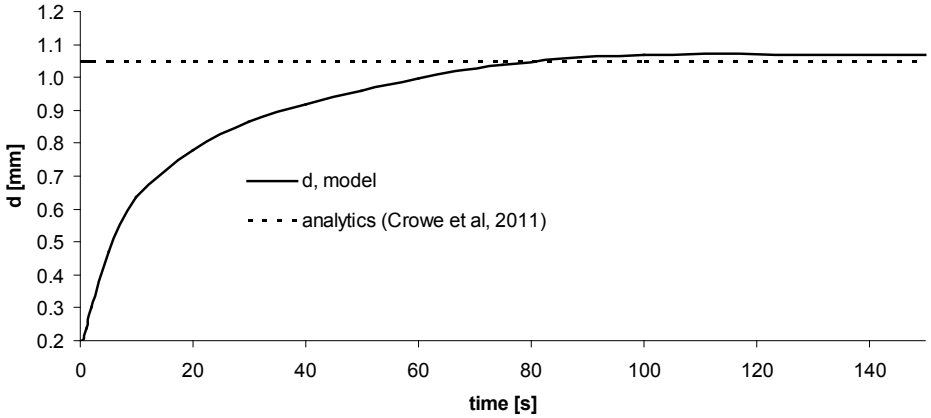

Figure 2: Average size of agglomerate as a function of time. The simulation results are compared with analytical expression given in Crowe et al., 2011.

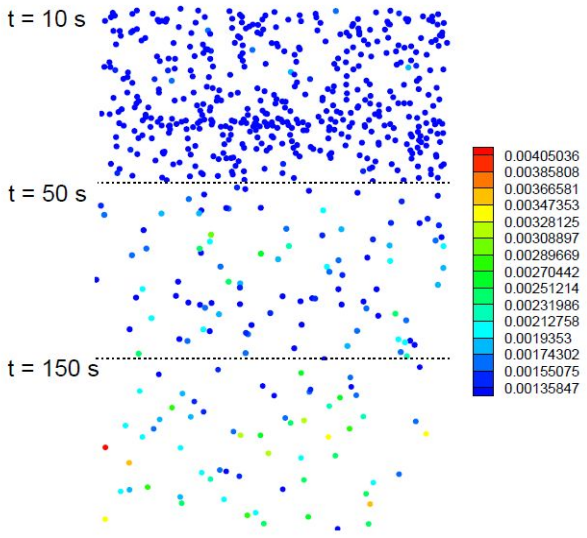

Figure 3: Agglomerated particles in the computational domain at 10, 50 and 150 s of the process. Colour scale illustrates particle size in m.

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MULTI-SCALE MODELING OF HYDROCARBON INJECTION INTO THE BLAST FURNACE RACEWAY

Christian MAIER[1] , Christian JORDAN[1], Christoph Feilmayr[2], Christoph Thaler[2], Michael HARASEK[1]

[1] Vienna University of Technology, Institute of Chemical Engineering, 1060 Vienna, Austria

[2] voestalpine Stahl GmbH, 4020 Linz, Austria

Corresponding author's e-mail: chmaier@mail.tuwien.ac.at

Keywords: Multiphase heat and mass transfer, multiscale, Lagrangian methods, blast furnace, direct injection.

ABSTRACT

The majority of liquid raw iron is produced via the blast furnace route, traditionally utilizing metallurgical coke as the main reducing agent. Aiming at a reduction of primary resources, using alternative reducing agents such as liquid hydrocarbons, natural gas and waste plastics contributes to the reduction of coke rates. In the blast furnace these agents also serve as fuels by combustion with hot blast, delivering heat necessary for melting processes as well as endothermic reduction reactions.
To optimize the utilization of the input material, thorough examination of the impact of fuel injection is necessary. However, due to the extreme conditions in the shaft of blast furnaces, the application of experimental techniques is very limited. A promising alternative is to conduct numerical experiments applying the methods of computational fluid dynamics. In this work, models are developed to study the process on multiple scales. The implemented setup includes the description of various phases such as solid coke, gases, injected liquid hydrocarbon and plastic particles, accounting for heterogeneous heat and mass transfer phenomena. Non-equilibrium between the slowly descending bed of metallurgical coke and counter-currently ascending gases is considered by solving separate sets of conservation equations.
The injection of liquid hydrocarbons and plastic particles is modeled applying tracking schemes in a Lagrangian frame of reference. Heating rates are computed accounting for contributions from laminar and turbulent fluid flow as well as radiation. The release of droplet mass from the liquid fuels to the gas phase is computed applying a multicomponent evaporation model based on temperature dependent saturation pressures of solution components. Further cracking of oil vapor to form smaller gas constituents as well as combustion is modeled in the gaseous regime. Rates of homogeneous gas-phase reactions are calculated considering educt species mixing on finest scales of turbulent eddies. In accordance to experimental observation the pyrolysis of injected plastics takes place at very high specific heat transfer rates, resulting in high characteristic Biot numbers. Therefore, internal radial temperature profiles of injected plastic particles are very steep in the vicinity of the particle surface, while temporal thermal conditions in the particle center can be approximated to remain constant. A pyrolysis model was implemented to properly describe the mass release of the plastics mixture used for injection.
Heterogeneous reactions of coke with gas components are evaluated accounting for major reaction routes such as oxidation, steam and CO_2 gasification and methanation. Reaction rates are calculated regarding educt species transport on a particulate scale, accounting for boundary layer diffusion, diffusion in the porous coke structure and intrinsic reaction kinetics.
Species concentration and temperature profiles are evaluated in terms of efficient feedstock utilization, aiming at the comparison of various operating conditions and injection lance configurations.

10th International Conference on CFD in Oil & Gas, Metallurgical and Process Industries
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CFD Modelling of a Plasma Reactor

Sverre G. JOHNSEN[1*], **Are J. Simonsen**[1]

[1] SINTEF Materials and Chemistry, 7465 Trondheim, NORWAY

Corresponding author's e-mail: Sverre.G.Johnsen@sintef.no

Keywords: Metal refining, Plasma, Process metallurgy, Reactor

ABSTRACT

The PPM (Plasma Production of Materials) reactor developed at SINTEF has previously been utilized for production of e.g. carbon nano-tubes. The reactor is presented in several publications, most recently by Andreas Westermoen. Due to novel employment of the plasma reactor to produce new materials, a CFD study was undertaken to assess the reactor temperature field with special focus on optimizing substrate surface temperature, and for designing the substrate holder.
The reactor geometry was approximated by a 2-dimensional axisymmetric model. The CFD model employed a *Source Domain* model for the plasma arc, assuming a steady state time-averaged shape and electric current distribution. A momentum source due to the Lorentz force and an energy source due to Ohmic heating, within the plasma arc, were implemented by user defined functions. The *Discrete Ordinate* model was employed for the radiation field in the reactor. The reactor gas is considered single-component (Argon or Helium) and single-phase, and no chemical reactions or precipitation/dissolution was considered.
A sensitivity study was performed to evaluate the importance of various key experimental parameters with respect to temperature.

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CFD modeling of pollutant emissions due to syngas combustion in a semi-industrial HiTAG

M. Saffari Pour[1*], W. Yang[1], W. Blasiak[1]

[1] Division of Energy and Furnace Technology, KTH Royal Institute of Technology, Brinellvägen 23 SE 100-44, Stockholm

Corresponding author's e-mail: mohsensp@kth.se

Keywords: Renewable Energy, CFD modelling, Syngas combustion, Pollutant emission, NO_X

ABSTRACT

Renewable and clean resources are highly important for industrialized countries to gain more efficient and clean energy. In order to attain more efficiency, the overview of developed countries is directed to switching fuels from traditional fossil fuels to something renewable. Nowadays, gasified biomass is become more attractive topic for researchers in gasification and combustion processes. Combustion of gasified biomass is applicable in huge furnaces such as blast and tunnel furnaces. In this Paper, gasified biomass is introduced as an alternative fuel for natural gas.
Computational Fluid Dynamic (CFD) methods together with experimental measurements are applied to model a syngas combustion chamber. In order to investigate syngas combustion, produced gas from a high temperature air gasifier (HiTAG) with 0.5 MW capacity is combusted in a secondary chamber. The temperature at the highest part of the gasifier could achieve 1500°C and the injected syngas to secondary chamber could achieve 900°C. A low NO_X emission burner together with secondary air injection system is used to fulfill a stable flame in a secondary chamber with 0.45 m^3 volume. The measurements set up are consisted of thermocouple with a gas analyzer to detect the gas composition and temperature fields. The comparison of numerical data with experimental measurements shows convenient results through the computational domain. The calculated amounts of pollutant emissions show a reasonable system for producing direct heat as well as heat recovery for huge power plan.

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SINTEF, Trondheim, Norway
17-19 June 2011

CFD SIMULATION OF A BURNER HEAD IN A SECONDARY REFORMER FOR AMMONIA SYNTHESIS

Jakub BUJALSKI[1] , Justas DAUPARAS[2]
[1] Yara International ASA, CCC Process Technology, Hydrovegen 67, 3936 Porsgrunn, NORWAY
[2] Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Wilberforce Road, CB3 0WA, UK

Corresponding author's e-mail: jakub.bujalski@yara.com

Keywords: reaction, ammonia synthesis, material damage, geometry modification.

ABSTRACT

Due to the construction of the chemical plant it is almost impossible to visualise the system during normal operation. For this reason Computational Fluid Dynamics (CFD) has been found to be an useful tool by providing information on the flow patterns inside the equipment. With the current computational power CFD gives the engineer the possibility of analysing more complex physics in industrial scale equipment. It is no longer used just of simulation of "what if" scenarios in change in geometry and load. In industry is also gaining an acceptance as an investigation tool to gain insight in investigations to determine the root cause of unscheduled plant shutdown.

As an example of such an investigation this paper presents the CFD simulations that were carried out to examine the hydrodynamics and performance of a burner head of an ammonia plant secondary reformer reactor to determine the root cause of the damage sustained by the reactor. The simulations investigated the effect of production load, geometry modification, on the behaviour of the of the reactor. To accurately model the reactor the CFD simulations included reactions, heat transfer and radiation in the full production scale. The simulations showed that under normal operation there is no problem with excessive temperatures and potential damage occurring in the reactor that were found during post shutdown inspection of the reactor. This lead to a further simulation investigation of the potential scenarios that could lead to the observed damage. This work showed that slight changes in the geometry that deviated from the construction could lead to the equipment damage that was found during the post incident inspection. The root cause of the damage to the reactor was found and solution to this problem was implemented.

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Numerical investigation of the vertical plunging force of a spherical intruder into a granular bed

Y. (Yupeng) Xu[1], J.T. (Johan) Padding[1]*, M.A. (Martin) van der Hoef[2], J.A.M. (Hans) Kuipers[1]

[1] Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, 5600 MB, Eindhoven, The Netherlands

[2] Department of Science and Technology, University of Twente, 7500 AE, Enschede, The Netherlands

Corresponding author's e-mail: j.t.padding@tue.nl

Keywords: Fluidized granular bed; impact cratering; moving internals; gas effect; Immersed Boundary Method.

ABSTRACT

Studies of forces resisting a big intruder moving through a granular medium can help us to understand phenomena such as footprints on sand and the craters of the lunar surface. When an intruder moves through a granular bed, the force on the intruder shows complex behavior caused by the inhomogeneity of the force propagation and the requirement for grain reorganization. Phenomenological models have been proposed to account for experimental results of the force acting on a vertically falling object impacting onto a horizontal bed of granular particles. Different force profiles were measured in different experiments and different force laws were deduced. Clearly, the form of the force experienced by an impacting intruder is still not unified, and detailed understanding of this problem remains limited. At the same time, new questions arise, such as what the relative role is of the interstitial gas phase for systems with relatively large (Geldart B) granular particles.

In this work, we first numerically study the impact of a large sphere dropping into a prefluidized granular bed using a state-of-the-art hybrid Discrete Particle and Immersed Boundary Method (DP-IBM). For the first time, both the gas-induced drag force and the contact force exerted on the intruder are investigated separately. Our results show that even for relatively large granular particles of 0.5 mm diameter and an intruder of 1 cm, the drag exerted by the interstitial gas accounts for up to 5 % of the total force experienced by the intruder. Our simulation results match well with existing experimental observations.

The further investigation of the plunging of a large sphere into a prefuidized granular bed with various constant velocities show a concave-to-convex plunging force as a function of depth and in the concave region the force fits to power-law with exponent around 1.3, which is in good agreement with existing experimental observations.

This work shows that the current simulation scheme could become a powerful tool to investigate the effect of interstitial gas on the dynamics of projectile impact cratering. More generally, the method allows for accurate simulation of the hydrodynamic effects of large internal objects moving through (pre-)fluidized granular beds.

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SAMPLE RESULTS

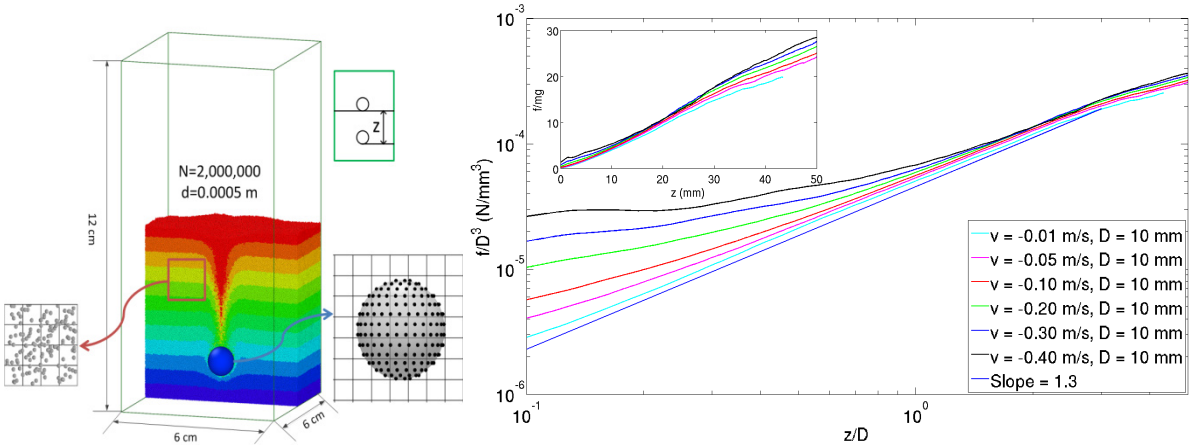

Figure 1: Left: Schematic representation of the discrete particle and immersed boundary methods. representation of the DP and IB methods. In the DP model the motion of the suspended small particles is solved, taking into account detailed solid-solid contact forces, as well as drag forces caused by motion relative to the interstitial gas phase. The particles are smaller than the grid on which the gas phase equations are solved (left), requiring the use of empirical drag relations. On the contrary, the intruder is much larger than the gas grid. Coupling between the intruder and the gas phase is accomplished through the IB method, which enforces no-slip boundary conditions by homogeneous distribution of force points across the surface of the intruder (right). Schematic representation of the bed geometry is also shown in this figure, prior to moving the large intruder, the granular bed is fluidized and slowly de-fluidized. Only half of the bed is shown and the particles are colour coded according to their initial position in z direction.

Right: Plunging force f of a 10 mm intruder with different intruding velocities as a function of penetration depth z

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OPERATING EXPERIENCE WITH A HIGH-TEMPERATURE PSEUDO-2D FLUIDIZED BED REACTOR DESIGNED ESPECIALLY FOR DETAILED LOCAL DATA COLLECTION

Abdelghafour ZAABOUT[1*], Schalk CLOETE[2], Stein Tore JOHANSEN[1] & Shahriar AMINI[1]

[1]Department of Flow Technology, SINTEF Materials and Chemistry, Norway

[2]Department of Energy and Process Engineering, Norwegian University of Science and Technology (NTNU), Norway

*E-mail: abdelghafour.zaabout@sintef.no

ABSTRACT

This paper reports practical experience from the high-temperature operation of a pseudo-2D fluidized bed reactor running redox reactions typically occurring in a Chemical Looping Combustion process. The reactor was designed for the primary purpose of providing detailed local data for the validation of reactive multiphase flow models. For this purpose, the pseudo-2D bed was equipped with multiple measurement ports which allowed for the simultaneous measurement of temperature, pressure and gas composition at various positions within the bed. Multiple unforeseen challenges were encountered and solved (within practical limits) during this first-of-a-kind experimental campaign. Extensive recommendations are given to guide future experimental campaigns aiming to build on this work. In spite of these challenges, initial comparisons between experiments and simulations show reasonable agreement.

Keywords: Fluidized bed reactor, validation, experiments, Two Fluid Model.

INTRODUCTION

Fluidized bed reactors find application in a wide range of process industries where efficient gas-solid reactions, heat transfer and/or mass transfer, is desired. The very large exposed surface area and excellent mixing displayed by these reactors makes them ideal for this purpose. However, fluidized bed reactors typically display very complex hydrodynamics which directly influences the mass and heat transfer occurring within the bed. This complexity makes design, scale-up and operation challenging.

Due to the continued exponential increase in computational power and availability, fluidized bed reactor modelling using the Kinetic Theory of Granular Flows (Jenkins and Savage, 1983, Lun et al., 1984, Gidaspow et al., 1992, Syamlal et al., 1993) is now becoming a viable strategy for improving the understanding of the complex multiphase flow in fluidized bed reactors and thereby accelerating the design and scale-up of these processes. The traditional Two Fluid Model approach to fluidized bed flow modelling has been under development for a number of decades now and has been proven to result in reliable hydrodynamic predictions (Taghipour et al., 2005, Ellis et al., 2011, Cloete et al., 2013), but such validation studies are largely absent for reactive systems. This absence is of significant concern because such reactive validation campaigns are crucial to the development and widespread acceptance of reactive multiphase flow modelling as a tool for accelerating the development and scale-up of fluidized bed reactors.

There are good reasons for the absence of such work to date. Reactive validation studies are much more difficult to perform because of the high temperatures which are typically involved. The detailed local flow measurements necessary to properly evaluate model performance are also much more challenging to collect from such high-temperature systems. It is therefore to be expected that reactive validation campaigns involve a much greater risk of unexpected additional complexities, costs and unforeseen problems with data collection.

In recognition of these challenges, the work reported in this paper aims to greatly reduce these resistances to dedicated validation campaigns for reactive multiphase flow modelling by presenting a detailed account of the operating experiences in such a campaign. The purpose of this work is

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HEAT TRANSFER IN GAS-SOLID FLUIDIZED BED THROUGH AN INTEGRATED DIA/PIV/IR TECHNIQUE

Amit.V. Patil, Elias.A.J.F., Johannes.A.M. Kuipers

Multiphase Reactor Group, Department of Chemical Engineering, 5600MB Eindhoven, THE NETHERLANDS
Corresponding author's e-mail: A.V.Patil@tue.nl

Keywords: Fluidized beds, Multiphase heat and mass transfer, PIV, New Techniques, Infrared thermography, Gas-solid flow.

ABSTRACT

A new combined IR (infrared)/PIV (particle image velocimetry)/DIA (digital image analysis) measuring technique for studying heat transfer in gas-solid fluidized bed is presented. The infrared images are coupled with visual images that are recorded simultaneously using an external trigger system. This gives instantaneous thermal and hydrodynamic data of a pseudo 2D fluidized bed that can be used to validate simulations of heat transfer in such a bed.
The well-established technique of DIA/ PIV (Jong et al, 2012) can be applied on visual images to get hydrodynamic information and its combination with IR images gives the thermal dynamics. Since the visual and infrared images were recorded with different cameras with different image sizes mapping of the images is needed to obtain a good superposition. It will be shown that the used method result in a good superposition and synchronization of hydrodynamic and thermal data. The combined technique was used to get insightful information into issues like the mean temperature of particles as function of time, spatial temperature distributions as function of: particle sizes, bed aspect ratio and background gas velocity. The measured data from the technique can also be used to get heat fluxes inside the bed alongside mass flux. These experimental results can be used to validate CFD models on heat transfer in gas-solid fluidized beds.

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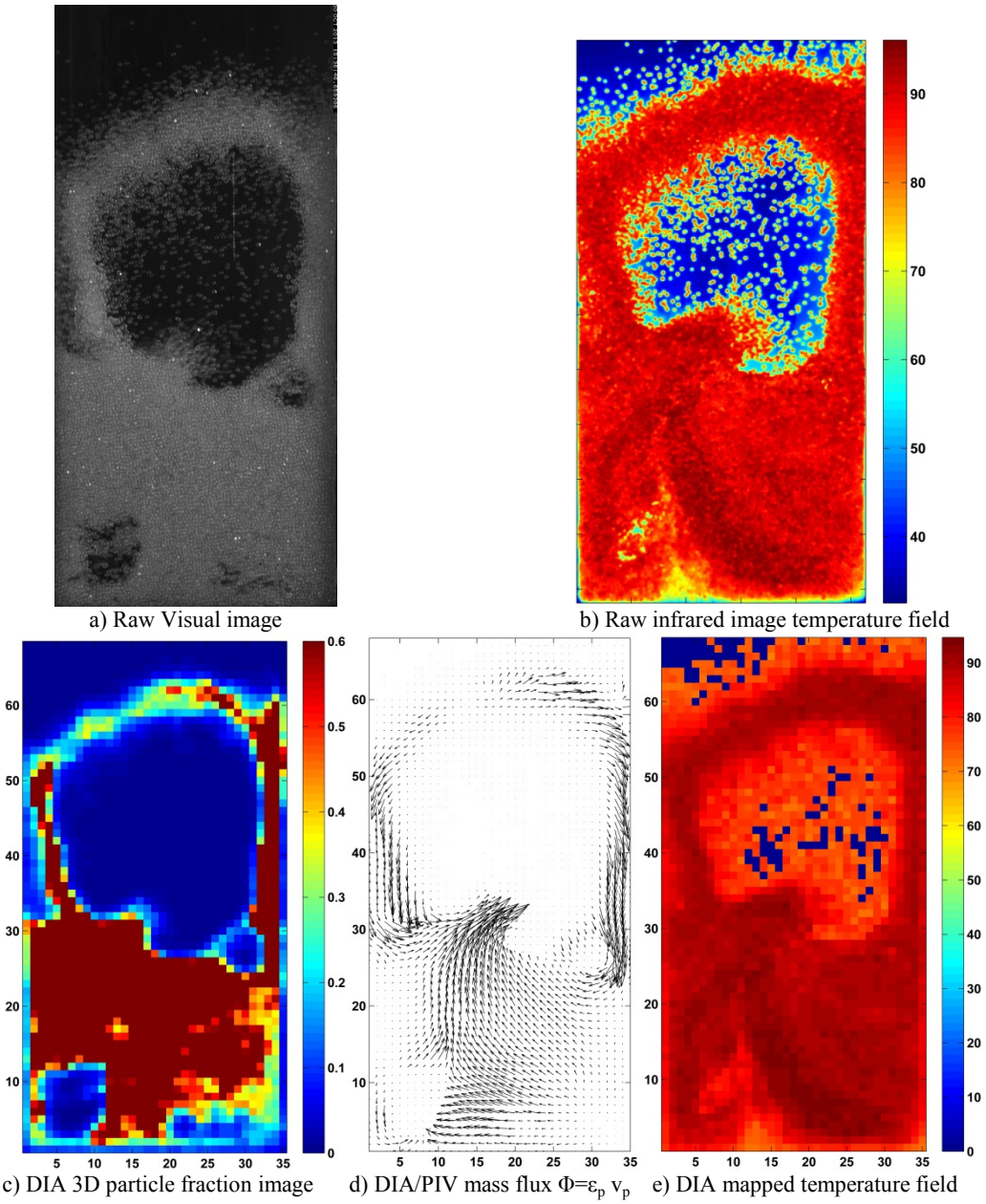
SAMPLE RESULTS



a) Raw Visual image

b) Raw infrared image temperature field

c) DIA 3D particle fraction image

d) DIA/PIV mass flux $\Phi=\varepsilon_p v_p$

e) DIA mapped temperature field

Figure 1: Visual and infrared image processing procedure leading to the combining of DIA/PIV/IR to get mass flux, energy flux and temperature distribution within the gas-solid fluidized bed system.

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HYBRID EULERIAN-LAGRANGIAN MODELLING OF BI-DISPERSE FLUIDIZED BEDS

Simon SCHNEIDERBAUER[1], Stefan PUTTINGER[1], Stefan PIRKER[1*]

[1] Dep. Particulate Flow Modelling, Johannes Kepler Univ., 4040 Linz, AUSTRIA

Corresponding author's e-mail: stefan.pirker@jku.at

Keywords: CFD Fundamentals and Methodology, Fluidized Beds, Eulerian Two-Fluid Model, Lagrangian Particle Model, Poly-disperse Materials.

ABSTRACT

Most industrial applications of fluidized bed reactors include poly-disperse materials. Thus, it is important to understand the mixing and segregation of particles classes in the reactor to evaluate its efficiency. Since the total number of particles involved in most practically relevant fluidized beds is extremely large, it may be impractical to solve the equations of motion for each particle. It is, therefore, common to investigate particulate flows in large process units using averaged equations of motion, i.e. two-fluid models (TFM), which include the inter-particle collisions statistically by kinetic theory based closures of the particle stresses. However, in poly-disperse flows each particle class requires additional momentum and continuity equations, leading to high computational costs which might be prohibitive for pragmatic industrial simulations.

In this paper, we, therefore, present a hybrid model for the numerical assessment of poly-disperse gas-solid fluidized beds. The main idea of such a modelling strategy is to use a combination of a Lagrangian discrete phase model (DPM) and an Eulerian kinetic theory based TFM to take advantage of the benefits of those two different formulations. On the one hand, the local distribution of the different particle diameters, which is required for the gas-solid drag force, can be obtained by tracking statistically representative particle trajectories for each particle diameter class. On the other hand, the contribution from the inter-particle stresses, i.e. inter-particle collisions, can be deduced from the TFM solution. These then appear as additional body force in the force balance of the DPM. Note that in a first step we solely consider diameter averaged solids stresses since the drag force is at least on order of magnitude higher than the solids stresses in fluidized beds.

Finally, the numerical model is applied to a fluidized bed of a bi-disperse mixture of glass particles (0.5 mm and 2.5 mm particles) and with a cross-section of 0.15 m x 0.02 m. The results are then analysed with respect to experimental data of Puttinger et al (2014). This comparison demonstrates that the computed bed hydrodynamics (including bed expansion, segregation and channelling) is in fairly good agreement with the experiment. However, the results also suggest that sub-grid drag and sub-grid stress corrections (Schneiderbauer et al., 2013; Schneiderbauer et al., 2014) for poly-disperse fluidized beds are required to make the numerical investigation of industrial scale fluidized bed units accessible.

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SAMPLE RESULTS

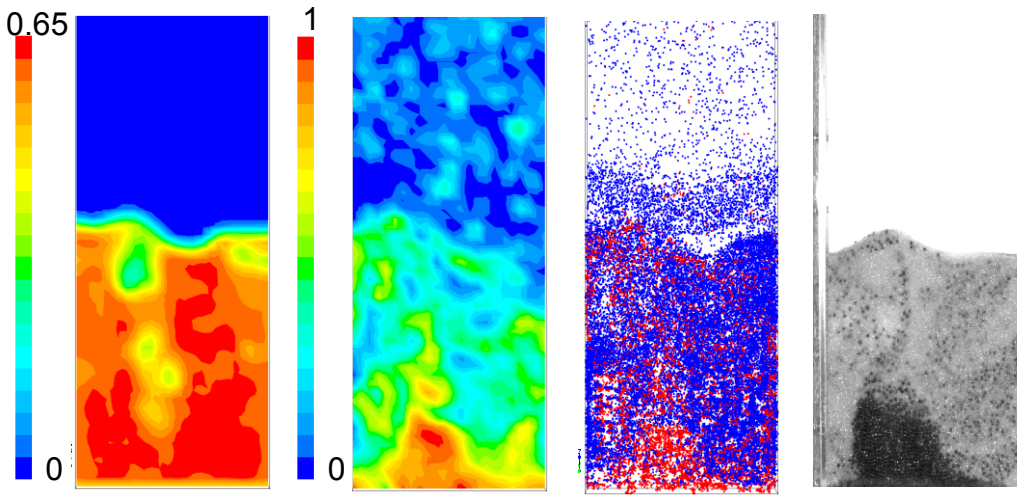

Figure 1: Validation example – Partial de-fluidization in a bi-disperse fluidized bed due to de-mixing of two particle classes: Large (black) particles form a non-uniform packed bed just above the distributor plate; process gas channels to the upper part of the bubbling fluidized bed of small (gray) particles. Our hybrid simulation model is able to reproduce this critical behaviour: (from left to right) solid-phase volume fraction, fraction of large particles, tracer particles colored by their size, experimental observation

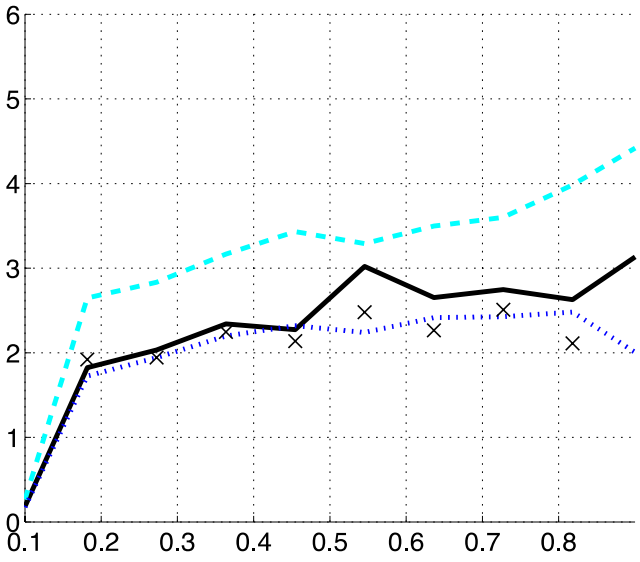

Figure 2: Computed bubble rise velocity as a function of the bubble diameter:
x fine grid simulation, − with sub-grid stress correction (Model B),
• • • with sub-grid stress correction (Model A),
- - - w/o sub-grid stress correction
(see Schneiderbauer et al., 2013; Schneiderbauer and Pirker, 2014)

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COMPARING EULER-LAGRANGE AND EULER-EULER BASED CFD MODELS FOR FLUIDIZED BEDS

Dr. Markus Braun[1], Dr. Markus Lambert[1], Dr. Shailesh Ozarkar[2], Dr. Jay Sanyal[2], Dr. Mohan Srinivasa[3], Shitanshu Gohel[3]

[1] ANSYS Germany GmbH, Birkenweg 14a, D-64295 Darmstadt, Germany

[2] ANSYS Inc., 275 Technology Drive, Canonsburg, PA, 15317, US

[3] ANSYS Software Pvt. Ltd, 32/2 Rajiv Gandhi Infotech Park, Pune, 411057, India

Corresponding author's e-mail: shailesh.ozarkar@ansys.com

Keywords: Lagrangian Methods, DEM, Euler-Lagrange and Euler-Euler based Models

ABSTRACT

Simulation of gas-particle flows in commercial scale devices such as fluidized beds is of an interest to many industries including chemical processing, oil and gas, and energy. For simulation of such flows, traditional Euler-Euler model based on Kinetic theory of granular flow (KTGF) along with classical or modified form of gas-particle drag laws [1-4] have been extensively used in literature. With recent advances in computing power and computational algorithms, there is a growing interest in using Euler-Lagrange models as these models efficiently handle particle size distribution in comparison to KTGF based Euler-Euler models.

In this study, we performed the validation of Euler-Lagrange model as well as KTGF based Euler-Euler model using experimental data of two fluidization challenge problems [5] that were proposed by National Energy Technology Laboratory (NETL). The first fluidization challenge problem was based on laboratory scale fluidized bed while second fluidization challenge problem was based on pilot scale circulating fluidized bed. All simulations were performed using ANSYS Fluent. It was found that both models qualitatively captured the trends observed in experiments. Along with validation results, we will also highlight simulations of few industrial applications using Euler-Lagrange model.

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AGGLOMERATION STUDY IN THE INLET SECTION OF A LARGE SCALE SPRAY DRYER USING STOCHASTIC EULER-LAGRANGE MODELLING

Sandip PAWAR[1], Johan T. PADDING[1], Niels G. DEEN[1], Alfred JONGSMA[2], Fredrik INNINGS[2], J.A.M. KUIPERS[1]

[1]Multiphase Reactors Group, Department of Chemical Engineering and Chemistry,
Eindhoven University of Technology , P.O. Box 513, 5600 MB Eindhoven, THE NETHERLANDS
[2] Tetra Pak CPS, Heerenveen, THE NETHERLANDS
*Corresponding author, E-mail address: J.T.Padding@tue.nl; Tel: (+31) 40 247 3674;
Fax: (+31) 40 247 587

ABSTRACT

Spray drying is an essential unit operation for the production of powders from liquid slurry. Main events occurring inside the spray dryer are droplet drying and interactions between droplets and fine particles, leading to bouncing collisions, coalescence, agglomeration, and satellite droplet formation. In recent years, there has been growing interest to use computational fluid dynamics (CFD) for exploring such phenomena inside spray dryer systems. Researchers have extensively investigated single droplet-droplet and single particle-particle interactions using numerical and experimental methods. However, the literature on droplet-particle interactions with a quantitative description of agglomeration in spray drying is scarce, and mainly qualitative.

In this paper, we explore the development of an Euler-Lagrange model with a stochastic approach for the prediction of collision, coalescence and agglomeration of partially wet particles in a spray dryer. In this approach, the dynamics of the gas phase is solved by an Eulerian equation as a continuum and the dynamics of the solid phase is solved by a Lagrangian equation as a dispersed phase, with conventional gas-solid coupling. Inside the spray chamber, the turbulent gas flow has an effect on the particle interactions. In a spray dryer, the number density of droplets is usually more than 10^{11} per cubic meter, effectively ruling out a deterministic approach in which each particle is individually tracked. We introduced a stochastic Direct Simulation Monte Carlo (DSMC) approach in which each particle searches randomly, in a local and spherical searching scope, for another particle to collide with during a particle time step. In a spray dryer, different kinds of events can occur when a pair of particles collide. We use elementary models for collision, coalescence, break-up, drying and agglomeration, validated by experimental results from the literature and industrial data. In this paper we present details of the modelling approach using sub-models and preliminary simulation results. The ultimate aim of this project is to develop a simulation tool that can provide the particle size, velocity and flux distribution for a section of a large-scale spray dryer. These results ought to be used as boundary conditions for even coarser simulations, which will be used to design more efficient spray dryers that can produce higher throughputs.

KEYWORDS: Agglomeration, Break-up, Spray Drying, Stochastic Modelling

SAMPLE RESULTS:

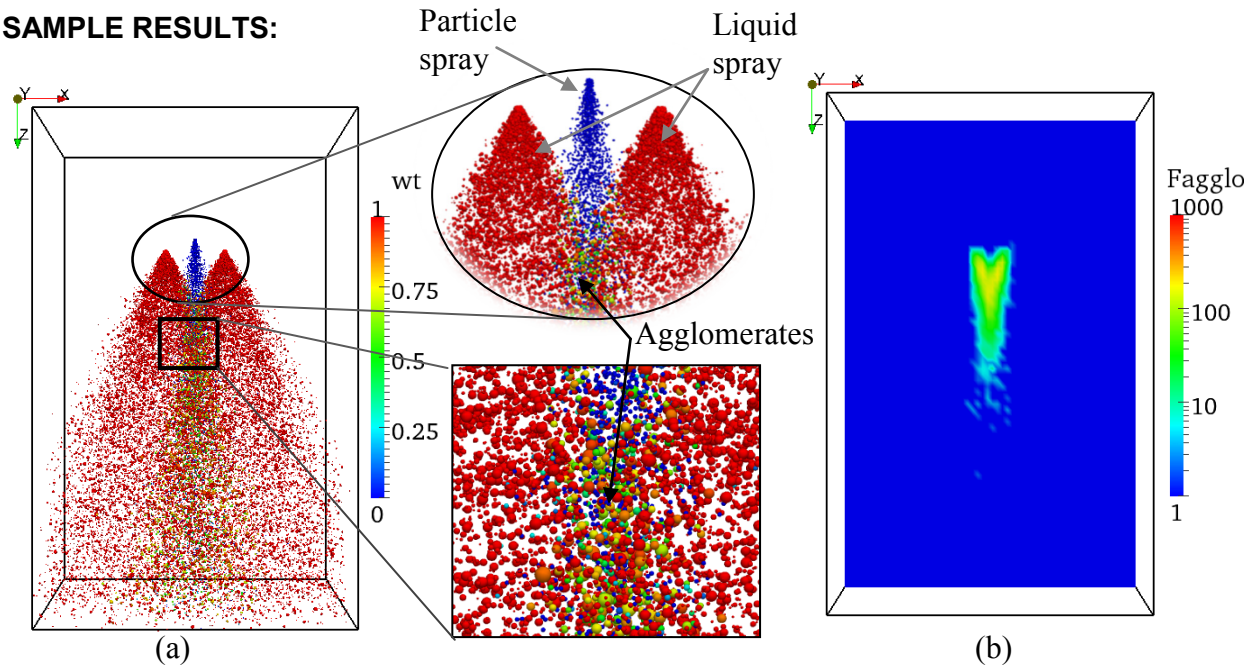

Figure 1: a) Two droplets sprays and one primary dry particle spray at the center. Droplets and particles collide and agglomerates are formed. Colors indicate wetness (wt) of the agglomerates (blue = completely dry, red = completely wet). b) Local frequency of agglomeration (F_{agglo}) events for the system shown in (a).

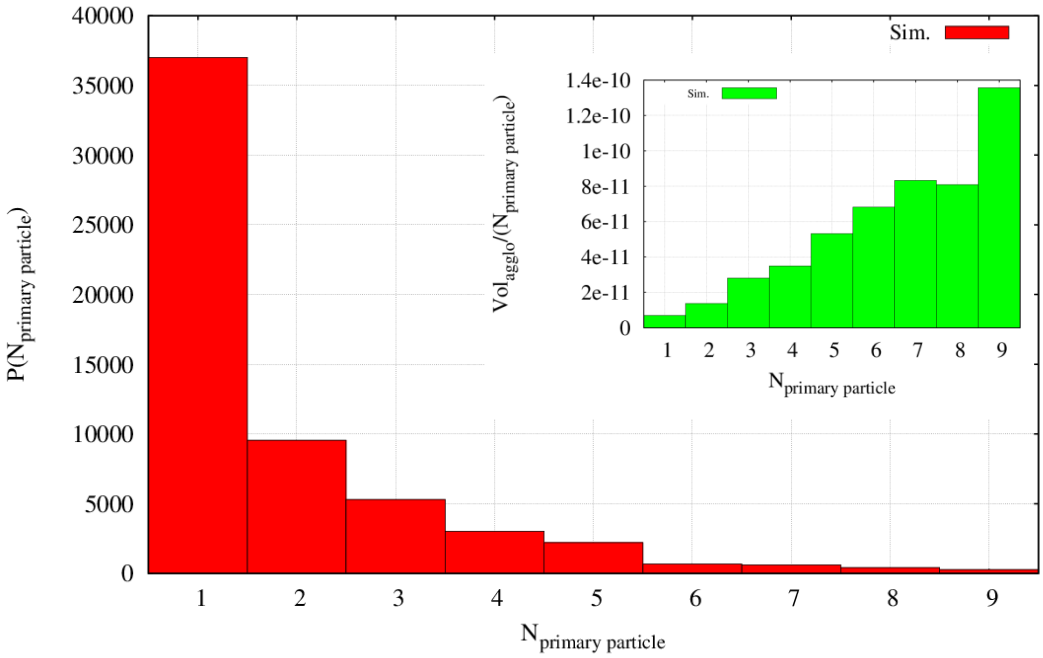

Figure 2: *Main figure: histogram of the number of primary particles per agglomerate. Inset: average volume of the primary particles as a function of the number of primary particles in an agglomerate. This shows that agglomerates with more primary particles also tend to contain larger primary particles.*

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STATE OF THE ART OF MAPPING SCHEMES FOR DILUTE AND DENSE EULER-LAGRANGE SIMULATIONS

Begona CAPA GONZALES,[1] Christoph GONIVA,[2,3] Stefan PIRKER,[2] Stefan RADL[1*]

[1]Inst. f. Process and Particle Engineering, Graz University of Technology, AUSTRIA
[2]DCS Computing GmbH, Linz, AUSTRIA
[3]Dept. of Particulate Flow Modelling, Johannes Kepler University Linz, AUSTRIA

*Corresponding author's e-mail: radl@tugraz.at

Keywords: Lagrangian methods; Separation; Jets, sprays and burners

ABSTRACT

Objective
Euler-Lagrange (EL) simulations are an extremely important tool for academia and industry to better understand gas-particle flows. In case the particle population is polydisperse, and particles are non-spherical, EL simulations are currently the only reliable tool to investigate cluster formation, mixing or segregation effects. Unfortunately, the use of inadequate numerical schemes may lead to inaccurate results. This paper aims on discussing recent developments in the field of mapping schemes, and on improving their robustness.

Scope
We present simulation results for various gas-particle flows using a variety of Lagrangian-to-Euler mapping schemes. Specifically, we have combined the idea of "smoothening" the exchange fields (as proposed by Pirker et al., as well as Capecelatro and Desjardins) to design a new generation of robust mapping schemes that allow implicit time marching. Our schemes enable EL simulations of highly loaded gas-particle flows in which particles have a broad size distribution. We will also discuss the virtues and merits of these new mapping schemes, and benchmark them against "perfect" mapping based on (ii) Voronoi tessellation (Rycroft), and (ii) an accurate geometrical reconstruction of the local particle volume fraction. Simulations were performed using "CFDEMcoupling" (www.cfdem.com), and "LIGGGHTS" (www.liggghts.com).

Results
The performance of the mapping schemes discussed in our paper is benchmarked for the case of (i) a bubbling bi-disperse fluidized bed, (ii) a freely sedimenting polydisperse suspension, as well as (iii) cross flow gas-particle injection in a turbulent flow. Performance was assessed in terms of computation speed, robustness, and ability to reproduce the "perfectly" mapped particle volume fraction.

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SAMPLE RESULTS

Figure illustrates results from our cross-flow simulation setup. In this simulations mono-disperse particles with a diameter of 15 µm are injected into an air flow (from left to right) with a mean velocity of 16.8 [m/s]. The mass loading, i.e., the ratio of the particle and gas injection rate, is ca. 21, and a significant change of the flow pattern can be observed.

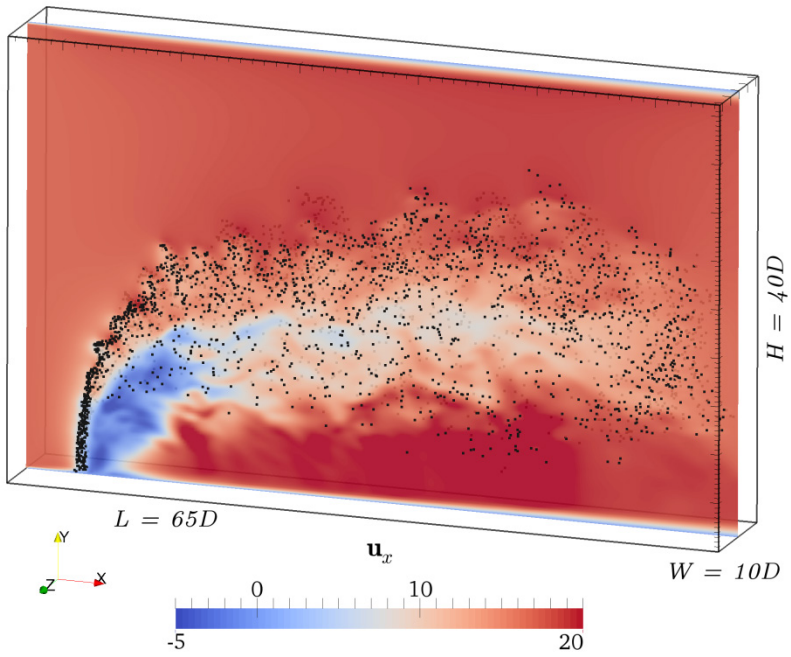

Figure 1: Simulation results (i.e., streamwise velocity field) for the cross flow gas-particle injection case using the standard "divided" mapping scheme.

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Numerical Simulation of Ice Accretion on Vessels and Structures due to Sea Spray

Mihaela Popescu and **Stein Tore Johansen**
Department of Process Technology, Flow Technology, SINTEF Materials and Chemistry, Trondheim, Norway, 7046
Corresponding author's e-mail: Mihaela.popescu@sintef.no

Keywords: CFD, marine icing, two phase flow, droplets

In the Arctic area, wave impacts against vessel hulls and solid structures result in sea sprays. At low ambient temperatures the spray droplets may deposit on surfaces and solidify, which can lead to hazardous ice accumulation. As ice accretion on vessels and off-shore structures may cause severe stability problems, predictive models are critical for safe operations in the Arctic.

We simulate the transport of the droplets, caused by the wave impacts. Effects of the droplet size and wind characteristic (speed and direction) is studied using two phase flow theory - using the Euler-Lagrangian method to simulate the flow and deposition of the droplets. The sea spray is simulated as a discrete mass and momentum source of droplets, localized in given volumes close to the hull of the vessel. The accumulation rate of the droplets which drive the ice accretion is simulated based on the idea that ice accretion only takes place if the velocity is below some critical limit. If the droplet impact velocity is very high, the contact time with the surface is short and main parts of the droplets will rebound and will not contribute to ice accretion.

The present study is done using a fixed mass and mass flow rate of the wave induced spray source. The spray droplet size distribution is mono-disperse in order to be able to investigate the direct effect of droplet drop size, and the wind on the ice accumulation. The result shows that droplets smaller than 1.0 mm have the greatest contribution to the ice accretion. The wind velocity has a direct effect on accumulation of the ice on the vessel superstructures: larger wind speed create a larger ice accumulation on the superstructures, not on the entire ship.

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MULTI-SCALE MODELLING OF TURBULENT FLOWS BY EMBEDDED LATTICE-BOLTZMANN CO-SIMULATION

Stefan PIRKER[1*], Stefan PUTTINGER[1], Simon SCHNEIDERBAUER[1]

[1] Dep. Particulate Flow Modelling, Johannes Kepler Univ., 4040 Linz, AUSTRIA

Corresponding author's e-mail: stefan.pirker@jku.at

Keywords: CFD Fundamentals and Methodology, Multilevel/Multi-scale, Pragmatic Industrial Modelling, Finite Volume Simulation, Lattice-Boltzmann Simulation.

ABSTRACT

Turbulent flows are of crucial importance for many industrial processes. However, in an industrial context it is often not possible to resolve three-dimensional coherent turbulent structures due to limited computational resources. As a consequence Reynolds averaged turbulence models are commonly applied, although their restricted predictive capabilities are well known.

In this paper we present a pragmatic approach which overcomes these limitations in cases when the turbulent core phenomenon is restricted to a special sub-region of the computational domain. While the global computational domain is covered by a conventional finite volume simulation with Reynolds averaged turbulence modelling, a lattice-Boltzmann patch is additionally placed in the sub-region of interest. This embedded lattice-Boltzmann co-simulation actually resolves coherent turbulent structures by a Large Eddy Simulation at smaller length and time scales. At regular communication interrupts this detailed information on turbulent structures is transferred back to the global simulation by a fortified Navier Stokes approach. Note, that this scale ascending communication step needs time averaging and spatial filtering.

We have implemented this multi-scale modelling approach into the commercial software ANSYS/Fluent by adding an in-house lattice-Boltzmann code by the way of pre-defined interfaces (called user defined functions, udf's). Communication between a classical Fluent simulation and the embedded lattice-Boltzmann co-simulation is realised by many to many MPI parallelization. For activating this multi-scale turbulence model one only has to define the region of interest.

After validation by focusing on the turbulent structure of a round jet, we applied this concept on several industrial flow configurations including gas cyclones (Pirker et al., 2013), submerged entry nozzles and computer cooling by synthetic jets. Summarizing we can state that this concept delivers accurate results of turbulent flows at very low computational costs. We expect that this hybrid simulation concept will become more prominent in future because it is able to efficiently harness upcoming computer architectures due to the high parallel scalability of the embedded lattice-Boltzmann code.

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SAMPLE RESULTS

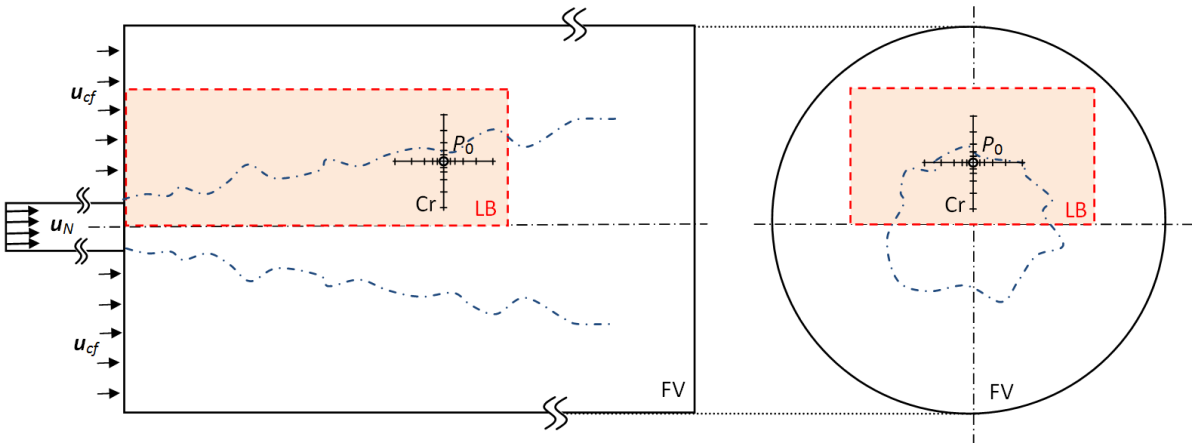

Figure 1: Validation example – hybrid simulation of a turbulent co-jet; *FV*: Finite Volume domain, *LB* embedded Lattice Boltzmann domain; *Cr*: crosshairs for evaluating axial and radial turbulent length scales.

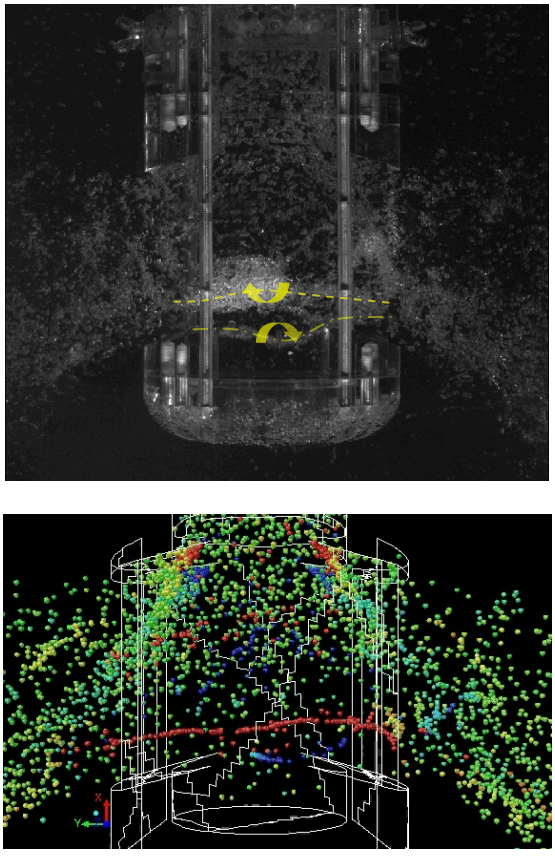

Figure 2: Application example – water model and multi-scale simulation of submerged entry nozzle flow in continuous casting of steel; the mean flow triggers secondary vortices which are visualized by air bubbles; our embedded lattice-Boltzmann co-simulation is able to resolve this behavior within a global Reynolds averaged turbulence model (bubbles are colored by y-vorticity); the lattice-Boltzmann patch covers only the region of flow deflection; additional computational costs account for 8%.

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Lifetime distributions of turbulent flow structures in chemical process equipment

Farideh GHASEMPOUR[1*], Ronnie ANDERSSON[1], Donald J. BERGSTROM[2] and Bengt ANDERSSON[1]

[1] CTH Chemical and Biological Engineering Department, 4296 Gothenburg, SWEDEN

[2] U of S Mechanical Engineering Department, Saskatchewan, CANADA

Corresponding author's e-mail: farideh@chalmers.se

Keywords: Turbulent flow, Vortex characterization, LES, Lifetime

ABSTRACT

Common phenomena in chemical engineering processes are coalescence, break-up, mixing and fast chemical reactions. These phenomena occur very fast, often within a few milliseconds, and are significantly influenced by the hydrodynamics and interfacial interactions of phases. Therefore, their modeling is complex and requires a detailed description of the turbulence spectra [1]. One of the main mechanisms of coalescence, break-up and mixing is the interaction of fluid particles with single or paired vortices in which the timescale is too short. Due to the lack of enough interaction time, fluid particles may only interact with single vortices and thus, using the average turbulence properties to model these phenomena becomes invalid. Consequently, the interaction should be described by the distribution of properties of single-turbulent vortices. To date, the properties of individual turbulent vortices such as lifetime, core volume, vorticity, growth rate, enstrophy and turbulent kinetic energy within the vortices of various sizes have not been addressed adequately [2].

The objective of the present study is to quantify several vortices' lifetime using the vortex-tracking algorithm developed. For this purpose, a new vortex-tracking algorithm that allows the details of the single turbulent vortices to be visualized and quantified is developed by the authors. The algorithm can track individual vortices over their lifetimes as they interact with mean flows and other coherent structures. It also helps to define different properties attributed to the vortices. Moreover, turbulence was modeled using large-eddy simulation with the dynamic Smagorinsky-Lilly subgrid scale model. The simulation was performed for a denser region in a straight pipe flow including 248×138×572 cells. The flow in the pipe was water at the Reynolds number of 20000, resulting in mean Taylor microscale Reynolds number of 80. The turbulent vortices were resolved at the flow condition of a low Taylor microscale Reynolds number, concluding a very narrow inertial subrange. However, this low Reynolds number is close to what is common in chemical process equipment and motivates a detailed study. The simulation assessments were conducted by mesh convergence study, analyzing the ratio of the resolved turbulent kinetic energy to the total turbulent kinetic energy, two-point correlation, wall y plus and SGS turbulent viscosity ratio. The results showed that the LES simulation was a well-resolved simulation. Furthermore, the vortex tracking algorithm was applied for studying the lifetimes of several number of vortices. The analysis of these several number of vortices reveals new information about their lifetimes. It is concluded that the lifetime determined from $\tau=k/\varepsilon$ is an underestimation mainly close to the wall.

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10th International Conference on CFD in Oil & Gas, Metallurgical and Process Industries
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Modeling of Post Combustion inside the Off-Gas Duct System Of the Ovako Electric Arc Furnace

Niloofar ARZPEYMA[1*] , Mikael ERSSON[2] , Pär JÖNSSON[3]

[1] Department of Materials Science and Engineering, Royal Institute of Technology (KTH), 100 44, Stockholm, SWEDEN

[2] Department of Materials Science and Engineering, Royal Institute of Technology (KTH), 100 44, Stockholm, SWEDEN

[3] Department of Materials Science and Engineering, Royal Institute of Technology (KTH), 100 44, Stockholm,, SWEDEN

Corresponding author's e-mail: arzpeyma@kth.se

Keywords: Duct System; EAF; Off- Gas; Post Combustion.

ABSTRACT

In order to study the post combustion (PC) inside the duct system of an electric arc furnace (EAF), a three-dimensional computational fluid-dynamics (CFD) model was developed. The reactions between the off gas species (oxygen and hydrogen) and oxygen which was leaked through the air gap was considered. The off-gas composition, the off – gas velocity and the outlet pressure were considered as parameters affecting the PC. The results showed that there was a considerable amount of the uncombusted CO to be captured. The highest CO concentration was found at the central part of the duct. The results also showed that a higher off-gas mass flow rates and a higher power of the outlet fans led to a higher combustion of CO and H_2. An off-gas analysis probe was then installed after the air gap, where the tip of the probe was placed according to the predicted high CO concentration area found in the simulations. The measured off gas composition was then used to predict the off-gas composition at the outlet of the EAF.

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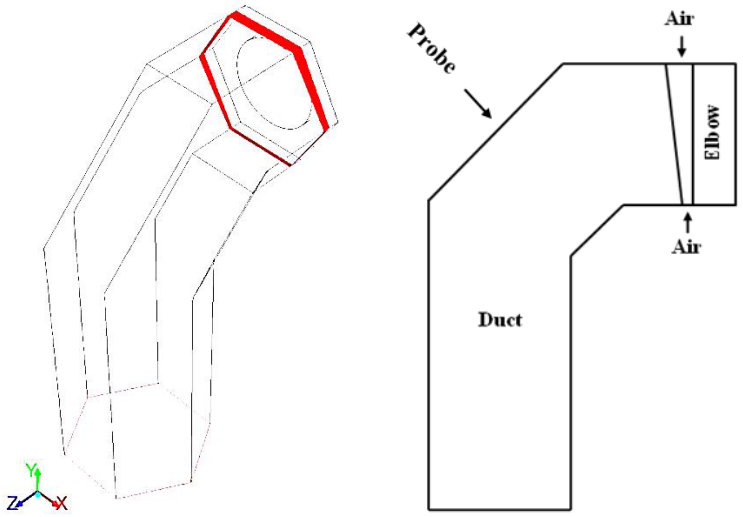

Figure 1. (a) The computation domain of the duct model; **(b)** the cross sectional view of the domain, showing the boundary conditions and the probe position.

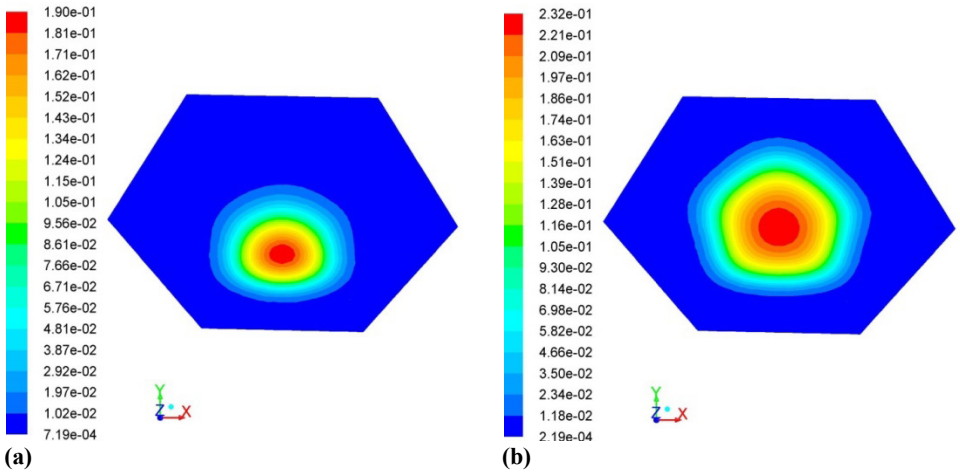

Figure 2. CO distribution in mole fraction in the plane at the probe direction **(a)** pressure -300 Pa and **(b)** pressure -100 Pa.

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Modelling of the Ferrosilicon furnace: Effect of boundary conditions and burst

Balram Panjwani[1] and Jan Erik Olsen[1]

[1] SINTEF Materials and Chemistry, 7465 Trondheim, NORWAY

Corresponding author's e-mail: balram.panjwani@sintef.no

Keywords: CFD, process gas, NOx, SiO_2, Dust, Ferrosilicon

ABSTRACT

In a Ferrosilicon furnace, process gas mainly consisting of SiO and CO with some moisture are the by-products of a reduction process (SiO2 (silica) + C (Coal)). Hot process gas from the reduction zone escape through the charge surface into a furnace hood. Simultaneously, air is sucked into the hood through various open areas due to the pressure drop, and reacts with the process gas. A steady state and transient CFD model solving for continuity, momentum, energy, species and turbulence equation have been developed for the furnace hood. Modelling the process inside the furnace hood is very challenging due to the complex interaction among, flow, buoyancy forces, radiation and turbulence. Another challenge also faced by modellers is the selection of proper boundary conditions, especially, the boundary condition used for the charge surface, which is neither a wall surface nor a mass flux. Traditionally, this boundary condition is modelled as a mass flux boundary, without considering the effect of roughness due to uneven distribution of charge material (Silica and Coal). Although, it is possible to account the roughness effect in the CFD geometry and mesh in a pre-processing step, this will be a time consuming process. In the present study, the charge gas surface is modelled as a wall surface, where roughness effects are accounted with roughness height and flow of process gas is modelled as an appropriate source term in continuity, momentum, energy, species and turbulence equations. This approach is compared with the traditional mass inlet boundary condition. The process gases (SiO and CO) react with air and produces SiO_2 (s) and CO_2, this reaction is very exothermic and generates temperature of 2300-2700 ^{0}C inside the furnace hood, which is indeed a favourable condition for thermal NOx formation. Furthermore, escaping of process gas from the charge surface is non-uniform, where strong burst of SiO and CO have been observed inside the furnace. These bursts are responsible for higher local temperature and NOx formation. The present study accounts for modelling these bursts, which has not been modelled yet as per best of our knowledge. The studies show that both the strength of the burst and its location play a significant role in the NOx production.

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A STUDY OF BREAKAGE BY SINGLE DROP EXPERIMENTS

Jannike SOLSVIK, Reza FARZAD, Hugo A. JAKOBSEN
Department of Chemical Engineering, NTNU, 7491 Trondheim, NORWAY

Corresponding author's e-mail: jannike.solsvik@chemeng.ntnu.no

Keywords: population balance equation; drop breakage; single drop experiment; drop dynamics; breakage closures; breakage time

ABSTRACT

In dispersed multiphase flow modeling using population balances (PB), the dispersed phase system is considered as a population of entities of the dispersed phase distributed not only in physical space but also in an abstract property space. The population balance equation (PBE) is a useful modelling tool which uses a density function defined in a phase space (i.e. spatial space + property space) in order to balance a population of entities that may evolve through the influence of entity-entity and entity-continuous phase interactions. In its original form, the PBE holds an accumulation term, a convection term for each dimension of the phase space, and source terms that account for birth and death of the entities. The key challenge associated with the formulation of predictive PB models is the determination of the submodels of the PBE. For example, the contradictory prediction of the breakage frequency function for fluid particles: Some authors argue that the breakage frequency profile should go through a maximum as the parent drop diameter increases, others have anticipated that the breakage frequency should be monotonically increasing with increasing parent drop size (Solsvik et al. 2013). The number of daughters produced in a breakage event is commonly set equal to two in PB modelling although experimental data have indicated that this number can be higher.

In the present work, the entities of the population are oil drops in a continuous water phase. Numerous single drop breakage events are collected by use of high-speed camera. The single drop experiments allow us to study the detailed mechanisms of drop breakage. That is, the time taken from the deformation of the drop until it breaks can be determined along with the average number of daughter particles produced in the breakage. These data can be used to evaluate the existing literature models for drop breakage. A similar experimental investigation has been performed by Maass and Kraume (2012) for toluene/water and petroleum/water systems. The present study is extended to consider other oil/water systems.

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SAMPLE RESULTS

Fig. 1 illustrates the breakage of an oil-drop.

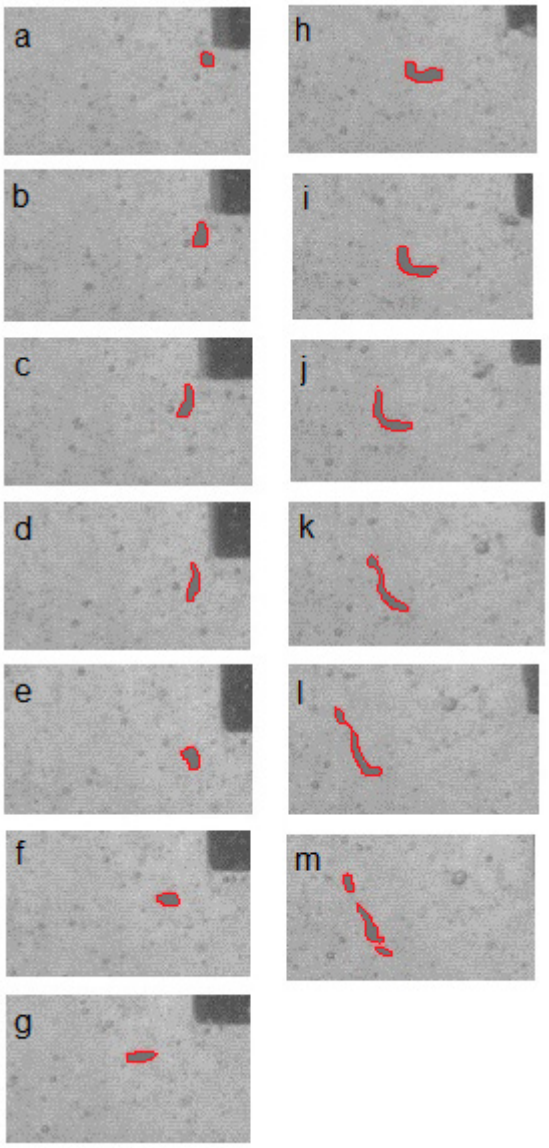

Figure 1: Time series of a mother oil-drop breaking into three daughters.

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MODELLING OF BUBBLE SIZE DISTRIBUTION BY USING HOMOGENEOUS AND INHOMOGENEOUS POPULATION BALANCE APPROACHES

Lilunnahar DEJU[1], Sherman C. P. CHEUNG[1], Guan H. YEOH[2,3] and Jiyuan TU[1*]

[1] School of Aerospace, Mechanical and Manufacturing Engineering, RMIT University, VIC 3083, AUSTRALIA

[2] Australian Nuclear Science and Technology Organization (ANSTO), NSW 2234, AUSTRALIA

[3] School of Mechanical and Manufacturing Engineering, UNSW, NSW 2052, AUSTRALIA

Corresponding author's e-mail: Jiyuan.Tu@rmit.edu.au

Keywords: Bubble column, Homogeneous MUSIG, Inhomogeneous MUSIG, Bubble breakup, Bubble coalescence.

ABSTRACT

To account the coalescence and breakup phenomenon of gas-liquid bubbly flows, the population balance equation (PBE) has to solve along with continuity and momentum equations within the two fluid modelling framework. Previous study by Deju et al. (2013) has been carried out to assess the performance of different population balance approaches in tracking the changes of gas void fraction and bubble size distribution under complex flow conditions. This reveals that the behaviour of breakup and coalescence kernels have dominant effect on solution method of PBE.

Nonetheless, the study assumes all bubbles travel in one single velocity field which may not valid in practical systems. In this paper, the inhomogeneous MUSIG approach has been applied to obtain a deeper understanding of the flow structure in the bubble column reactor that helps to describe the breakup and coalescence of bubbles and the evolution of bubble size distribution. The inhomogeneous MUSIG model enables consideration of different velocity fields for bubbles with different sizes. Meanwhile, the bubble breakup and coalescence phenomenon can be also modelled to capture the bubble interactions and its impact on the bubble size distributions. Two breakage kernels were chosen; the widely adopted breakage kernel by Luo and Svendsen (1996) along with more recent one by Wang et al. (2003). On the other hand, the coalescence kernel by Prince and Blanch (1990) was applied. The results from homogeneous and inhomogeneous MUSIG models were compared against the experimental data from the TOPFLOW test facility at HZDR (Lucas et al. 2010). Furthermore, the performance of different breakage and coalescence kernels and its coupling effects with multiple velocity fields were also assessed.

Numerical results have shown that lateral separation of small and large bubbles is in well agreement with the experimental measurements. The evolution of bubble size and its associated bubble migration due to the lift forces is well described by the inhomogeneous MUSIG approach.

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SAMPLE RESULTS

Figure 1 shows the radial gas volume fraction profile for the test case T107 for different kernel combinations at a close distance from the bottom of the pipe L/D=1.7 and at a longer distance of L/D=39.9. Two kernel combinations are implemented. For the combination 1, with the breakage kernels by Luo and Svendsen (1996) and the coalescence by Prince and Blanch (1990); the inhomogeneous MUSIG model clearly shows a separation between small and large bubbles. Driven by the lift force, small bubble sizes showed a wall peak volume fraction profile while a core peak profile was found for large bubbles. In the comparison to the homogeneous MUSIG, the predicted volume fraction profiles seem to be in better agreement with the experimental data.

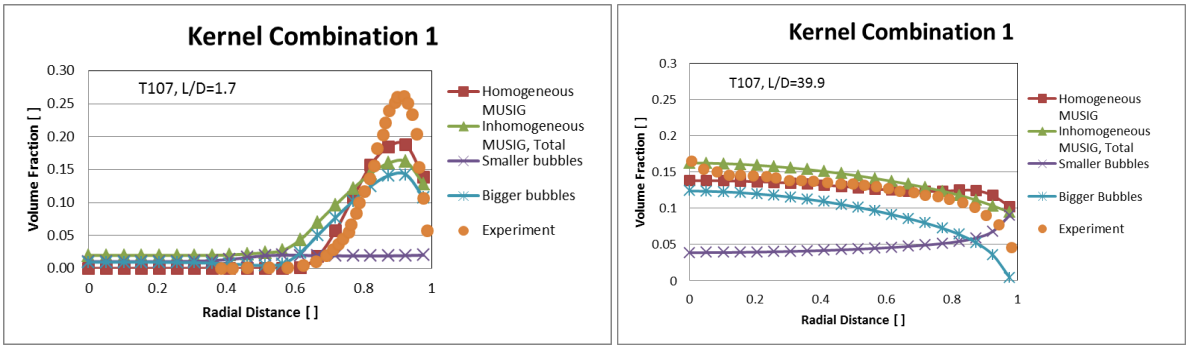

Figure 1: Radial void fraction profile by homogeneous and inhomogeneous MUSIG compared with experimental data for flow condition T107 with kernel combinations 1.

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SIMULATION OF POLYDISPERSE GAS-LIQUID SYSTEMS WITH QUADRATURE-BASED MOMENT METHODS

Antonio BUFFO[1] , Daniele L. MARCHISIO[1], Marco VANNI[1], Julia HOFINGER[2], Peter RENZE[2]

[1] Department of Applied Science and Technology, Politecnico di Torino, 10129 Torino, ITALY

[2] Department for Chemical and Process Engineering, BASF SE, Ludwigshafen, GERMANY

Corresponding author's e-mail: antonio.buffo@polito.it

Keywords: population balance modelling, gas-liquid systems, quadrature-based moment methods.

ABSTRACT

Different industrial scale dispersed gas-liquid system can be successfully described by considering that gas bubbles are polydisperse, namely the gas phase is characterized by a distribution of bubbles with different velocity, size and composition. Phase coupling issues can be properly overcome by considering the evolution in space and time of such bubble distribution, which is dictated by the so-called Generalized Population Balance Equation (GPBE) (Marchisio and Fox, 2013), with the inclusion of specific mesoscale models for taking into account momentum, heat and mass exchange with the liquid phase, as well as bubble coalescence and breakage. The choice of these mesoscale models is of crucial importance for the prediction of the relevant properties of a gas-liquid system. A computationally efficient approach for solving the GPBE is represented by the quadrature-based moment methods, where the evolution of the entire bubble population is recovered by tracking some specific moments of the distribution and the quadrature approximation is used to solve the "closure problem" typical of moment-based methods. Among these methods, the Conditional Quadrature Method of Moments (CQMOM), is particularly interesting. Following up on our previous work on this topic, this contribution focuses on three different aspectst: (1) role played by the different interface forces (i.e., drag, lift and virtual mass); (2) improvement of the drag force mesoscale model, accounting for turbulence and bubble swarm effects; (3) crucial details of the implementation of these methods into the opensource CFD code OpenFOAM.

The investigation of the first two points is motivated by the final aim of our work, which is the development of a very general (and fully predictive) methodological approach, useful to simulate very different gas-liquid equipment. As a matter of fact, only with reliable mesoscale models for the different interfacial forces, this goal can be achieved. The last point is motivated by the necessity of efficiently implementing the transport equations for the moments satisfying the properties of conservation, realizability and boundedness, consistently with what done with the other conserved transported variables (e.g. gas volume fraction). The methodology is here validated by considering very different gas-liquid systems, mainly bubble columns and aerated stirred tank reactors, for which experimental data are available (Laakkonen et al. 2006, Kulkarni et al. 2007, Diaz et al. 2008). For validation purposes, the local measurements of Bubble Size Distribution (BSD), local axial liquid velocity and gas hold-up profiles, together with global measurements of gas hold-up are eventually compared with the simulation results, showing in general a good agreement with the experimental data for all the system reproduced.

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SAMPLE RESULTS

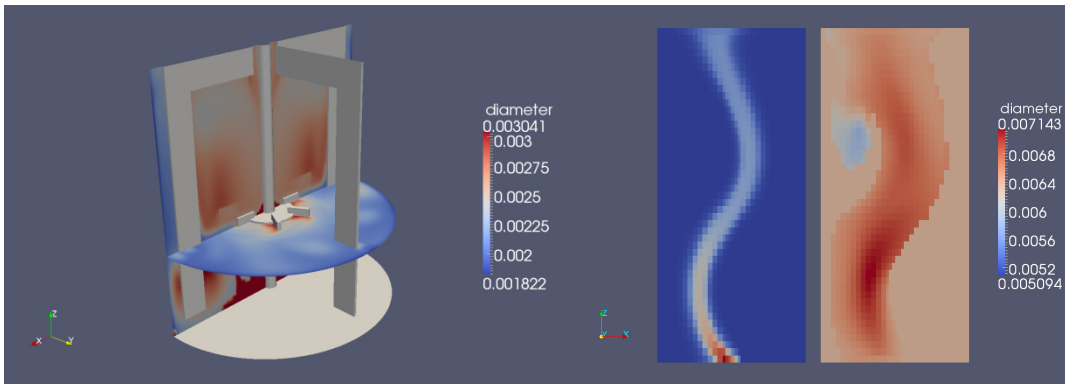

Figure: Contour plot of mean Sauter diameter for an aerated stirred tank reactor (left) and an instantaneous contour plot of volume fraction and mean Sauter diameter for a pseudo 2D rectangular bubble column.

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CFD simulations of a Wankel pump performance with moving and static grids

Jason LEONG Yu Chuan[1],BA Te[1], Stephen WAN Yee Ming[1], ZHAO Yuqiao[2], KANG Chang Wei[1], LOH Wai Lam[2], Arthur LIM Teck Bin[1*]

[1] IHPCFluid Dynamics, 138632 SINGAPORE

[2]NUSDepartment of Mechanical Engineering, 117576 SINGAPORE

Corresponding author's e-mail: limtba@ihpc.a-star.edu.sg

Keywords: Positive displacement pump;Computational fluid dynamics;Downhole equipment; Hydraulic performance

ABSTRACT

This paper presents the numerical analysis of a Wankel pump using 3 different CFD techniques. The Wankel pump is a positive displacement pump which consists of an eccentrically rotating rotor in a housing that can be described by an epi-trochoid (see Figure 1). Although this has been a well-known internal combustion engine design, its use as a pump has not been much investigated numerically. The 'Wankel pump' can be classified as a rotary action positive displacement pump. Considering the use of this design as an internal combustion engine, the Wankel pump, as with most positive displacement pumps, is expected to perform even when subjected to high gas volume fractions. This would be a marked advantage over centrifugal pumps which tend to gas lock when exposed to highly gassy flows. As such, there is therefore good potential for the use of the Wankel pump as a multiphase pumpfor useful application in production from gassy wells of high gas fractions..

For a Wankel pump typical design, however, the tight clearances between the rotor and the housing and the unconventional rotor trajectory, not definable by a stationary rotational axis alone, presents some technical challenges that cannot be resolved by conventional CFD techniques, such as the MRF or sliding meshing that are normally applied for turbomachinerysimulations. In light of the novel nature of the pump and the shortcomings of conventional CFD methods, three different approaches - each respectively available in the proprietary CFD codes, FLUENT, CFX and FLOW3D - were attempted here for the analysis of the performance of the Wankel pump. The dynamic meshing capabilities in FLUENT were used to morph the mesh according to the topological changes with respect to the rotation of the rotor. The immersed solid method was used in CFX. This technique used two overlapping grids to identify the location of the solid rotor. Finally, in FLOW3D, the free gridding technique was used where the geometry building and grid generation are independent operations.

In this paper, the single phase pump performance was investigated for a series of varying housing-rotor clearance and running speed, for a comparative studies on the numerical results from the 3 different approaches. This study will serve as the foundation for subsequent multiphase flow performance analysis in the Wankel pump in future work.

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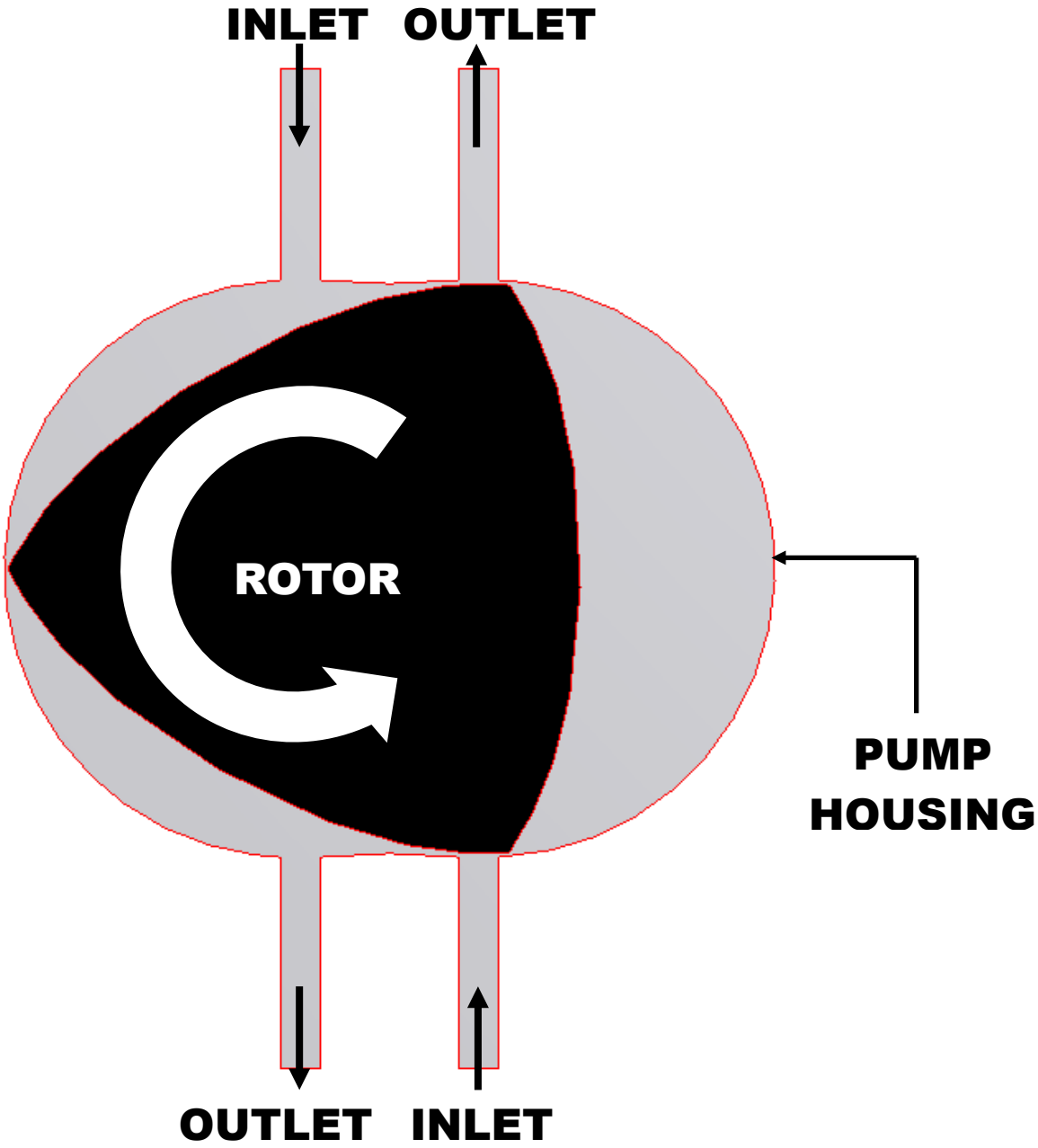

Figure 1: Schematic diagram of Wankel Pump

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CFD STUDY OF THE INFLUENCE OF PRE-ROTATION OF MULTIPHASE FLOW ON PUMP PERFORMANCE

Mikhail P. STRONGIN
Xylem Inc. AWS, Morton Grove, IL 60053, USA
mikhail.strongin@xyleminc.com

Keywords: Pump, pre-rotation, multiphase, separation.

ABSTRACT

Pre-rotation is a common phenomenon in industrial applications of pumps. It may have a significant influence on pump performance [1]. Even though the number of CFD works was done for liquid only with pre-rotation, such as [2], a CFD study of behaviour of liquid-solid mixture with pre-rotation in the pump is practically non-existent.
This work compares the influence of pre-rotation flow on pump performance for homogenous and multiphase flows.
Two stages of vertical mixed flow pump were modelled. The fluent 14.5.7 commercial code was used for simulations. The mixer multiphase model was chosen for the mixture model. The SST k-ω model for turbulence was taken. The gravity was taken into account. A multi-reference frame approach was used for rotation domains. The primary phase was water. The secondary (solid) phases were silicon spherical particles of 0.2mm diameter. The volume fraction of solid particles in the mixture ranged from 0.5% to 10%. The swirling number on the inlet was 1. The total number of mesh cells was 9 million.
By definition, the pump head was determined by the liquid phase. The mixture pump head and the pure water pump head were compared when both had the same flow rate and the same swirling number. The pump heads displayed a difference of approximately 1%. For the head of the first sage or the pump the difference is slightly more visible: approximately 1.5%. The efficiency of the pump with high solid phase load was much lower than the efficiency of the pump with pure water with the same flow rate. For 10% of solid particles volume fraction, this difference is more than 10 percentage points. The difference in the head ratio between stages with pre-rotation on the inlet was relatively high: from 10% to 25%.
Efficiency is determined as a ratio of power added by the pump to both liquid and solid phases to the total power consumed by the pump. The power added to the liquid was determined by the head. The power added to the solid phase was determined by the difference between the power of solid phase on an outlet versus an inlet. Results were as expected: they showed this difference to be less than 1% of head power for all solid phase loads. The difference between losses in homogenous and multiphase flows was due to power consumed by particle separation.
These results will be helpful in the design of liquid-solid pumps with pre-rotations.

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PARAMETRIC MODEL OF THE S809 WIND TURBINE BLADE BY CFD ANALYSIS TO PREDICT BEST ANGLE OF ATTACK

Nurul HASAN
CEO, Don Computing, 39/385 Bourke St, Melbourne, VIC 3000, Australia

Corresponding author's e-mail: drnhasan@doncomputing.com

Keywords: optimization, turbine, parametric study.

ABSTRACT

The recent development in increase of simulation driven design, associated with the progress of the numerical methods for predicting wind turbine performances, allows vital improvement in wind turbine blade design. This article of parametric modeling of S809 wind turbine blade presents a coupling between FRIENDSHIP-Framework and FLOW-3D CFD. In the first step S809 Blade is drawn in FRIENDSHIP Framework with a fixed angle of the attack. Model is exported to the meshing software to generate the mesh around the blade. Designed model is coupled with the Flow-3D, a CFD package to analysis the coefficient of the lift and drag. This process is continued by the automation of FRIENDSHIP-Framework till finding the maximum sliding ratio (lift/drag ratio) in order to gain the maximum power from the wind turbine. By using this method significant saving is found.

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FORECASTING TURBULENT DRAG REDUCTION IN A PIPELINE FLOW ON BASIS OF TAYLOR-COUETTE DEVICE EXPERIMENTAL DATA

Dmitry ESKIN

SCHLUMBERGER DBR Technology Center, 9450-17 Ave., Edmonton, AB T6N 1M9, CANADA

Corresponding author's e-mail: deskin@slb.com

Keywords: Couette device, Drag reduction, Modelling, Polymer additive, Pragmatic industrial modelling, Pipeline Flows, Turbulence

ABSTRACT

Drag reducing polymer additives are widely employed for reduction of friction losses in turbulent pipeline flows. Such chemicals allow reducing the pressure gradient up to 80 %. Numerous flow loop experiments are usually conducted to characterize drag reducer performance under field conditions in a wide range of operation parameters. High flow rate tests are needed because high Reynolds number flow regimes are most important for drag reducer applications. An accurate model of the drag reduction effect allows a significant reduction of a number of relatively expensive measurements. A model of drag reduction in a pipe flow, based on a boundary layer concept, is developed. An approach of Yang and Dou (2010) for modelling a stress deficit in the laminar boundary sublayer, caused by drag reducing additives, is employed. In this case, the laminar sublayer thickness is calculated by an empirical equation as a function of the so-called drag reduction parameter. Use of a simple Prandtl Mixing-Length model of turbulence for derivation of model equations allows us to formulate the drag reduction model as a modified Prandtl-Karman correlation for the Fanning friction factor. The model developed contains only one parameter that must be identified from experiments. This parameter is a function of the drag additive type and concentration. The model predictions are in good agreement with the results obtained by a more complicated model of Yang and Dou (2010) that was verified experimentally. Note that only a couple of experiments at different Reynolds numbers are required for identification of the mentioned model parameter.

Application of a wide-gap Taylor-Couette device instead of flow loop for drag reducer performance studies is suggested. A laboratory Taylor-Couette device is compact, requires a small fluid amount and, therefore, can be efficiently used for rapid characterization of drag reducing additives. A turbulent drag reduction model is developed for a device, in which an inner cylinder rotates and an outer one is immobile. The basic principles of both the developed drag reduction model in a pipe and an engineering model of a turbulent Taylor-Couette flow (Eskin, 2010) are employed for deriving a model of drag reduction in a Taylor-Couette device. The drag reduction model parameter for a certain chemical additive can be identified from laboratory-scale experiments in a Taylor-Couette device and can further be used for drag reduction forecasting in industrial-scale pipe flows for a wide range of Reynolds numbers.

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SAMPLE RESULTS

Figure 1 shows a performance of a developed simple drag reduction model for a pipe flow vs. the more complicated model of Yang and Dou (2010).
In this Figure f is the Fanning friction factor, Re is the Reynolds number, α_{0*} is the identified parameter for the model developed, α_* is the identified parameter for the model of Yang and Dou (2010).

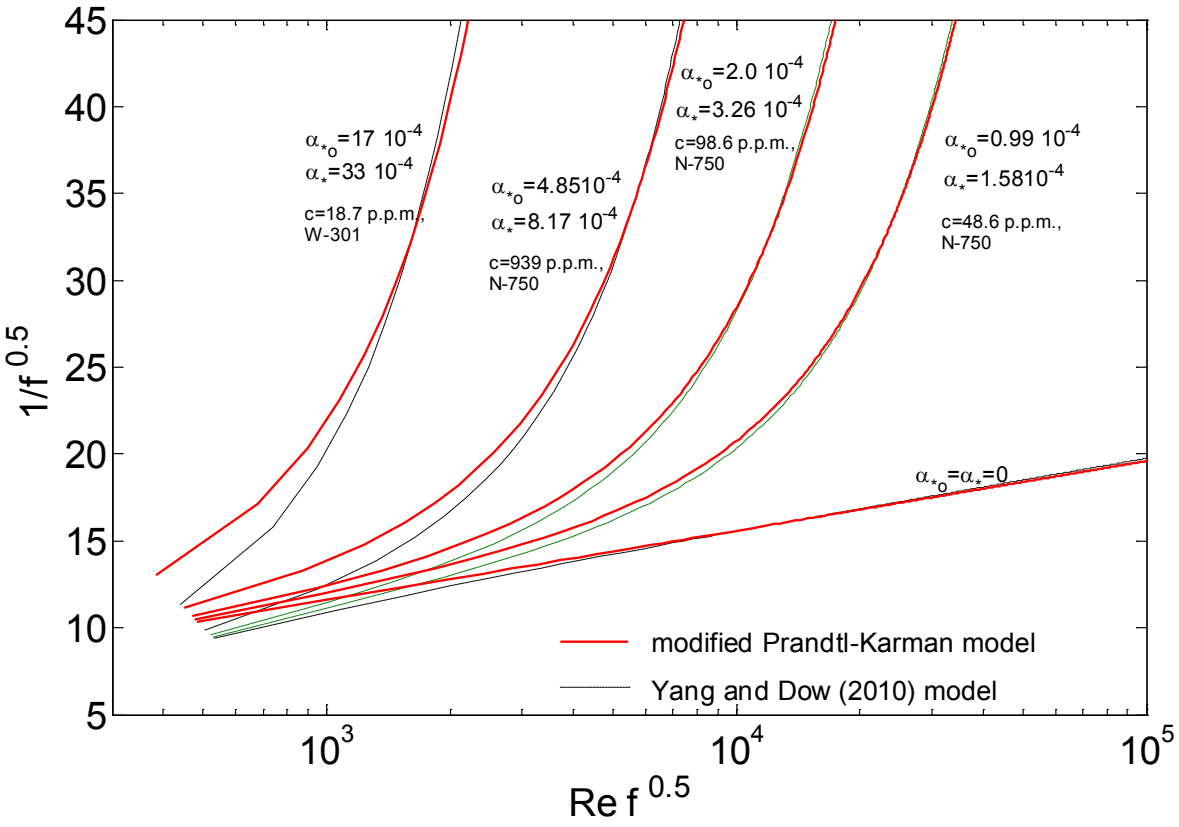

Figure 1: Dependence of the Fanning friction factor on the Reynolds number

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CFD MODELLING OF GAS ENTRAINMENT AT SLUG FRONT

Jinsong HUA and Martin Foss
Institute for Energy Technology, PO Box 40, NO-2027 Kjeller, NORWAY

Corresponding author's e-mail: jinsong.hua@ife.no

Keywords: multiphase pipe flow, gas entrainment, CFD simulation, VOF method.

ABSTRACT

Gas entrainment process at slug front contributes the aeration of liquid slug body in multiphase pipe flows. The transportation and distribution of small gas bubbles in liquid slug body changes the aeration status of liquid slug, which has strong effects on hydrodynamic behaviour of liquid slug moving inside pipes. Numerous experiments (Nydal and Andreussi 1991; Wang et al. 2012; Barnea et al. 2013) were conducted to investigate the gas entrainment rate and void fraction distribution in liquid slug. A mechanistic gas entrainment model was proposed in Skartklient et al. (2012). Due to the complex flow physics and the dynamic gas-liquid interface in the gas entrainment process, there are still many challenges in measuring the gas entrainment rate accurately. The experimental difficulties also hinder our physic understanding of the flow process and retard the development of a proper model to estimate the gas entrainment rate.

In this paper, we try an alternative approach to model the gas entrainment at slug front using a computational fluid dynamics method based commercial package Star-CCM+. As we know, the gas entrainment at slug front is a very complex and dynamic process, involving bubbles of different length-scales. Hence, the basic principle we are using now is to use fine mesh for resolve the different length scales and small time step size to resolve the dynamic features. In the CFD model, the VOF method is used to track the gas-liquid interface. The mesh grid size is set 1.0E-3m or finer and the time step size is set 1.0E-4s. With such fine mesh grid size and time step size, we are affordable to run a transient model for a 2D channel as shown in Figure 1. In order to let the slug front to stabilize in the computational domain, a moving reference frame is adopted with the translation speed of Taylor gas bubble. We initialize the Taylor gas bubble as rectangle shape, locating at the left end of the model, and the liquid fills up the rest part. The Star-CCM+ will calculate the transient development of liquid-gas interface, and gas entrainment process.

An example simulation result on the gas entrainment process at slug front of an air-water system is shown in Figure 2. The width of channel is 0.1m. The channel inclination is about 5 degree uphill. The mixture velocity is about 1.0 m/s. Small gas bubbles are produced at the gas-liquid interface nearby the liquid slug front. In the final paper, we will present more simulation results under effects of pipe inclination, Taylor gas bubble propagation speed, liquid layer holdup, and let layer jet velocity.

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SAMPLE RESULTS

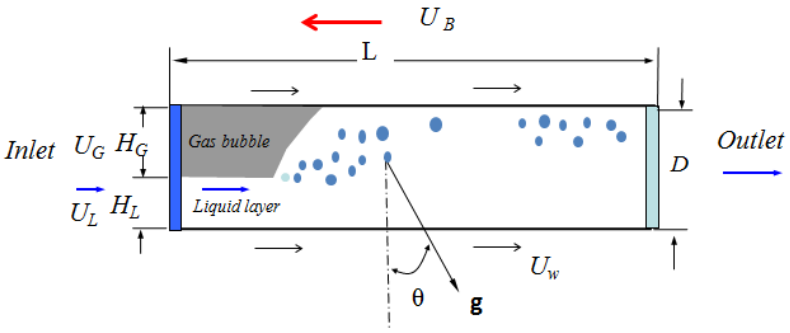

Figure 1: Schematic diagram of CFD model for the gas entrainment process in slug flow.

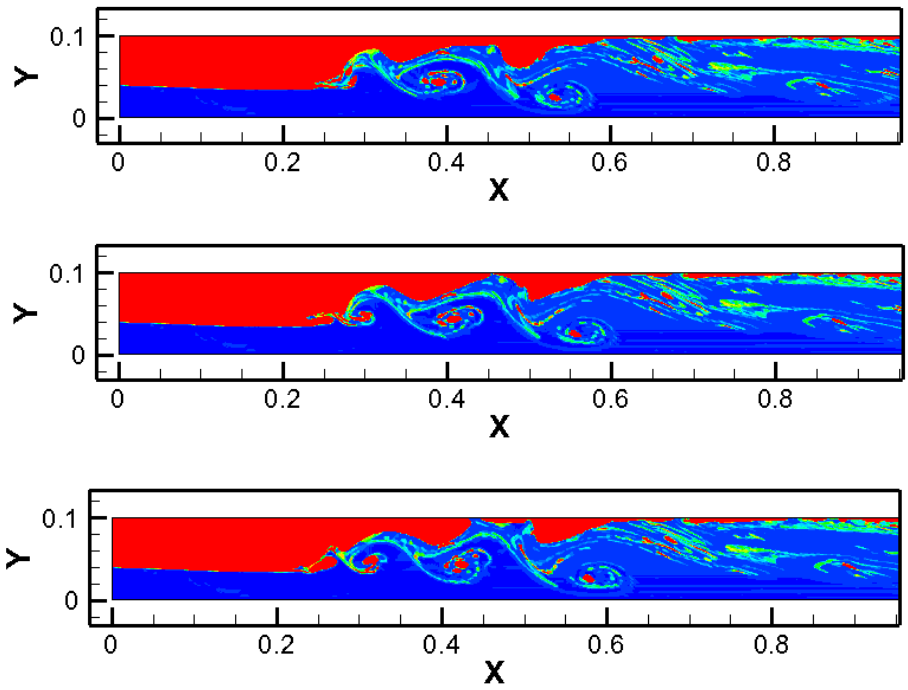

Figure 2: Predicted dynamic air-water interface behaviour at the slug front ($U_w = 1.5m/s$, $U_L = 1.0m/s$, $H_L = 0.04m$, $\theta = 5^\circ$, $D = 0.1m$, Air-water system).

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Computational modelling of subsea hydrates formation and associated risks and impact on flow assurance

Mathieu Labois, Djamel Lakehal, Chidambaram Narayanan

ASCOMP GmbH Zurich, SWITZERLAND
chidu@ascomp.ch

ABSTRACT

Subsea hydrate formation may cause blockages in oil production lines, and as such it remains today one of the main concerns to deepwater field developments. Hydrates form from a chemical reaction involving cold water (at high pressure) and methane, or oil light-components. The present strategy of operators consists in the deployment of prevention methods that aim at producing outside the hydrate domain, via pipeline insulation (for oil systems) or by means of chemical injection (for gas systems). Another strategy is to produce still inside the hydrate domain by transporting the hydrate phase as slurry of hydrate particles dispersed in the oil phase. Be it as it may, there is an incentive to develop advanced CFD/CMFD models to help design strategies to ensure restarting after a long shutdown due to hydrate blockage. While 1D models for hydrate-plug formation in flowlines are available and have been successfully applied for subsea tiebacks, full 3D CFD predictions are in fact rare in this area.

Another important context in which hydrates mitigation is vital relates to deepsea oil spills, which become a great concern today given the proliferation of oil production from wells at great depth (1500-3000 m below sea level). In the event of a spill, contingency plans including both capping and collection system have to be developed and validated. In particular, collection systems consisting of a simple dome and riser system can be critical in containing the environmental impact until a permanent solution such as a capping stack is ready for installation. The use of a collection system in deep sea is complicated by the thermodynamic conditions of high pressure and low temperature which results in rapid conversion of gaseous hydrocarbons to hydrates within a very short distance resulting in complete plugging of the dome. As is well known the containment effort of BP for the Deepwater Horizon oil spill was unsuccessful due to severe hydrates plugging. Typical response to a large oil well blowout is to cap the well. However, before capping can be achieved, relief wells have to be dug to intercept the existing well bore. This procedure is time consuming and can take up to 3 months, during which time other means of containing the oil and gas leak have to be implemented to minimize environmental damage. The capping of the well is slowed down by the logistics of the surface ships required such as a drilling rig, and several specialized surface vessels and by the availability of capping stacks. If the well integrity is compromised, further complications arise resulting in higher environmental damage unless a temporary solution is available that effectively collects the hydrocarbons thus preventing long-term contamination. It is clear that a canopy/dome and riser based collection system is an essential tool for the containment of well blowouts.

The current study introduces the hydrate physics module built in TransAT, and coupled to the N-phase multiphase flow model. The hydrates module includes models for hydrate formation and dissociation kinetics, formation enthalpy, hydrates rheology including effect of agglomeration and hydrates adhesion. The modelling was recently extended to include the possibility to simulate the mixing and dissolution of miscible liquids such as methanol and hot water as active mitigations mechanisms. Selected examples will be presented and discussed.

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PRESSURE AND TEMPERATURE PREDICTION IN PRESENCE OF HYDRATE

Nurul HASAN
CEO, Don Computing, 39/385 Bourke St, Melbourne, VIC 3000, Australia

Corresponding author's e-mail: drnhasan@doncomputing.com

Keywords: hydrate, sink/source term, Phase diagram.

ABSTRACT

Hydrate behavior has been under the continuous investigation and thousands of the experimental and modelling examinations have been published by researchers since its discovery. This main issue is the formation condition of hydrate that can be so different in a variety of circumstances such as inhibitor and promoters presence. Therefore, this topic has allocated an immense number of articles to itself. In this article, a two phase one dimensional model is solved for unsteady case. Heat of condensation/hydrate (CH_4/H_2O) formation is considered in the liquid phase. The properties of gas and liquid are continuously updated wrt to the T and P. Phase diagram is examined continuously to check the presence of the hydrate. The hydrate formation kinetics is considered as sink/source term in gas/liquid phase. The pressure and temperature in the pipe flow is validated with some other published data.

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CFD SIMULATIONS OF FLOW IN PACKED BEDS OF SPHERES AND CYLINDERS: ANALYSIS OF THE VELOCITY FIELD

Ferdaous DORAI[1*], Matthieu ROLLAND[1], Anthony WAchs[1], Manuel MARCOUX[2], Eric CLIMENT[2]

[1] IFPEN, Rond Point de l'Échangeur de Solaize, 69390 Solaize, France

[2] IMFT, 1 Allée du Professeur Camille Soula, 31400 Toulouse, France

Corresponding author's e-mail: ferdaous.dorai@ifpen.fr

Keywords: Chemical Reactors, packed beds, velocity distribution, probability density function

ABSTRACT

Small catalytic fixed bed reactors are commonly used to assess the performance of heterogeneous catalysts (typically spheres and cylinders). In this work, we are interested in a better understanding of the flow patterns that might affect local mass transfer and effective reactor performance. Packed beds of spheres or cylinders are simulated using the DEM (Discrete Element Method) code Grains3D (Wachs et al. (2012)). Solid objects are randomly inserted inside a horizontally bi-periodic container and then fall under gravity and collide with each other and the bottom of the reactor. Hydrodynamic simulations are performed with PeliGRIFF (Wachs (2010)), a Fictitious Domain/Finite Volume numerical model, with similar periodic boundary conditions as the DEM simulations in the horizontal directions, uniform inlet vertical upward velocity and uniform outlet pressure. Simulations parameters that have been varied are the bed height and the Reynolds number of the flow. Results are analysed in terms of the probability density function (PDF) of the normalized velocity components (P (V_i/V_{inlet})) and observations of the local flow with a special focus on stagnant zones and by-passes.

For a given bed, the analysis of regions of equal volume have given close to identical PDF curves except near the top and the bottom of the bed due to classical inlet and outlet effects (Dorai et al.(2012)). The work in progress consists in the comparison of the results in the same bed with different Reynolds numbers, with a focus on changes in velocity distribution (particularly low and high velocities). The distribution of the angle of the flow relative to the average vertical direction is studied as well. Finally we compare the velocity PDF for beds made of the same particles but packed differently, for two packed bed heights, and also compare velocity PDF obtained with spheres and cylinders. This gives insight on the variability of velocity inside a packed bed compared to the variability between two randomly packed ones.

Future work will focus on the relationship between flow and mass transfer / effective reactivity by solving the convection-diffusion equation in the same geometries.

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PORE-SCALE SIMULATION OF COLLOID DISPERSION AND DEPOSITION IN POROUS MEDIA

Gianluca BOCCARDO[1] , Matteo ICARDI[2,3,4], Tiziana TOSCO[2], Daniele L. MARCHISIO[1], Rajandrea SETHI[2]

[1] Department of Applied Sciences and Technology, Politecnico di Torino, 10129 Torino, ITALY
[2] Department of Environment, Land and Infrastructures, Politecnico di Torino, 10129 Torino, ITALY
[3] Division of Computer, Electrical and Mathematical Science and Engineering, King Abdullah University of Science and Technology, 23955-6900, Thuwal, SAUDI ARABIA
[4] Institute for Computational Engineering and Sciences, University of Texas at Austin, 78712-0027, Austin, USA

Corresponding author's e-mail: gianluca.boccardo@polito.it

Keywords: packed beds, mass transfer

ABSTRACT

The simulation of colloidal transport and deposition in porous media finds many important environmental and engineering applications: particle filtration [1], aquifer remediation [2], catalytic processes in packed beds and enhanced oil recovery, the latter two being of particular interest to the oil & gas and process industries.

The objective of this work is the development of robust computational tools for the simulation of three-dimensional porous media from the geometrical modelling to physics simulation, in a way to overcome the constraints often suffered by studies of this kind (assumption of Stokes flow and limitation to simplified geometries). Having obtained a framework for the efficient reproduction of arbitrary geometric models for the packing, accompanied by a particular care given to mesh generation and spatial discretization issues, simulations of transport and deposition of colloidal particles, in a wide size range, were performed.

A code for the rapid prototyping of many packing samples, diverse in porosity, grain size distribution and grain shape was developed, interfacing to the open source code Blender to manage the rigid-body physics. The open source finite volume CFD code OpenFOAM was used: first fluid flow is described with the Navier-Stokes equations, then an Eulerian approach has been used to analyze particle dispersion. Velocity distributions and hydrodynamic dispersion coefficients are obtained, and the validity of Fick's law in describing dispersion is assessed in each case. Moreover, particle deposition efficiency is calculated and compared to the results of a preliminary investigation [3] performed on more primitive geometric models.

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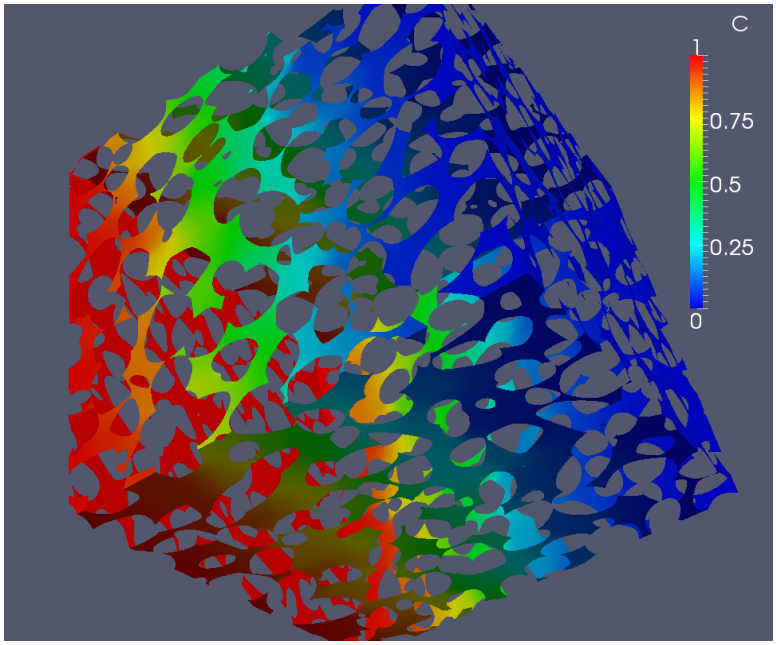

Figure: Contour plots of the solute concentration in the porous medium at one instant.

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17-19 June 2011

Automated Workflow for Spatially Resolved Fixed Bed Reactors with Spherical and Non-Spherical Particles

Nico JURTZ[1] , Thomas EPPINGER[1*]
[1] CD-adapco, 90411 Nürnberg, GERMANY

Corresponding author's e-mail: thomas.eppinger@cd-adapco.com

Keywords: DEM, Packed Beds, Chemical reactors, Process industries

ABSTRACT

Fixed bed reactors are widely used in the chemical and process industry amongst others for highly exothermic or endothermic catalytic surface reactions. Such reactors are characterized by a small tube to particle diameter ratio (D/d-ratio) to ensure a safe thermal management. For the design of such apparatuses the well-known correlations for packed bed reactors cannot be used, because these reactors are dominated by the influence of the confining wall, which affects the porosity and the velocity field and as a result also the species and temperature distribution within the bed.

For spatially resolved simulations of fixed bed reactors a randomly packed bed has to be generated and meshed. Special attention has to be paid on the mesh at the particle-particle and particle-wall contact points. We developed a method, which flattens the particles locally in the vicinity of the contact points and we could show, that this method does not affect significantly the bed properties and the fluid dynamics in terms of global bed porosity, radial porosity distribution and pressure drop.

Based on this published work we developed a workflow and a tool which allows an automated simulation: generation of a packed bed with DEM (discrete element method), meshing and solving the transport equations with a finite volume code. The whole workflow is done within the software package STAR-CCM+ by CD-adapco. The simulation time could be reduced significantly and depends on the number of particles (typically 1-2 days for 1500 particles).

Further we used the built-in DEM capability to generate random packings of non-spherical particles like cylinders and Raschig rings, which are more often used in the chemical industry, as a composition of spherical particles. For the meshing and the CFD calculation these approximated shapes are replaced by their original exact shape.

With the described workflow we have investigated spherical as well as non-spherical packings with a D/d-ratio between 2 and 10 and packing heights between 10d and 40d. The results are validated in terms of global bed porosity, radial porosity and velocity distribution and temperature profiles with experimental results from literature.

Based on these results the interplay between the flow field, the temperature, the species distribution and the chemical reaction in packed bed reactors can be investigated in detail.

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17-19 June 2011

A HYBRID NUMERICAL ALGORITHM FOR UNDERSTANDING FLOW IN FRACTURED ROCKS

Gerald G PEREIRA[1] , Vincent. LEMAILE[1] Paul W Cleary[1*]

[1] CSIRO Computational Informatics, Clayton, 3166, AUSTRALIA

Corresponding author's e-mail: Gerald.Pereira@csiro.au

Keywords: Multi-scale, meshless methods, fractures, oil and gas

ABSTRACT

In the dynamic process of fracture (e.g. hydraulic fracture or rock fracture for oil or gas recovery) the permeability of the rock changes as a function of shear stress. This is a complex, coupled dynamical process where the fracture affects the fluid flow, which ultimately determines the rock permeability. In this study we will address numerical modelling of this process from the continuum scale to the pore scale. Initially, we model the fracture of the rocks with a method capable of modelling large strains, which is the Smoothed Particle Hydrodynamics (SPH) method. This is done at the continuum (macro-scale) level and yields shear stresses throughout the medium. Given the stresses throughout the medium we can model the micro-scale re-arrangement of the individual grains through the Discrete Element Method (DEM). This not only gives the dilation in the material for the next strain rate calculation but also the capability to model micro-scale fluid flow and ultimately a permeability calculation using the Lattice Boltzmann (LB) method. The three numerical modelling techniques (SPH-DEM-LB) are combined into a hybrid multi-scale algorithm. We show how this model works on simple two-dimensional test cases and consider extension to more complicated systems.

10th International Conference on CFD in Oil & Gas, Metallurgical and Process Industries
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MODELLING THERMAL EFFECTS IN THE MOLTEN IRON BATH OF THE HISMELT REDUCTION VESSEL

Yuqing FENG[1], Peter J. WITT[1], and Mark P. DAVIS[2*]

[1] CSIRO Computational Informatics, Melbourne 3169, AUSTRALIA

[2] HIsmelt Corporation Pty Ltd, Kwinana 6966, AUSTRALIA

Corresponding author's e-mail: peter.witt@csiro.au

Keywords: CFD, Multiphase heat and mass transfer, Process metallurgy, HIsmelt process, Iron Making, Thermal Radiation.

ABSTRACT

Over a thirty year period the HIsmelt process has been developed as an alternative to the traditional blast furnace for the production of pig iron. This process involves the injection of fine iron ore and non-coking coal particles into a molten iron bath though a number of wall lances. These jets induce substantial mixing and splashing of molten droplets into the top space of the vessel due to the substantial volume of gas generated within the bath. Control of heat transfer, reactions and the complex multiphase fluid dynamics is critical to successful operation of the process. Since inception computational fluid dynamics has played an important role in scale-up and process optimisation (Davis and Dry, 2012).

A "Bath model" has been developed which focusses on the smelt-reduction processes occurring within the bath volume of the HIsmelt vessel (Stephens *et al.*, 2011). As this model is a transient multi-component Eulerian-Eulerian model with Lagrangian particle tracking for the coal and ore particles, it requires a substantial computational effort. For this reason (and due to the large thermal inertia of the liquid bath) earlier versions of the model have been isothermal.

Particles enter the molten iron bath at close to ambient temperature. Heating of both the particles and gas stream by the bath will require a finite time and cause local cooling around the particle jet. To investigate this effect the bath model has been extended to include convective heat transfer between the bath, gas and particles, and radiation within the gas cavity.

This paper reports on the incorporation of thermal effects into the model and presents results showing the impact of these on bath dynamics.

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10th International Conference on CFD in Oil & Gas, Metallurgical and Process Industries
SINTEF, Trondheim, Norway
17-19 June 2011

Design Optimization of Metal Tapping Room for Minimization of Dust Emission

Balram Panjwani[1], Bernd Wittgens[1], Stein Tore Johansen[1] and Benjamin Ravary[2]

[1] SINTEF Materials and Chemistry, 7465 Trondheim, NORWAY
[2] ERAMET NORWAY AS, 7037 Trondheim, NORWAY

Corresponding author's e-mail: balram.panjwani@sintef.no

Keywords: Tapping room, Dust, DPM, CFD

ABSTRACT

In the industrial tapping room, metal flows from the tapping hole through a Shute and poured into the ladles. Dust is formed in the ladles due to the oxidation of the metal, and this dust needs to be collected due to health and environment issue. In the tapping room, a suction system and air curtain are provided to capture the dust. The observed flow pattern and the accompanying dust distribution in the tapping area is unsteady and very complex, which hamper the process of dust collection. If the suction systems are not mounted at a proper location, the dust will be diluted with air and the capturing efficiency of the suction system is reduced considerably provided a given volume which can be extracted is constant. A main objective of the present study is to assess the effect of an installed air curtain and simultaneously investigate the proper location of a suction system in the tapping room of Eramet Sauda using a CFD-modelling approach. Initially, a 3D simulation of the tapping room has been performed to validate the existing system and verify that boundary conditions for the model are properly chosen and observed effects are modelled correctly. For validating the model, some visual experiments are performed. Simulation in 3D is computationally expensive, thus for parametric studies, a 2D simulation approach is proposed. The results from the 2D simulation is used for optimization of suction system location. Based on the 2D and 3D simulation approach, design of tapping room is suggested for achieving the maximum capturing of the dust.

VALIDATION OF CFD MODEL

The geometry of the tapping room is shown in Figure 1. As shown in Figure 1, there are two ladles in which metal is continuously poured through a Shute (not shown in the figure), when first ladle is completely filled with molten metal then the metal will overflow from the first ladle into the second ladle. Dust is generated inside the tapping room, due to the oxidation of metal, which will be collected by a suction system. Furthermore, an air curtain is also provided to prevent the dust going out from the tapping room. CFD model for the tapping operation is developed and is visually validated for three scenarios. In the first scenario, there was no tapping of the metal and the suction system was also switched off. In this scenario, only air curtain was switched on. In the second scenario, during a tapping operation, the air curtain was switched off, but a suction hood for collecting the dust was at full capacity (27 500 Nm^3/h). In the last case during the tapping operation: the air curtain, and the suction system for collecting the dust was in operation.

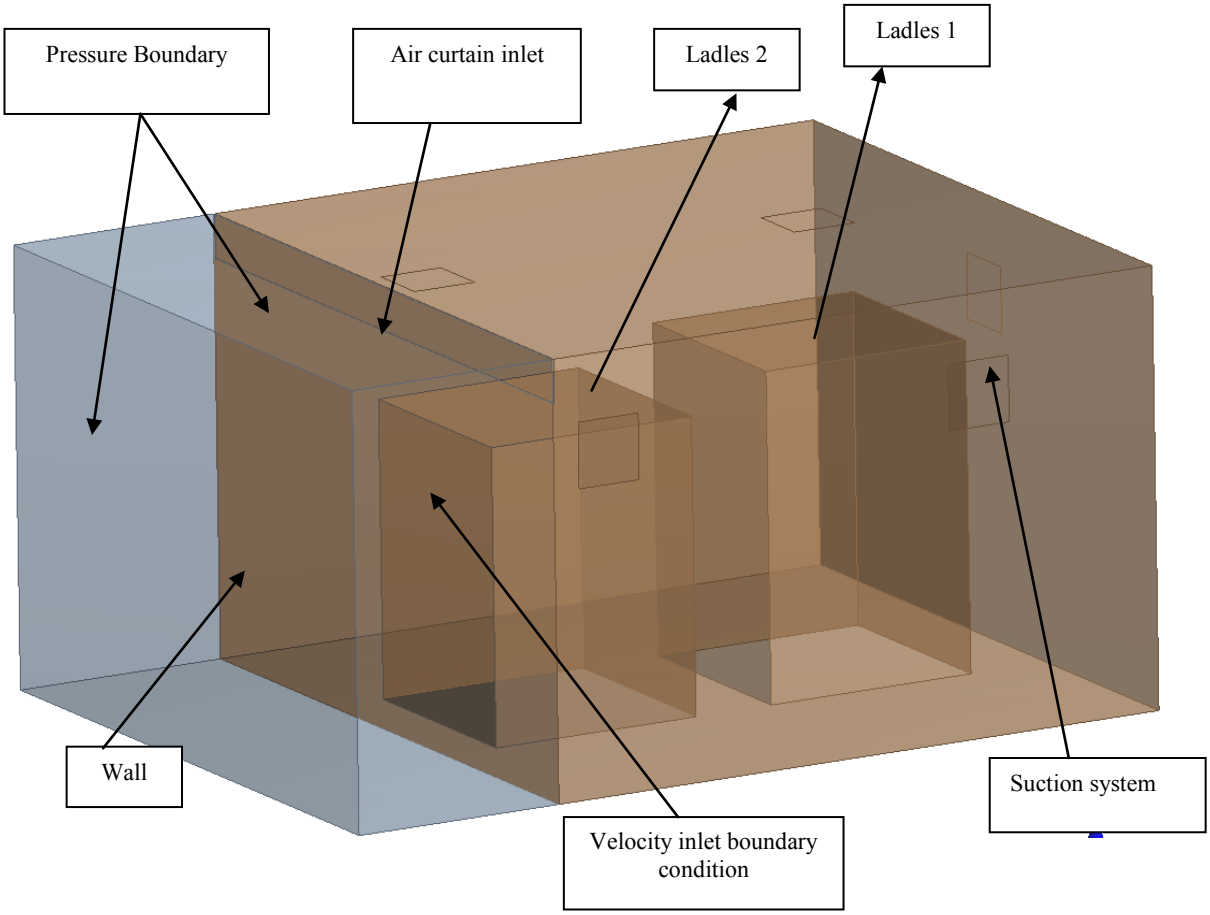

Figure 1 3D simplified tapping room along with the simplified surroundings

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CFD Simulation for Reactive Transport in Copper Heap Leaching

Liping CAI[1,2], Peyman MOSTAGHIMI[1,2], Gerard J. GORMAN[2], Stephen J. Neethling[1,2*]

[1] Rio Tinto Centre for Advanced Mineral Recovery, Department of Earth Science and Engineering, Imperial College London, London SW7 2AZ, UNITED KINGDOM

[2] Applied Modelling and Computation Group, Department of Earth Science and Engineering, Imperial College London, SW7 2AZ, UNITED KINGDOM

Corresponding author's e-mail: s.neethling@imperial.ac.uk

Keywords: Heap Leaching, Reactive Transport

ABSTRACT

Heap leaching is a hydrometallurgical approach which is used to extract a wide range of metals from ore. The aim of the work presented in this paper is the development of a CFD framework for the simulation of these complex systems. While a general framework is being developed, the specific implementation presented in this work is for a copper sulphide system. Predicting the behaviour of the fluid and chemical species inside heaps, involves understanding and modelling of the multiphase flow as well as the many coupled physico-chemical phenomena that occur within these systems, including mass transfer, heat transfer and chemical reaction.

A new multiphase fluid flow model has been implemented based on experimental work and particle scale simulations. This model accounts for the hysteresis observed in these systems. The model is solved implicitly for pressure and explicitly for saturation. Unlike most existing heap leaching models, this simulator has 2 way coupling between the gas and liquid. Mass and heat transport are solved using a mobile-immobile model, which, when compared to experiments, more accurately models the transport behaviour than the traditional advection-dispersion models.

A number of different chemical reactions are modelled, with 2 way coupling to the mass and heat transfer models. These reactions include chalcopyrite and pyrite dissolution, ferrous oxidation and precipitation reactions. In the reaction modelling both surface reaction rates and mass transfer limitations are considered.

The heap leaching models have been implemented within the Fluidity framework, which has allowed transient simulations to be carried out in up to 3D. A major advantage of using Fluidity is that it includes dynamic remeshing. This is important in heap leaching where small scale effects associated with, for instance, the initial wetting and final drying of the heap need to be resolved, but where efficient long term simulation is also required. The simulations are based on the control volume finite element method (CVFEM) which has the advantage over conventional FEM methods of being conservative, which is important when fluid flow, mass transport and heat transfer are strongly coupled.

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DESIGN AND IMPROVEMENT OF AN INDUSTRIAL AIRLIFT REACTOR USING COMPUTATIONAL FLUID DYNAMICS

Tao Song[1, 2], Kaixi Jiang[2], Junwu Zhou[2], Deyu Wang[3], Ning Xu[2], Yuqing Feng[4]

[1] School of Materials and Metallurgy, Northeastern University, Shenyang 110819, CHINA

[2] BGRIMM, Beijing General Research Institute of Mining and Metallurgy, 100160 Beijing, CHINA

[3] Shandong Gold Group, 250100 Jinan, CHINA

[4] CSIRO Computational Informatics, Clayton VIC 3168, AUSTRALIA

Corresponding author's e-mail: songtao@bgrimm.com

Keywords: Gas liquid flow; Airlift reactor; Air inlet design; CFD simulation

ABSTRACT

The airlift reactor performance in cyanide leaching relies on the good mixing between solid particles and reagents. As the increase of tank sizes, the design of efficient large scale reactors turns to be difficult. An Eulerian multi-fluid model with extra user defined subroutines has been developed and validated to provide insights into a big size airlift reactor used in gold leach plants. The CFD model enables the efficiency of the functions of several main design and/or operating parameters to be investigated, including gas inlet and circulating tube designs. Under a wide range of reactor designs and process conditions, the circulation velocities, gas hold-up in the tank and bubble residence time distribution were simulated and compared. In particular, a patented BGRIMM designed air nozzle which can produce high speed gas jet flow was evaluated in the industrial airlift reactor. CFD simulations demonstrated a better performance than the original reactor design. Some new reactor setups have been applied in a full-scale airlift reactor at a Shandong Gold Group leach plant in Laizhou China. Several operational factors make the application complicated, but the new designs still bring improvements in slurry circulation and bubble distribution.

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A CRITICAL COMPARISON OF SURFACE TENSION MODELS FOR THE VOLUME OF FLUID METHOD

Maike W. BALTUSSEN[1] , J.A.M. KUIPERS[1], Niels G. DEEN[1]

[1] Eindhoven University of Technology, Postbus 513, 5600 MB Eindhoven, THE NETHERLANDS

Corresponding author's e-mail: N.G.Deen@tue.nl

Keywords: Bubble and droplet dynamics, multi-scale modelling, direct numerical simulations, volume of fluid.

ABSTRACT

In many industrial practices, interactions of two immiscible fluids are frequently encountered. These interactions are often studied using a multi-scale modelling approach. In this approach, the largest scale models are used to simulate full-size industrial equipment, but these models need closure relations for the bubble-bubble and bubble-liquid interactions, which can be obtained by smaller scale models. The smallest scale model is Direct Numerical Simulations (DNS). In DNS models, the Navier-Stokes equations are solved on a sufficiently refined computational grid to capture the small scale flow features. In this work, we focus on the improvement on one of these smallest scale models: the model based on Volume of Fluid method (VOF). (van Sint Annaland et al., 2005)

The VOF model tracks the interface between the two-immiscible surfaces using a color function. Although the use of the color function ensures mass conservation, the use of the color function also poses a challenge with respect to the calculation of the surface properties, due to the reconstruction of the interface. In this work, three different surface tension models for the VOF model are tested: the Continuum Surface Force (CSF) model (Brackbill et al., 1992), the height function model (Gerrits, 2001) and the novel tensile force method inspired by the approach adopted in Front Tracking (FT) (Tryggvason et al., 2001, Baltussen et al, under review).

To select the best surface tension method, the models are compared in verification simulations and single bubble simulations. The performed verification tests (stationary bubble test, standard advection test and oscillating bubble test) show that the height function model and the novel tensile force method are an improvement on the generally used CSF model.

Although these verification test are very useful to determine the numerical implementation of the model, the real test for these models is the comparison with experimental data for single bubbles from the Grace diagram (Grace, 1976). The simulation results show that the height function model performs best for small bubbles ($Eo < 1$). The tensile force method works best for large bubbles ($Eo > 10$). For large bubbles, the curvature estimation in the height function model uses a stencil of 3 grid cells in the direction normal to the surface. This results in problems with the curvature calculation for highly deformed bubbles, which have a distance between two interface in the direction of the normal less than 4 grid cells. For the Eötvös region between 1 and 10, both surface tension models perform equally well.

The Morton number only has a small effect on the ranges in which the surface tension models are applicable. For very low Morton numbers ($\log Mo \leq -7$) , the ranges for both surface tension models change slightly (the height function model can be used for $Eo \leq 2$, while the tensile force method can be used when $Eo \geq 2$). While at very high Morton numbers, the height function model can also be used for bubbles with $Eo \geq 10$.

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SAMPLE RESULTS

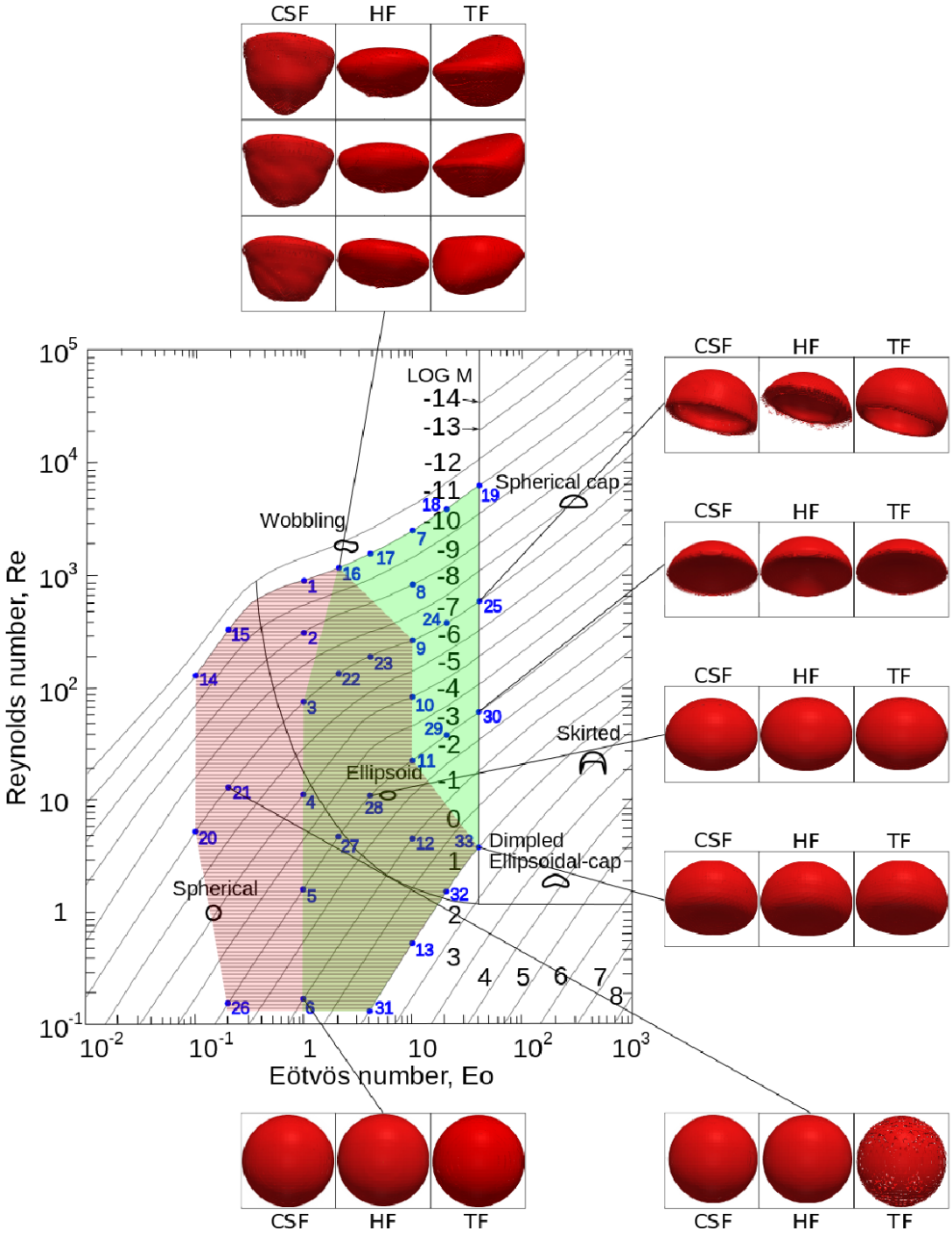

Figure 1: The performed single bubble simulations for several physical properties and bubble sizes. The figure shows the shapes of 7 bubbles for all the used surface tension models (Continuum Surface Force method: CSF, height function model: HF and the new tensile force method: TF). Furthermore the striped red area, the results using the height function model are within 10 % or the best performing model. While the tensile force method is within an 10 % accuracy or the best performing model in the filled green area.

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Numerical simulation of the influence of bubble bursting on a molten iron surface

Yonggui XU*, Mikael ERSSON, Pär G. JÖNSSON
Division of Applied Process Metallurgy, Royal Institute of Technology
(KTH), Brinellvägen 23, SE-100 44 Stockholm, Sweden

Corresponding author's e-mail: yonggui@kth.se

Keywords: CFD, VOF, bubble bursting, surface, molten iron

ABSTRACT

The transport of an argon bubble through a molten iron bath and across its free surface was investigated by CFD simulations. The Volume-of-Fluid (VOF) model was used to track the interface between argon and liquid iron as well as the free surface of the liquid iron. The bubbling dynamic inside the liquid phase was studied in terms of the bubble's terminal velocity and shape. For a bubble with a specific size, two groups of small metal droplets can be formed due to the bubble bursting on the liquid iron free surface. One group is the "film droplets" which are caused by the rupture of the liquid film when a bubble comes to rest and protrudes at the liquid surface. Another group "jet droplets", is due to the collapse of the remains after the bursting of a bubble cap. Simulations of both droplet types were qualitatively compared to experimental data and the agreement was found to be good. The influences of bubble size and liquid surface tension on the droplets were investigated systematically.

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AN ENHANCED FRONT TRACKING METHOD FEATURING VOLUME CONSERVATIVE REMESHING AND MASS TRANSFER

Ivo ROGHAIR[1], Martin VAN SINT ANNALAND[1], J.A.M. Kuipers[2*]

[1] Chemical Process Intensification and [2] Multi-scale Modelling of Multiphase Flows, Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, The Netherlands

Corresponding author's e-mail: i.roghair@tue.nl

Keywords:

- Bubble and droplet dynamics
- Multiphase heat and mass transfer

ABSTRACT

A chemical species transport model is developed and coupled to an improved Front-Tracking model, enabling dynamic simulation of gas-liquid mass transfer processes in dense bubbly flows.
Front-Tracking (FT) (Unverdi and Tryggvason (1992)) is a multiphase computational fluid dynamics technique where the location of a fluid-fluid interface is tracked via the advection of interface marker points, which make up a triangular mesh. A common drawback of FT implementations is that the volume enclosed by a mesh is not conservative during transient simulations. A remeshing technique is adopted to counteract these volume defects while keeping all physical undulations unharmed. The new remeshing procedures have been verified by comparison with results from the literature.
The model is used for a variety of hydrodynamic studies. In particular, the model is very suited to simulate (dense) bubbly flows due to the absence of artificial coalescence. A number of results, such as a closure of the drag force for bubbles rising in a bubble swarm (Roghair et al. (2011a), bubble-induced turbulent energy spectra (Roghair et al. (2011b)) and bubble-clustering (Tagawa et al. (2013)) will be outlined.
Species transport is modelled by a convection-diffusion equation which is discretized on a Eulerian grid, superimposed and possibly refined with respect to the grid used for the solution of the fluid flow equations. The velocity components have been interpolated to the refined grid using a higher-order solenoidal method. Enforcement of the Dirichlet condition for the concentration at the gas-liquid interface is achieved with an immersed boundary method, enabling the description of gas to liquid mass transfer. Careful validation of the newly implemented model, using synthetic benchmarks (exact solutions) and a comparison with correlations from the literature, has shown satisfactory results.
The liquid side mass transfer coefficient in dense bubble swarms, with gas fractions between 4% and 40%, has been investigated using the new model. The simulations have been performed in a 3D domain with periodic boundaries, mimicking an infinite swarm of bubbles. To prevent the liquid phase to become saturated with chemical species (with the consequence of a vanishing chemical species flux due to saturation of the liquid bulk), simulations have been performed using either artificial fresh liquid inflow, or a first order chemical reaction in the liquid phase. The results indicate that the liquid-side mass transfer coefficient rises slightly with increasing gas fraction. It has been shown that it is important to take mass transfer limitations into account when interpreting the simulation results.

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SAMPLE RESULTS

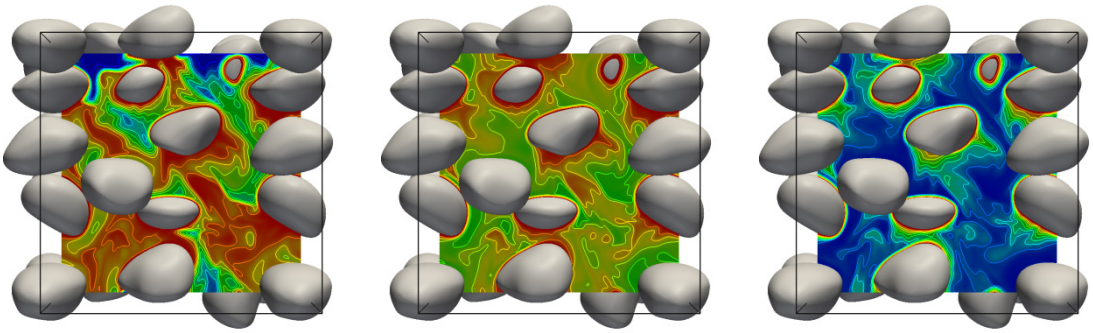

Figure 1: Mass transfer in a dense bubble swarm (30% void fraction) using different techniques to prevent species saturation in the liquid. From left to right: clean (zero-concentration) liquid inflow via top and bottom, slow chemical reaction and fast chemical reaction.

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A NUMERICAL STUDY OF DEFORMATION AND BREAKUP OF DROPS IN TURBULENT FLOWS

Benjamin LALANNE[1], Sébastien TANGUY[2], Jiří VEJRAZKA[3], Olivier MASBERNAT[1], Frédéric RISSO[2]

[1] Laboratoire de Génie Chimique, TOULOUSE

[2] Institut de Mécanique des Fluides de TOULOUSE

[3] Institute of Chemical Process Fundamentals, PRAGUE

Corresponding author's e-mail: Benjamin.Lalanne@ensiacet.fr

Keywords: Bubble and droplet dynamics, DNS, breakup modelling, turbulent flows, surfactants.

ABSTRACT

Modelling drop and bubble break-up in turbulent flows is an important issue in many industrial processes such as crude oil recovery or emulsification processes. Population balance models are often used to predict the size distribution of drops in turbulent flows, but such models do not account for the interface dynamics. The deformation of a drop is caused by continuous interactions with turbulent vortices; the drop responds to these interactions by performing shape-oscillations and breaks up when its deformation is critical[1]. Interfacial dynamics can be described by the theory of Miller and Scriven[2], but only under restrictive conditions, i.e. without considering the effect of gravity, without adsorbed surfactants and in cases of low deformation.

The purpose of this study is to extend this theory to situations of practical interest, based on experiments and direct numerical simulations. A numerical tool that solves the Navier-Stokes equations and tracks the interface with Level-Set and Ghost Fluid methods, is used for the simulation of drop deformation in flows.

First, we study numerically the shape-oscillations of rising clean drops[3] in a stagnant liquid. We prove that the rising motion increases strongly the damping rate of the shape-oscillations and we show that this is due to an increase of the dissipation in boundary layers near to the interface. Secondly, we consider experiments of the shape-oscillations of rising contaminated drops[4] and show that the presence of surfactants leads to a higher increase of the damping of the oscillations than that induced by gravity. Finally, we simulate the interaction between a rising clean bubble and an intense vortex, which involves a strong deformation of the bubble. The fast relaxation of its deformation proves that the bubble behaves as an overdamped oscillator in this case.

These elementary studies are necessary to accurately characterize the interface dynamics (characteristic times of eigenmodes of oscillation). Once this step is achieved, we present the ability of our approach to predict the breakup frequency of drops in turbulent flows[5] and the daughter drop size distributions, by comparison with experimental results.

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SAMPLE RESULTS

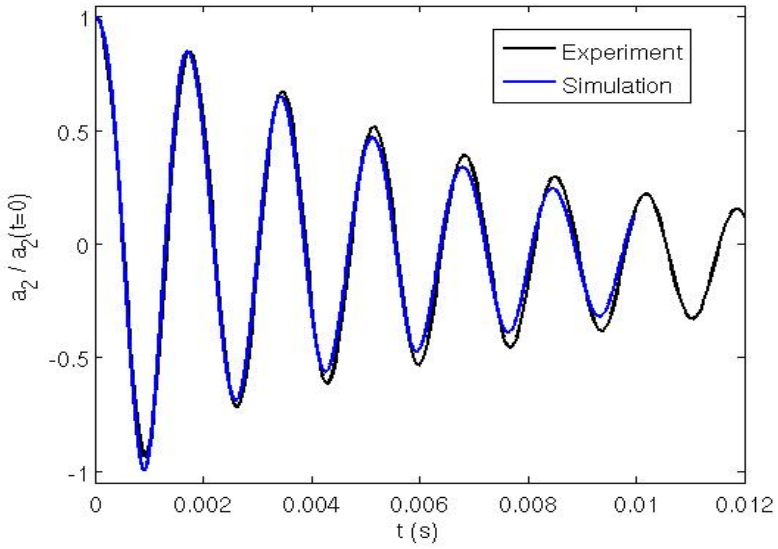

Figure 1: Interfacial dynamics: numerical and experimental evolution of the amplitude of oscillation of a drop.

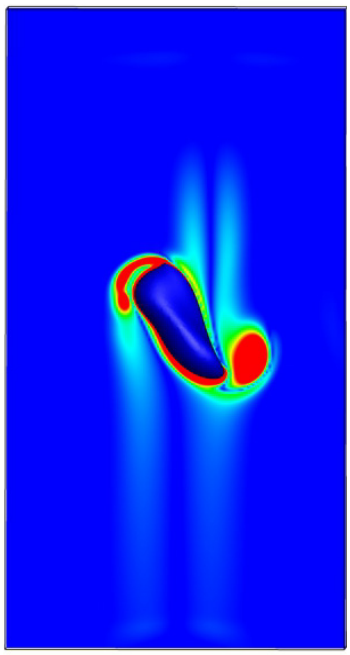

Figure 2: Simulation of the interaction between a rising bubble and an intense vortex (color represents vorticity).

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The parametric sensitivity of fluidized bed reactor simulations carried out in different flow regimes

Schalk CLOETE*, Jan H. CLOETE, Stein Tore JOHANSEN & Shahriar AMINI
[1] SINTEF Materials and Chemistry, 7465 Trondheim, NORWAY

* E-mail: schalk.cloete@sintef.no

Keywords: Fluidized bed reactors, Two Fluid Model, Kinetic Theory of Granular Flows, Specularity coefficient, Restitution coefficient.

ABSTRACT

Fluidized bed simulations carried out within the Kinetic Theory of Granular Flows framework utilize a number of model coefficients which are highly case dependent and difficult to determine accurately. The most important of these are the specularity coefficient (the degree of friction at the wall) and the particle-particle restitution coefficient (inelasticity of inter-particle collisions). This paper demonstrated that modification of these coefficients can trigger a regime change in very narrow and fast risers, thereby introducing a great amount of uncertainty. For situations sufficiently far from the dilute transport regime, however, sudden regime changes are not observed and the influence of these unknown parameters is more systematic. In the case of wide bubbling beds, the effect of these unknown model coefficients can become completely negligible, making these reactors highly attractive for simulation studies. Faster and narrower geometries, on the other hand, exhibit greater sensitivity to changes in the specularity coefficient and particle-particle restitution coefficient, thereby introducing ever-increasing quantities of uncertainty stemming from these unknown model coefficients.

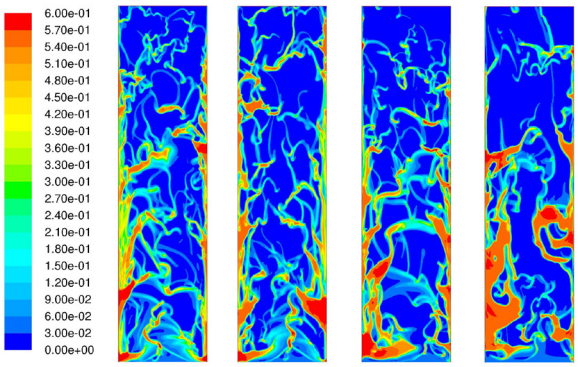

Figure 1: Instantaneous volume fraction profiles for the case with a fluidization velocity of 2.26 m/s. From left to right the specularity coefficients used are: 0.0001, 0,001, 0.01 and 0.1.

SAMPLE RESULTS

The potentially very large effect of the wall interaction settings is demonstrated via a narrow riser used to study CO_2 absorption in **Figure 1**. It can be seen that changes in the wall friction and particle wall restitution can completely alter the hydrodynamic and reactive behaviour of the reactor.

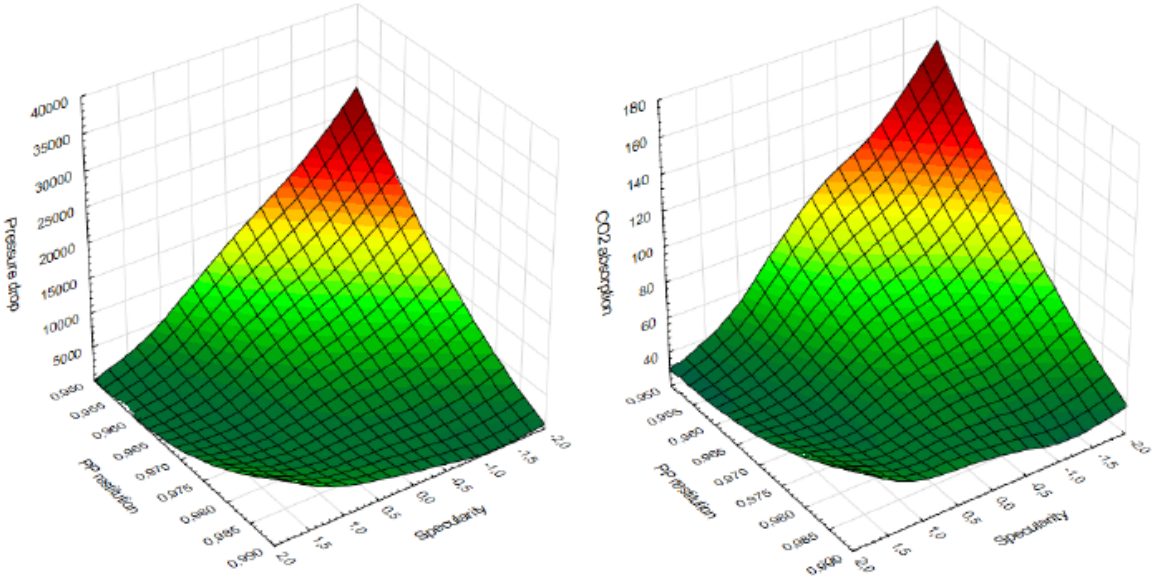

Figure 1: Effect of particle-particle restitution coefficient (PP restitution) and the specularity coefficient (friction) on the hydrodynamics (quantified via pressure drop) and the reactor performance (quantified via CO_2 absorption).

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Bed Expansion and Pressure Drop in a Bubbling Fluidized Bed

Kevin MANDICH* **, Robert CATTOLICA**
Department of Mechanical and Aerospace Engineering
University of California San Diego
9500 Gilman Drive, La Jolla, CA 92093
UNITED STATES

Corresponding author's e-mail: kevinmandich@gmail.com

Keywords: Experimental validation studies, Fluidized/packed beds

ABSTRACT

An experimental study of the bed expansion, pressure drop, and near-wall granular temperature in a lab-scale, gas-fluidized bed was conducted and the results compared with a computational fluid dynamics simulation. Bed expansion, pressure drop, and granular temperature were measured using a video recorder, pressure transducers, and acoustic shot noise via a wall-mounted accelerometer, respectively. These quantities were determined experimentally for particles of three different sizes and densities – 123 micros, 2.52 SG; 334 microns, 2.7 SG; 430 microns, 3.56 SG – all belonging to the Geldart B group classification. The fluid dynamics simulations were carried out using the Barracuda multiphase particle-in-cell computational method. The desired quantities were determined by performing an analysis on the relevant variables at each time step in the simulation. A parametric study with the computational simulation investigated the effect of changing the particle-particle restitution coefficient, particle-wall restitution coefficient, amount of slip allowed at the wall, and drag law.

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SAMPLE RESULTS

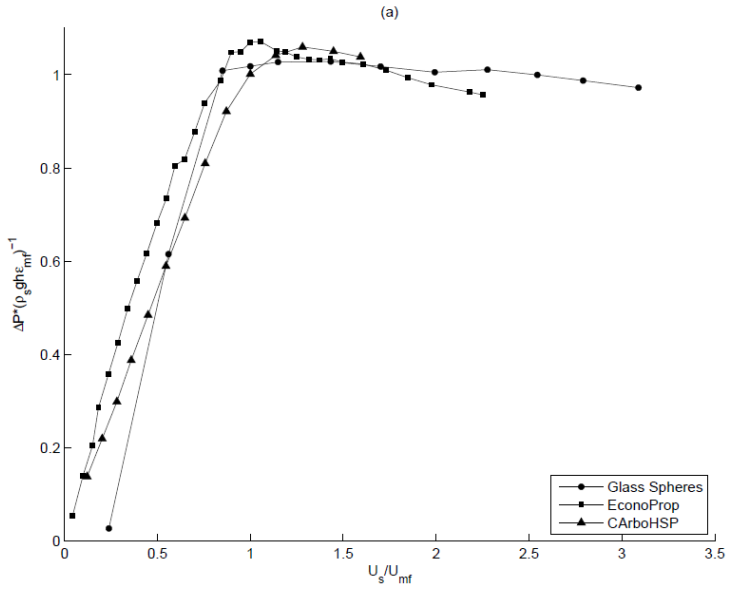

Figure 1: Experimentally-determined pressure drop, normalized by weight of the bed, vs. superficial gas velocity normalized by minimum fluidization velocity.

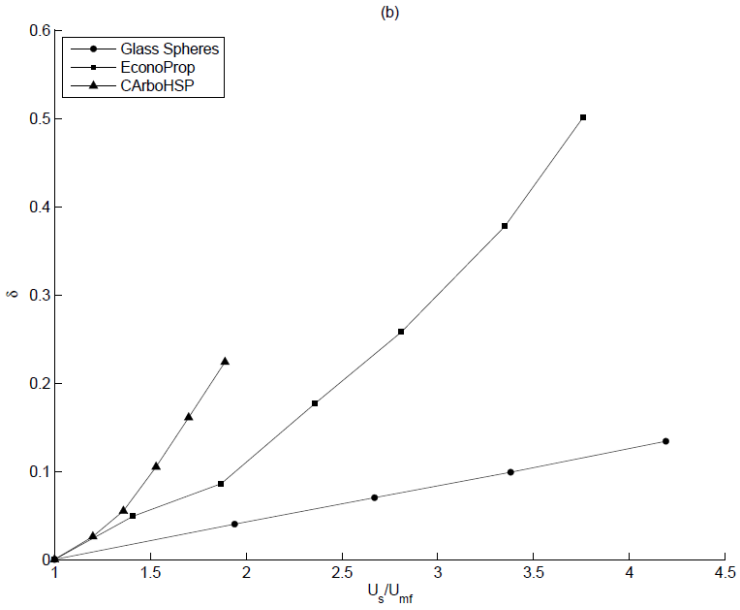

Figure 2: Proportional of bed height expansion from rest vs. superficial gas velocity normalized by minimum fluidization velocity.

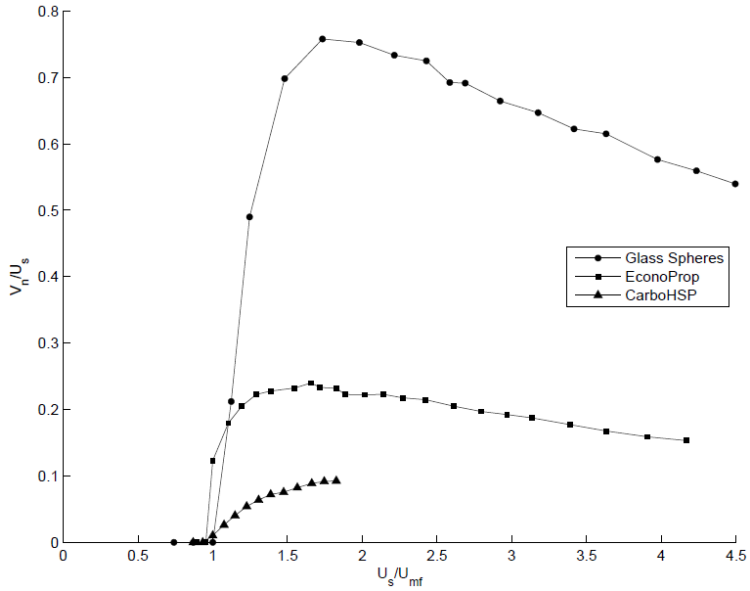

Figure 3: Experimentally-determined particle velocity normal to the wall, normalized by superficial gas velocity, vs. superficial gas velocity normalized by the minimum fluidization velocity.

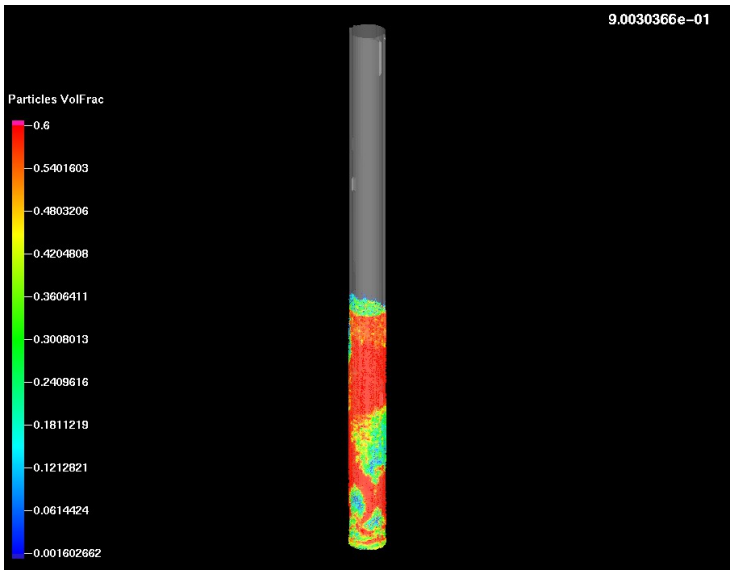

Figure 4: Snapshot of a simulation showing particles colored by local volume fraction.

In figure 2, the bed expansion is defined by:

$$\delta = \frac{h - \overline{h}}{\overline{h}} \tag{1}$$

Here, h is the bed height and $\overline{h}$ is the bed height at minimum fluidization.

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VALIDATION OF A 3D CYLINDRICAL CFD MODEL FOR GAS-SOLID FLUIDIZED BEDS

Vikrant Verma, Johan T. Padding*, Niels G. Deen, J.A.M. Kuipers
Eindhoven University of Technology; Dept. of Chemical Engineering and Chemistry
PO Box 513, 5600MB Eindhoven, The Netherlands

*T: 31-40-247-3674; F: 31-40-247-5833; E: J.T.Padding@tue.nl

Keywords: Fluidized bed, Two-fluid model, CFD validation

ABSTRACT

Gas-solid fluidized beds (FBs) are extensively used in process industries because of their impressive capabilities as a reactor, mixer and possibility of continuous operation. Understanding the dynamics of FBs is a key issue in improving efficiency and rational scale-up to a commercial scale. Traditionally two-dimensional (2D) or pseudo 2D CFD simulations are used to study the hydrodynamics of FBs on larger scales. Numerical integration on a very small time-step and for a longer period of time is still a challenge for full three dimensional (3D) fluidized beds, due to the high computational cost. With new developments in numerical methods and increasing computational power, large-scale 3D simulations are now attainable. However, validation of the computational models is highly necessary, specifically for 3D geometries. Experimental studies of 3D fluidized beds available in the literature provide details of bubble and solid flow characteristics at various operating conditions, and can be used to validate 3D numerical models. In this work we use an efficient two-fluid model (TFM) using Kinetic Theory of Granular Flow (Verma et al. 2013) to perform 3D simulations using a cylindrical mesh. Quantitative comparisons of simulation with experimental results are performed. Our study shows that CFD can predict the bubble and particle flow characteristics in close agreement with experimental observations. The bubble size distribution shows that smaller bubbles are located in the bottom section of the bed and significantly larger bubbles and fewer smaller bubbles in the top section of the bed. The porosity distribution plot reveals the gas-extraction process, where the emulsion phase is getting denser from bottom to top due to presence of large bubbles in the top section of the bed. All these observations are in agreement with the two-phase theory of fluidization. The particle circulation patterns are in fair agreement with the experimental work of Laverman et al. 2012. The time-averaged particle velocities at different heights in the bed are comparable with experimental results, with small differences near the wall and in the bottom section of the bed. This shows that improved wall boundary conditions may be required for some particle characteristics. The equivalent bubble size obtained from simulations shows a fair agreement with X-ray tomographic measurements and with correlations of Darton et al. 1977 and Werther 1975. The bubble rise velocity predicted from simulations shows close agreement with experimental results. The Hilligardt and Werther 1986 correlation can accurately predict bubble rise velocity for nearly ideal particles, such as glass, but deviates significantly for inelastic particles. When comparing fluidization at high pressure, the simulations show agreement with the experimental work of Godlieb et al. 2012, where the bubble size decreases with increase in pressure. Homogeneous fluidization takes place at very high pressures. Overall, this work shows that TFM can successfully predict the flow behaviour of a 3D gas-solids fluidized bed under different operating conditions. We also find that for more dissipative particles TFM requires more detailed stress closures to predict different regimes of fluidized bed, taking into account particle sliding and rotation friction.

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SAMPLE RESULTS

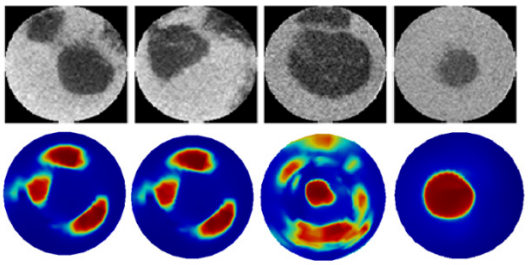

Figure 1: Bubble shape in the horizontal cross section plane: (top) X-ray imaging, (bottom) TFM simulations.

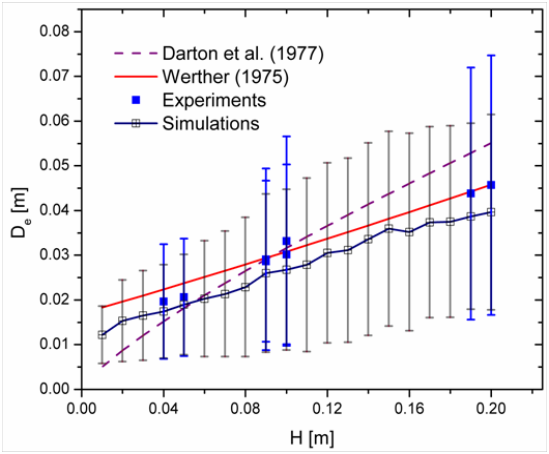

Figure 2: Equivalent bubble size as a function of height from the bottom. Comparing simulations with experiments and literature correlations.

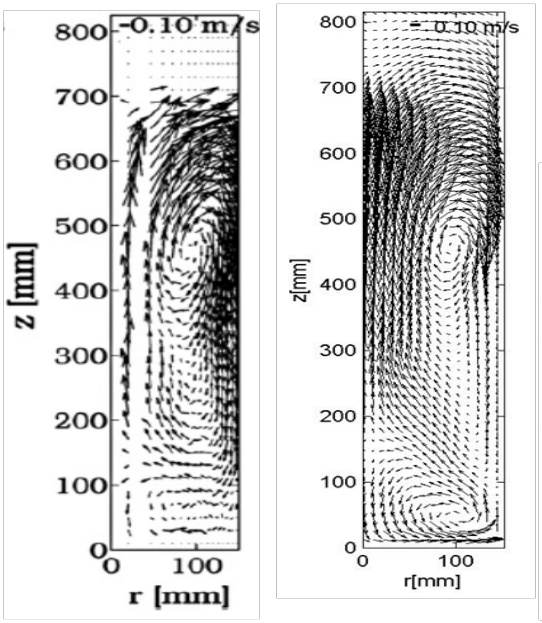

Figure 3: Azimuthally and time-averaged solids circulation patterns, (left) experiment Laverman et al. 2012 (right) TFM simulation.

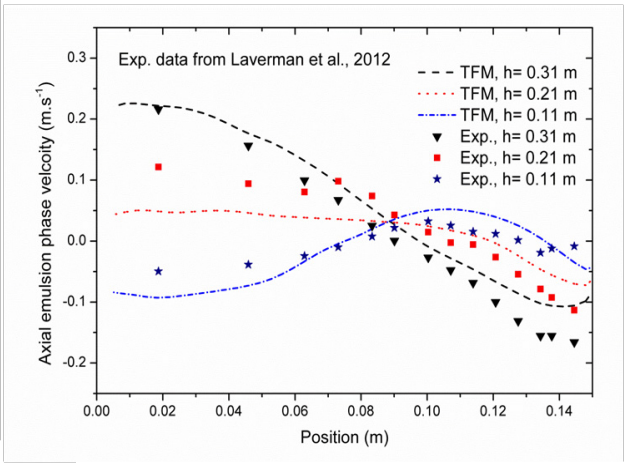

Figure 4: TFM simulations and experimental comparison of the azimuthally and time-averaged lateral profile of solids axial velocity at three different heights above the distributor.

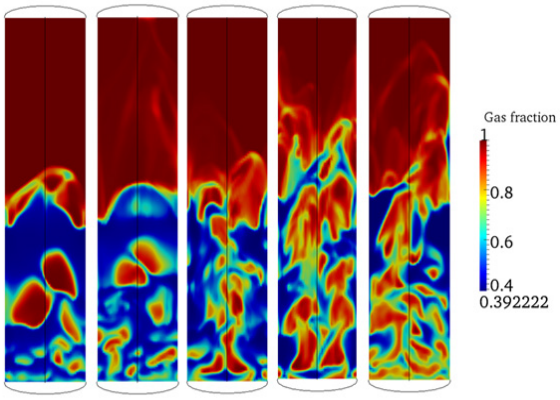

Figure 5: Arbitrarily selected instantaneous porosity plots at operating pressure of 2, 4, 8, 16 and 20 bars (from left to right).

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PROCEDURAL METHOD FOR SIMULATING AN INDUSTRIAL UREA GRANULATION PROCESS

Philipp LAU[1], Matthias POTTHOFF[2], Matthias KIND[1]

[1] Department of Thermal Process Engineering, KIT, 76131 Karlsruhe, GERMANY

[2] Uhde Fertilizer Technology B.V., 6042 NW Roermond, THE NETHERLANDSY

Corresponding author's e-mail: matthias.kind@kit.edu

Keywords: Fluidized/packed beds, Granular flow, Multiphase heat and mass transfer, Process industries, Stirred tanks

ABSTRACT

The process of fluidized bed spray granulation unites the steps of solid creation and solid formulation in one apparatus and is used for the continuous industrial urea granulation process.
In this connection the granulator is build up by connecting several granulation chambers in series using dividing walls and many nozzles in each chamber.
Thereby the hot urea melt is atomized with nozzles and sprayed into the fluidized bed which contains granulate particles of the same material. The droplets deposit on the particles near the spray zone and form a film which solidifies to a crystalline layer in the cold fluidization air. Step by step a raspberry-like product is formed. Besides drop deposition there are two more important mechanisms which influence the particle growth. On the one hand attrition due to particle-particle collisions and on the other hand dust integration on wet surfaces.

The tailored product size distribution can be obtained by a downstream Screening-Crushing process. Granules larger than the desired product size are crushed in a mill and fed back to the granulator together with small particles.

The aim of this development is to minimize the recirculation of particles behind the screen deck. Therefore it is necessary to get information about the growth and attrition rates of the granules to solve the population balance equation to calculate the development of the particle size distribution during the process. Hence, a 3d-multiphase model is developed to extract information which are not available in experimental research, e.g. particle exchange streams, particle size dependent growth rates and particle residence time. Due to the large number of nozzles and the large dimension of such a device, a granulator cannot be described completely using a numerical simulation tool.

Using Two-Fluid Model (TFM) and two periodic boundary conditions the fluid dynamics, granulation mechanisms (implemented with user-defined functions) and energy equations are solved in a representative domain in each chamber. The interactions between particles and air can be described with the model of Gidaspow (1994). The particle-particle momentum exchanges are modeled with the equations of Syamlal and O'Brien (1987). Obtaining important information of CFD simulation and coupling the granulation chambers with exchange streams, finally the population balance can be solved.
In this research a 3d-multiphase model is developed to generate growth and attrition rates of the granules to calculate the particle size distribution in the large-scale granulator. With this information it is possible to optimize process parameters and minimize recirculation.

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COOL DOWN SIMULATIONS OF SUBSEA EQUIPMENT

Atle Jensen, Stig Grafsrønningen
FMC Flow Assurance and Operability, 1386 Asker, NORWAY

Corresponding author's e-mail: atle.jensen@fmcti.com

Keywords: Pragmatic industrial modelling, uncertainty quantification

ABSTRACT

In the subsea oil and gas industry, thermal insulation of equipment is often used as a method to slow down cooldown, and to facilitate shut-down procedures. Great effort is spent on predicting the thermal behaviour of hydrocarbon production systems in order to identify and prevent hydrate formation in the production fluid during normal production, and during planned or unplanned shut downs.

Subsea equipment generally cannot be fully insulated for different reasons; avoid overheating of electronic components, facilitate ROV access, clearance, and various other reasons. The uninsulated parts of the subsea equipment create cold-spots which may have a severe effect on the thermal performance. Detailed thermal analyses are required to assess the effect of these cold-spots and to make sure the equipment is adequately insulated. An increasingly larger fraction of the detailed thermal analyses within the subsea industry nowadays are conjugate heat transfer CFD simulations.

Engineering flows are generally turbulent and laminar flows are seldom encountered. One exception is natural convection, i.e. buoyancy driven flow. During cool down of subsea equipment laminar, transitional and turbulent flow may occur simultaneously within the same domain. RANS-turbulence models, which is the only feasible level of turbulence treatment in CFD for engineering purposes on full scale equipment, are developed for high Reynolds number flow and are generally unable to predict the correct solution if the actual flow is laminar or transitional.

CFD simulations are often used in the design process of the insulation on subsea equipment in the subsea industry. However, the accuracy and uncertainty of the simulations are seldom reported, nor are the results verified against experimental data. The use of mainstay engineering CFD approaches introduces an uncertainty due to the inadequacy of the RANS-models to capture laminar to turbulent transitions and relaminarizations.

An assessment of the effect of using turbulence models on such flow has been performed in order to shed some light on the uncertainty of thermal CFD cool down simulations.

This article presents results from conjugate heat transfer cool down CFD simulations with comparison against cool down tests with a particular focus on the effect of using RANS turbulence-models on a buoyant flow which is laminar, transitional, and turbulent, within a single fluid domain.

SAMPLE RESULTS

Figure 1 show results from a cool down test and accompanying CFD results of a geometry resembling subsea equipment. The figure shows the mean vertical velocity along a horizontal line in a vertical 143mm ID pipe which emulates a dead-leg in a subsea production system.
The experimental data shown in figure 1 is obtained using PIV. The CFD simulations were performed in CFX v14.5.

The flow in the vertical section is turbulent at the beginning of the cool down, but approaches a laminar state as the fluid inside the geometry cools down. CFD simulations both with and without turbulence models were performed too see if there were any significant differences in the results.

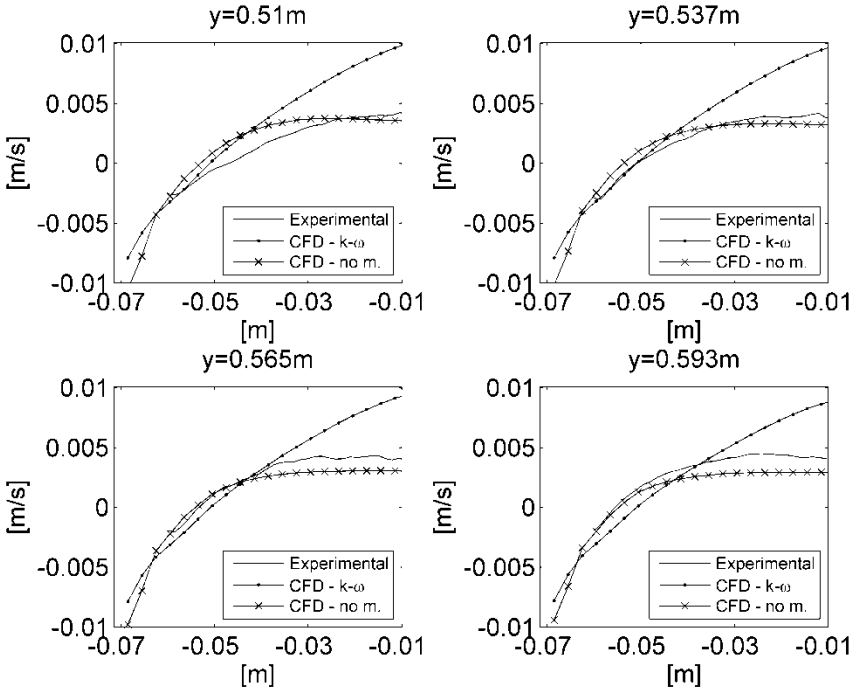

Figure 1: Vertical velocity in vertical pipe - 30 min cool down, comparison between experimental data and CFD simulations.

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Predicting emulsion pressure drop in pipes through CFD multiphase rheology models

Nathanael J. INKSON[1] , Jose PLASCENCIA[2] , Simon LO[1]

[1] CD-adapco , Trident House, Trident Park, Basil Hill Road, Didcot, OX11 7HJ, UK.

[2] GE Oil & Gas, Eyvind Lyches vei 10, 1338 Sandvika, Norway.

Corresponding author's e-mail: nathanael.inkson@cd-adapco.com

Keywords: Bubble and droplet dynamics, Rheology, Emulsion physics, Surfactants and interphases, Multiphase pipeline transport, Mixing, Oil & Gas.

ABSTRACT

A rheology model has been developed that fits shear stress and viscosity data of both suspensions and stabilized water in oil emulsions using a shear-thinning Generalized Newtonian model combined with a yield stress that blends the two limits of high and low strain-rate relative viscosity curves.

The rheology modelling shows that suspensions and emulsions share some similar physics, although the rate of shear-thinning and the development of yield stress are different.

Combining the relative viscosity models with the Morris and Boulay model of suspension stress in the context of Eulerian multiphase flow in a commercial CFD code: STAR-CCM+, it has been possible to quantitatively model the pressure drop of salt water in crude oil emulsions during pipe flow with minimal fitting. The Morris and Boulay model with negative normal stresses was required to correctly estimate the pressure drop, as models that use only shear relative viscosity overestimate the effect.Name of author(s) goes here: *Nordman and Xie*

10th International Conference on CFD in Oil & Gas, Metallurgical and Process Industries
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A transient CFD model for predicting reaction forces during safety valve blowdown in surface well testing

Barbara ZIELINSKA , Francis ALLOUCHE, Laurence FRASER, Naveed ZAFAR

Etudes et Productions Schlumberger
1, rue Becquerel, BP 202
92142 Clamart CEDEX, FRANCE

Corresponding author's e-mail: zielinska@slb.com

Keywords: Oil & Gas, Surface Well Testing, relief line, safety valves, gas blowdown, transient CFD

ABSTRACT

Pressure of gas arriving at rig surface must be carefully controlled by flow valves. Relief line and safety valves are mandatory on any pressure vessels (such as separators or surge tanks) used in surface well testing. They preserve the equipment integrity in case of overpressure due to unexpected events. Severe transient effects occur when the pressure safety valves open suddenly. These effects, which are typically very short in duration, produce substantial reaction forces and can tear off the line securing creating dramatic events. Reaction forces on pipes due to the fluid flow can be calculated using existing industry standards and recommendations. These standards express reaction force in terms of gas pressure, velocity and density which are not easy to predict. Moreover the transient effects due to reflection of shock fronts from piping elements like bends or cross section changes can modify the flow field.

Because of the high pressure and size of well testing installation there are relatively few full scale test data available. Also because of emergency nature of this equipment, field experience is scarce. Advances in modern computers allow routine use of Computational Fluid Dynamics methods to model transient flows. Here we present a transient CFD model for predicting forces acting on the conduit in case of sudden valve opening. Commercial software Fluent v.14 with density based solver and explicit time stepping is used. The model is axis symmetric and is validated with test data from shock tube classic experiment [1]. Furthermore the results are compared to relief valve experimental data presented in [2] and [3].

We apply this method to realistic relief line geometry and propose a method to calculate the reaction forces from CFD data. Furthermore we study the effect of design parameters (like the flow section opening angles, number of flow section changes, conduit diameter and length) on the induced forces.

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3. Muschelknautz S. and Wellenhofer A. (2003), "Flow Reaction Forces upon Blowdown of Safety Valves", Chem. Eng. Technol. vol. 26, p.7.

SAMPLE RESULTS

Figure 1 shows pressure shock advance in a sample relief line where a valve with 2.85" diameter suddenly opens to 6" and 10" flow line. The pressure ratio is 10 to 1 and the gas is methane.

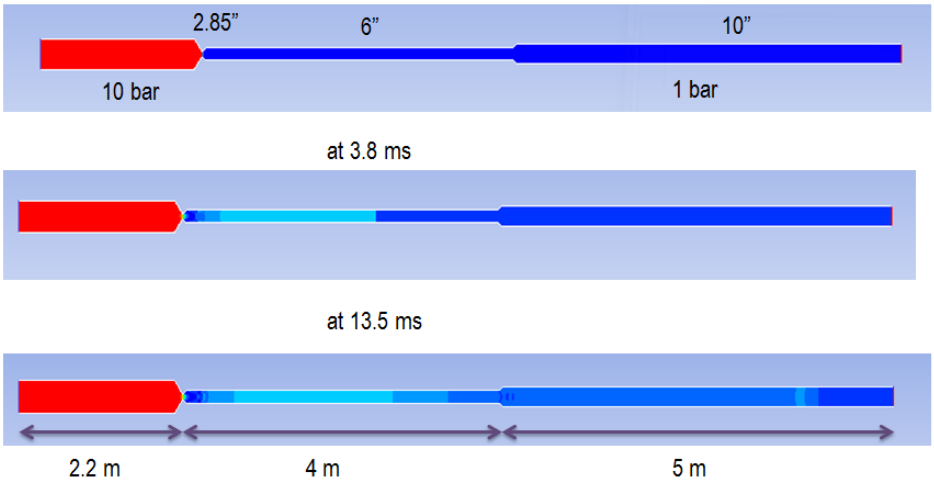

Figure 1: Pressure contours of a sample relief line function of time.

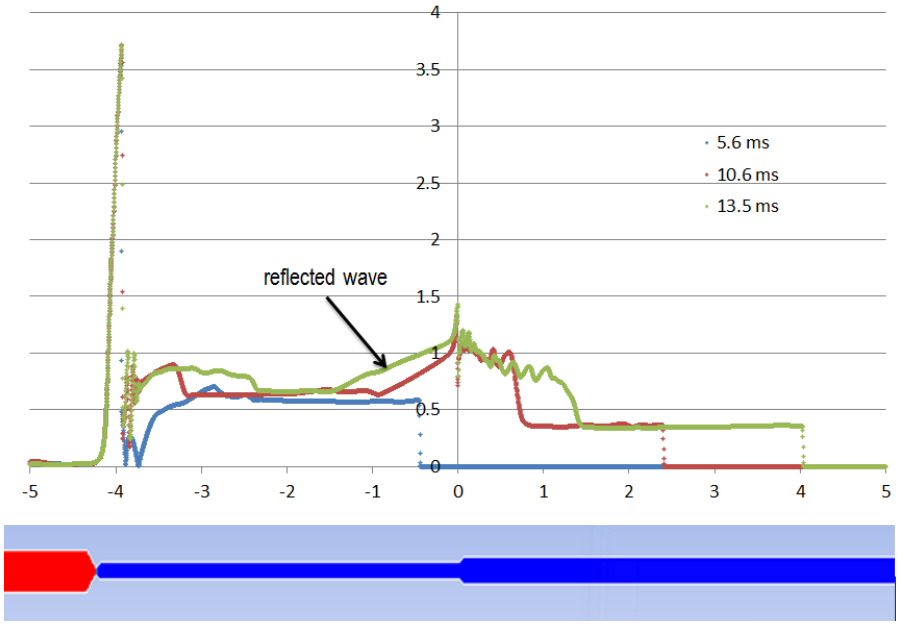

Figure 2. Mach number along the symmetry axis function of time

Figure 2 presents the Mach number along the symmetry axis for three time instants. Since the flow downstream of the initial shock wave is subsonic a reflected wave propagates back from the cross section perturbation.

The detailed knowledge of pressure, velocity, density and temperature fields in the relief line allows a precise calculation of reaction force as sum of pressure and momentum forces.

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ABSTRACT NO. (Will be filled in by organizer)

TOWARDS A MECHANISTIC MODEL FOR SUBCOOLED FLOW BOILING AT LOW-PRESSURE

Sara VAHAJI[1] , Sherman Chi Pok CHEUNG[1], Guan Heng YEOH[2,3], JiYuan TU[1*]

[1] School of Aerosapce, Mechanical and Manufacturing Engineering, RMIT University, Victoria 3083, Australia

[2] Australian Nuclear Science and Technology Organisation, Locked Bag 2001, Kirrawee DC, NSW 2232, Australia

[3] School of Mechanical and Manufacturing Engineering, UNSW, Sydney, NSW 2052, Australia

Corresponding author's e-mail: jiyuan.tu@rmitl.edu.au

Keywords: Multiphase heat and mass transfer; subcooled boiling flow; wall heat partitioning

ABSTRACT

For the modeling of subcooled flow boiling at low pressures in upward vertical channels, special consideration needs to be done on the dynamic behavior of two-phase flow and bubbles experiencing breakup, coalescence, and condensation in the bulk subcooled liquid as well as on the characterisation of the heat transfer occurring in the near-wall region. In terms of demonstrating the latter physics, several empirical models have been proposed for predicting the heat flux partitioning in subcooled flow boiling (Tu and Yeoh (2002)).

In this paper, a more mechanistic model is proposed for computing the active nucleation site density, bubble sliding and lift-off diameters, and bubble frequency and is implemented in the two-fluid model along with the population balance equation to solve governing equations. The first parameter is determined through the fractal hypothesis (Xiao and Yu (2007)) and the rest are calculated through the force balance model (Yeoh et al. (2008)). In this model, the additional heat flux at the heated wall caused by surface quenching of sliding bubbles is included. For the sake of better understanding and more comprehensive study, this model along with a set of selected empirical correlations is compared against experimental measurements of the axial and local distributions of void fraction and bubble Sauter mean diameter. The selected experiments (Zeitoun and Shoukri (1996); Lee et al. (2002)) cover a wide range of different inlet subcooling temperatures and heat and mass fluxes.

The results show that not one single combination of empirical correlations can acceptably predict all the assessed axial and local conditions. Also, the proposed mechanistic model clearly demonstrates the impact of subcooling temperature on the activation of the nucleation sites at the heated wall. The calculated wall superheat temperature is constantly under-estimated by the selected combinations of empirical correlations while predictions by the current model are in satisfying agreement with experiments. It has been found out that the bubble sliding along the heated wall has a high influence on heat partitioning and surface quenching during the process of subcooled flow boiling.

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ENABLING CFD CODES TO PERFORM SYSTEMATIC PARAMETER CONTINUATION AND STABILITY ANALYSIS FOR REALISTIC APPLICATIONS

N. Cheimarios [1], E.D. Koronaki[1*], H. Laux[2], A. G. Boudouvis[1]

[1] School of Chemical Engineering, National Technical University of Athens, 15780, GREECE
[2]OSRAM Opto Semiconductors GmbH, 493055, Regensburg, GERMANY

*E-mail: ekor@mail.ntua.gr

ABSTRACT

A computational framework is presented for enabling commercial, "black-box" Computational Fluid Dynamics codes to perform certain nonlinear analysis tasks that contribute significantly to the understanding of the studied physical problem. Among those tasks are parameter continuation along entire solution branches and stability analysis. The former, is important for the identification of ranges of operating parameters where multiple solutions exist. The stability of each solution is determined as a by-product of the method. When among the multiple solutions there are periodic orbits, the main idea is adjusted to compute the frequency and amplitude of the oscillation. The additional tasks do not require any alteration of the CFD model or intervention on the solver. The illustrative example here is that of a flow around a cylinder, where for varying Re numbers a branch of periodic solutions emanates from a branch of stationary ones. Stable and unstable, stationary and periodic states are computed for the same parameter values.

Keywords: Nonlinear phenomena, CFD software, solution multiplicity, periodic solutions

NOMENCLATURE

Greek Symbols

ρ	Mass density, [kg/m^3].
ν	Kinematic viscosity, [m^2/s].
λ	physical parameter
$\boldsymbol{\varphi}$	function of initial value, period T

Latin Symbols

r	Cylinder radius [m]
d	Cylinder diameter [m]
U	Velocity far from cylinder [m/s]
ps	Pressure, [Pa].
u	Velocity field, [m/s].
Re	Reynolds number
t	time [s]
$\mathbf{U}^n$	Solution vector at iteration n
F	time-stepper function
P	invariant subspace of dominant eigenvalues
Q	orthogonal complement of **P**
P	projector of $\mathbf{R}^N$ on **P**
Q	projector of $\mathbf{R}^N$ on **Q**
p	projection of **F** on **P**
q	projection of **F** on **Q**
N	dimension of the problem
Z	basis of **P**
I	identity matrix
H	reduced jacobian matrix
n_{max}	maximum number of iterations n
N	arc-length condition
s	solution branch arc-length
T	period of oscillation
x	solution of dynamic system
s_p	phase condition
M	monodromy matrix
y	eigenvectors of full problem
$\mathbf{y_Z}$	eigenvectors of **H**
St	Strouhal number
f	frequency

Sub/superscripts

n	iteration index
l_Z	dimension of basis **Z**

INTRODUCTION

In the past several years Computational Fluid Dynamics (CFD) codes have established themselves as valuable tools both for industrial and academic use. This is due to the combined effect of the advances in the numerical methods that contribute to fast and efficient solvers, the specialization of commercial CFD codes in a wide range of subjects and finally the availability of low-cost computational resources. It is now feasible and economical to tackle realistic, complex problems with a commercial CFD code.

10th International Conference on CFD in Oil & Gas, Metallurgical and Process Industries
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17-19 June 2011

ABSTRACT NO. (Will be filled in by organizer)

ON THE EXTENSION OF A SERIAL 3D TWO-PHASE CFD CODE TO PARALLEL EXECUTION OVER MPI BY USING THE PETSC LIBRARY FOR DOMAIN DECOMPOSITION

Åsmund ERVIK[1]*, Svend Tollak MUNKEJORD[2], Bernhard MÜLLER[1]

[1] NTNU Department of Energy and Process Engineering, NO-7491 Trondheim, NORWAY

[2] SINTEF Energy Research, P.O. Box 4761 Sluppen, NO-7465 Trondheim, NORWAY

*Corresponding author's e-mail: asmund.ervik@ntnu.no

Keywords: Parallelization, Oil/water separation, Surfactants and interfaces, Bubble and droplet dynamics

ABSTRACT

To leverage the last decade's transition in High-Performance Computing (HPC) towards clusters of compute nodes bound together with fast interconnects, a modern scalable CFD code must be able to efficiently distribute work amongst several nodes using the Message Passing Interface (MPI) or equivalent parallelization constructs[1, 2]. While MPI can enable very large simulations running on very large clusters, it is necessary that the bulk of the CFD code be written with MPI in mind. This is an obvious obstacle to parallelizing an existing serial code.

In this work we present the results of extending an existing two-phase 3D Navier-Stokes solver, which was completely serial, to a parallel execution model using MPI. The 3D Navier-Stokes equations for two immiscible incompressible fluids are solved by aid of the ghost fluid method [3]. The location of the interface is determined by the level-set method [4].

We employ the PETSc library [2] for domain decomposition (DD), using it to create a framework where only a fraction of the code needs to be aware of DD/MPI. The remainder of the code stays virtually unaltered, thereby significantly reducing the programming effort. We study the strong and weak scaling of the resulting code and report the speedup obtained and the overhead from communication. The cases we consider are relevant to the fundamental understanding of oil/water separation in electrocoalescers.

ACKNOWLEDGEMENT

This work was funded by the project Fundamental understanding of electrocoalescence in heavy crude oils coordinated by SINTEF Energy Research. The authors acknowledge the support from the Petromaks programme of the Research Council of Norway (206976), Petrobras, Statoil and Wärtsilä Oil & Gas Systems.

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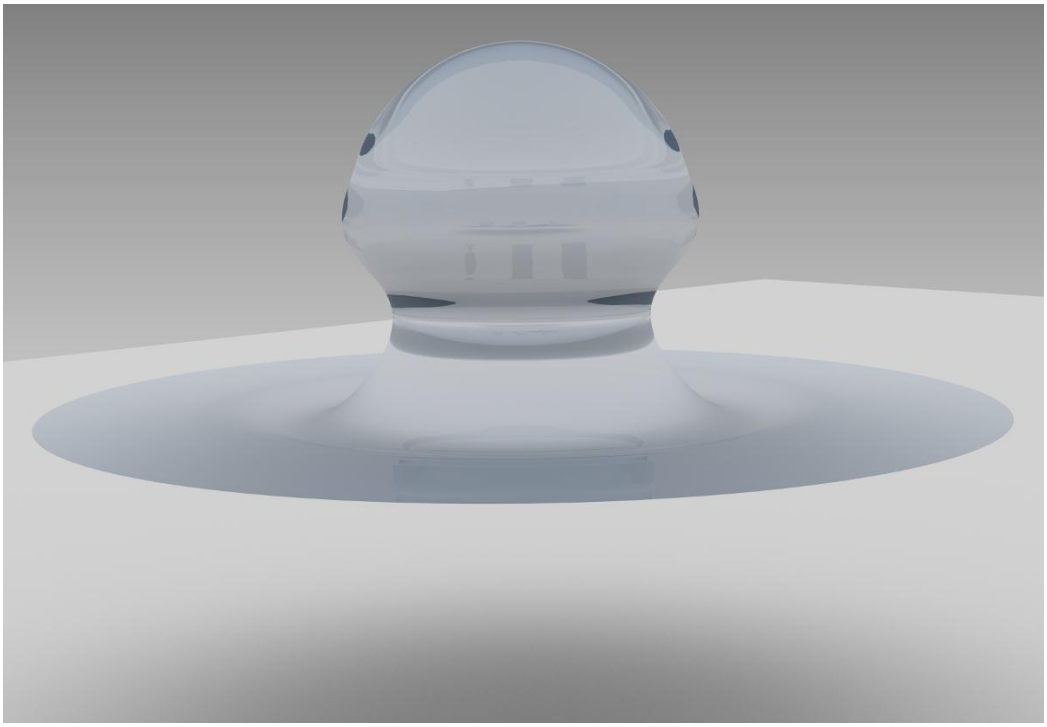

Illustrasjon 1: Example of a simulation result from the existing serial code. A 1.1 mm diameter drop of water falls through a polybutene/decane mixture and merges with a pool of water. This simulation was run in 2D axisymmetry, since the runtime in 3D for the serial code would have been measured in weeks.

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Space-Time hp-Adaptive DG-FEM Scheme for One-Dimensional Multiphase Flow Models

Joost S.B. VAN ZWIETEN[1*] , Ruud A.W.M. HENKES[23], Duncan R. VAN DER HEUL[1], Patricio I. ROSEN ESQUIVEL[3], Benjamin SANDERSE[3], C. (Kees) VUIK[1]

[1] Delft Institute of Applied Mathematics, TU Delft, Delft, THE NETHERLANDS

[2] Department of Process and Energy, TU Delft, Delft, THE NETHERLANDS

[3] Pipelines, Flow Assurance and Subsea Systems, P&T, Shell, Amsterdam, THE NETHERLANDS

Corresponding author's e-mail: j.s.b.vanzwieten@tudelft.nl

Keywords: multiphase flow, one-dimensional, implicit time integration, space-time DG-FEM, hp-adaptive, shock capturing.

ABSTRACT

Multiphase flow plays an important role in many industrial processes, such as oil and gas recovery, chemical processing, power generation and various civil applications. For the design of very long multiphase pipeline systems, the industry relies on time-dependent one-dimensional hyperbolic models. Earlier attempts to solve these models numerically, based on finite difference and finite volume schemes and a conservative drift flux model for the interaction between the phases [Romate, 1998], often fail to accurately predict the onset and propagation of unstable flow, such as terrain slugs and hydrodynamic slugs. In this presentation we show how to improve on this by using both an existing, more detailed model and a high-order space-time Discontinuous Galerkin Finite Element Method (DG-FEM) discretisation.

DG-FEM differs from traditional FEM in that solutions in the former are discontinuous at element edges. At the edges an FVM-like numerical flux needs to be applied. DG-FEM allows a mesh to be refined locally and allows the order of the basis functions to vary per element. Using high-order basis functions and coarse elements in regions where the solution to the Partial Differential Equations is smooth and a fine mesh and low order basis functions in regions where discontinuities appear, may yield a considerable reduction of the number of coefficients needed to achieve a certain accuracy compared to a structured mesh with constant order of the basis functions.

Compressible multiphase flow models may generate fast pressure waves, which are less important for our application. The CFL-condition for an explicit Runge-Kutta scheme yields a very small time step compared to the length of the required simulation. To overcome this restriction we use the space-time DG-FEM method [Rhebergen et al., 2008]. This allows us to refine the mesh and the order of the basis functions in space and time simultaneously, in a unified way.

We apply an adaptive procedure to obtain a discrete solution. First a solution on a coarse mesh with high-order basis functions is computed. Then, elements where discontinuities are detected are refined, the order of the basis functions is reduced and the solution is computed again on the locally refined mesh. In this presentation we show that the hp-adaptive scheme is more efficient than constant-order, structured discretisations for several test problems.

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SPOUT FLUIDIZED BED GRANULATOR: HEAT AND MASS TRANSFER STUDIES

Vinayak S. SUTKAR [1*], Niels G. DEEN [1], Vitalij SALIKOV [2], Sergiy ANTONYUK [2], Stefan HEINRICH [2], J.A.M. KUIPERS [1]

[1] Multiphase Reactors Group, Department of Chemical Engineering and Chemistry,

Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, THE NETHERLANDS

[2] Institute of Solids Process Engineering and Particle Technology, Hamburg University of Technology, 21071 Hamburg, GERMANY

*Corresponding author: E-mail: V.S.Sutkar@TUe.nl; Tel.: +31 40 2478028; Fax: +31 40 2475833

Keywords: spout fluidized bed, liquid distribution, wet restitution coefficient, discrete particle model, infrared thermography and heat and mass transfer.

ABSTRACT

Spout fluidized beds are often utilized in the pharmaceutical, food and chemical industries for granulation, coating and polymerization operations involving physical and/or chemical transformations with simultaneous heat and mass transfer. This is because these beds combine advantages of both spouted and fluidized beds. During these operations a small amount of liquid is atomized through the nozzle to form granules via. particles-droplets collisions followed by a fast drying to prevent unnecessary liquid absorption inside the particle. However, small change in the liquid injection often results a significant change in heat and mass transfer rate hence overall bed performance.

A detailed understanding of the bed dynamics along with flow transition and heat and mass transfer is of primary importance for a design and scale-up. This can be either achieved by performing experiments or numerical simulations. However, it is troublesome to perform experiments on an industrial scale, because it is difficult to access the relevant areas experimentally. Even though simulation tools offer a solid platform that can be used to obtain better insights, it is necessary to validate the model prediction before it can be confidently applied for design and scale-up purposes. Model validation can be achieved by comparing model results with experimental data obtained by utilization of preferentially non-intrusive techniques. Hence our research approach comprises the following elements:

Experimental investigations: Experiments were performed in a pseudo 2D spout fluidized bed (W x D x H = 0.08 x 0.018 x 0.15 m^3) to investigate the effect of liquid injection through the dual nozzle on the bed dynamics of glass and γ-aluminum oxide particles using high speed visual and infrared cameras. The obtained images were used to determine particulate flow pattern, particle velocity and volumetric particle flux through particle image velocimetry (PIV) and digital image analysis (DIA). The liquid distribution in the bed was determined using an infrared camera (FLIR system, SC7000).

Numerical investigations: A discrete particle model (DPM) with a variable restitution coefficient was used to simulate the bed dynamics. The gas phase dynamics were described by solving momentum, energy and species balance equations whereas the motion of individual spherical particles were described by Newton's law of motion with a soft sphere collision model. The heat and mass transfer from the fluid to the particle were determined using overall energy and species balance equations. The convective heat and mass transfer coefficients were evaluated using empirical Nusselt and Sherwood correlations. Simulations results were compared with the experiments.

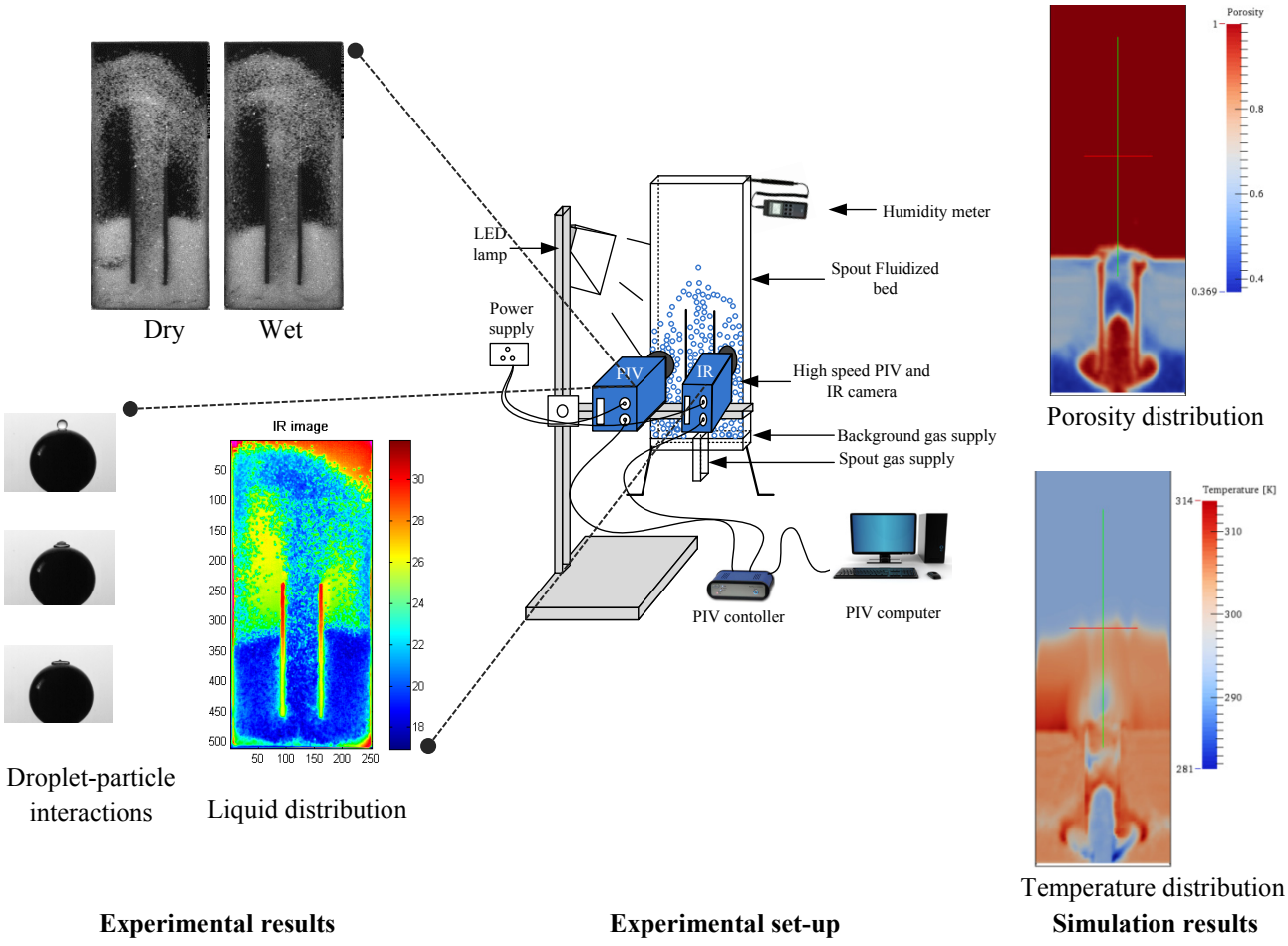

Figure: Experimental set-up comprising a spout fluidized bed with a combined high speed visual and infrared cameras. The obtained results for a fluidized bed-spouting-with aeration (dispersed spout) regime with a continuous water injection in terms of the flow patterns, liquid and droplet distribution are also shown for glass particles (d_p = 1 mm) at 60 °C. Also typical simulations results obtained from DPM in terms of porosity and fluid temperature are shown on the right hand side.

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ABSTRACT NO. (Will be filled in by organizer)

Simulation of Rectangular Fluidized Bed with Geldart D Particles

Mohit Tandon[1*] , Aditya Karnik[1]

[1] Cd-adapco Private Limited, Pune, INDIA

Corresponding author's e-mail: mohit.tandon@cd-adapco.com

Keywords: Bubbling fluidized bed, Geldart D particle

ABSTRACT

In this study simulations were carried out on a rectangular fluidized bed for which experiments were conducted by The Department of Energy's (DOE) National Energy Technology Laboratory (NETL). This problem was announced as Small Scale Challenge Problem (SSCP-I) in 2013 [1]. The objective of this numerical study is to evaluate the reliability of multi-fluid computational models available in literature.

The experimental measurements of the fluidized bed investigated are 3"x9"x48". The bed material for the experiment is Geldart group D particles of uniform size and high sphericity. The simulations for this study were carried out using multi-fluid model in Star-CCM+. Granular temperature calculations were performed by solving its transport equation. Simulation results were validated for vertical component of velocity, horizontal component of velocity, granular temperature and axial pressure gradient. Simulations were performed for all three variations of gas velocity (U = 2.19, 3.28 and 4.38 m/s) for which experiments were conducted. Simulations were carried out to study the effect of different drag laws (Syamlal, Gidaspow and Arastoopour) and the effect of wall boundary conditions on the simulation results.

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HYDRODYNAMIC INVESTIGATION INTO A NOVEL IC-CLC REACTOR CONCEPT FOR POWER PRODUCTION WITH INTEGRATED CO2 CAPTURE

Abdelghafour Zaabout*, Schalk Cloete, Shahriar Amini

SINTEF Materials and Chemistry, Flow Technology Department, 7034 Trondheim, NORWAY

Corresponding author's e-mail: Abdelghafour.zaabout@sintef.no

Keywords: Fluidized bed; Chemical Looping Combustion; Simulation-Based Reactor Design

ABSTRACT

This paper reports a preliminary investigation on the feasibility of an innovative CLC concept for power generation with integrated CO_2 capture. This concept will drastically reduce the technical complexities and the large investment costs involved in the traditional interconnected fluidized bed CLC concept. The concept consists of an internal circulating fluidized bed (IC-CLC) where a single reactor is divided into two separate sections in a way that oxidation and reduction of the oxygen carrier take place separately. This concept allows for large flexibility in term of designing the partition between the fuel and the air zones and thereby the resulting configuration from the partition will have a direct impact on the reactor performance. Since the two reactor sections are connected to allow for internal circulation and transfer of the oxygen carrier, an inevitable gas leakage will take place between them. A large amount of undesired leakage will naturally reduce the concept ability to capture and generate high CO2 purity. Therefore a reliable reactor design should be able to result in minimized gas leakage between the two reactor zones.

To reduce the risks fundamental multiphase flow models (based on the Kinetic Theory of Granular Flow KTGF) have been used first to investigate the hydrodynamics in different reactor designs and identify the most optimized configuration before building the experimental unit. The performance of each configuration has been evaluated through a quantified parameter which is the volumetric gas/solids leakage ratio between the two reactor sections. The results have been compared for the different configurations and the most efficient design has been selected for further simulation through a dedicated central composite design of operating conditions where the reactor performance response to the change in the static bed height and fluidization velocity has been evaluated.

Ultimately the configuration which resulted in minimal leakage has been selected for the experimental concept demonstration. The constructed experimental setup consists of a pseudo-2D cold flow unit where the front plate is made from Plexiglas to allow for using the PIV-DIA technique in order to determine the solids circulation rate between the reactor zones. Holes are created on the back plate of the unit for pressure measurements and gas extraction for quantifying the leakage. First tests on the experimental unit showed successful operation where continuous solids circulation between the reactor sections has been proved. However thorough and detailed quantitative results are still required to demonstrate the potential of this concept to be safely applied for CLC process.

SAMPLE RESULTS

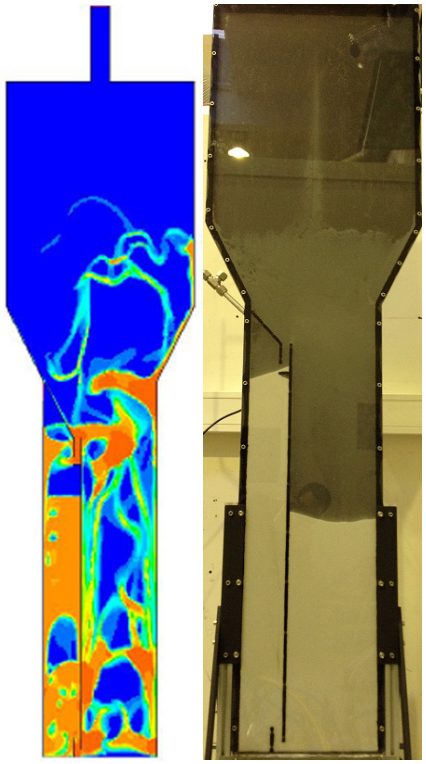

Figure 1: Internal circulating fluidized bed for chemical looping combustion application. Left: simulated cold flow; right: experimental pseudo 2D setup.

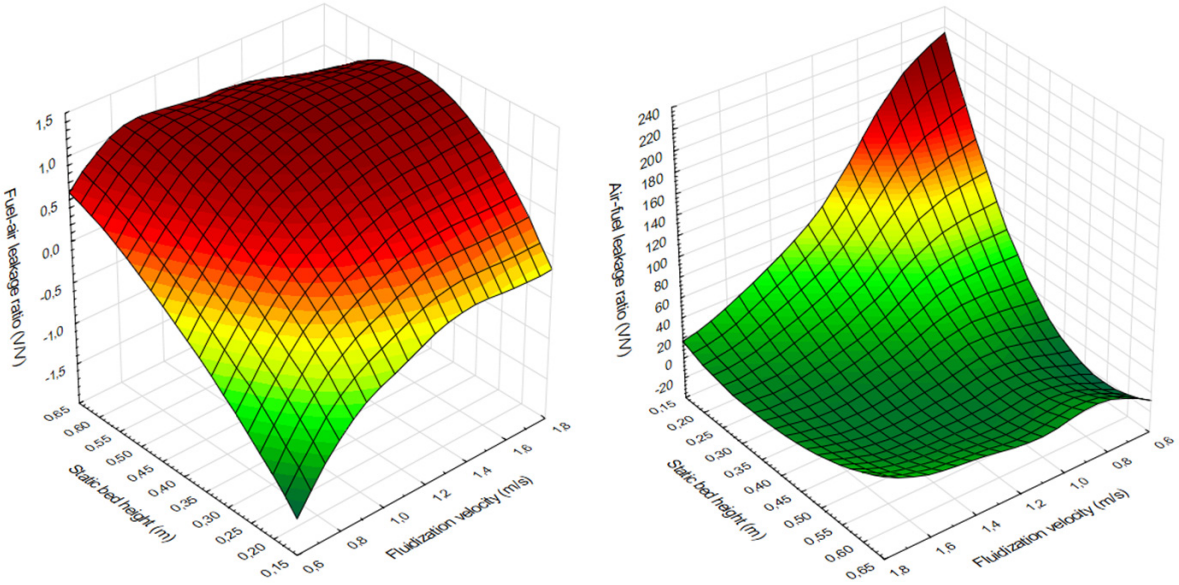

Figure 2: Response of the gas/solids leakage ratio to the change in the static bed height and fluidization velocity. Left: from the fuel to the air section; right: from the air to the fuel section.

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CFD MODELLING OF HEAT SUPPLY IN FLUIDIZED BED FAST PYROLYSIS OF BIOMASS

Pelle MELLIN[1] , Efthymios KANTARELIS[1], Weihong YANG[1]

[1] KTH Royal Institute of Technology, Division of Energy and Furnace Technology, 100 44 Stockholm, SWEDEN

Corresponding author's e-mail: pmellin@kth.se

Keywords: CFD, Fast pyrolysis, Pyrolysis oil, Biomass, Fluidized bed.

ABSTRACT

Fast pyrolysis of biomass to produce a liquid refinery feedstock is a new and interesting method to combat Greenhouse Gas (GHG) emissions from the transportation sector. The concept has been introduced previously with experimental results [1] and a CFD model [2, 3]. The main idea is to use steam, which according to [1] will produce deoxygenated oil, which in turn improves stability, acidity and calorific value.

The CFD method is based on ANSYS Fluent and use of the eulerian multiphase framework. Corrections for the granular bed material and the biomass particles are implemented in the simulation. ser Defined Functions (UDF) are extensively used to describe interactions of heat and momentum between the phases and a comprehensive chemistry model is employed to describe the chemical products from the pyrolysis.

The purpose of this paper is further use of CFD to investigate the heat supply to the biomass, which undergoes pyrolysis in the fluidized bed. Since the technology will be further developed, a solution for the heat supply in a large-scale reactor must be conceived. The primary target is to achieve a process which do not need any extra heat.

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SAMPLE RESULTS

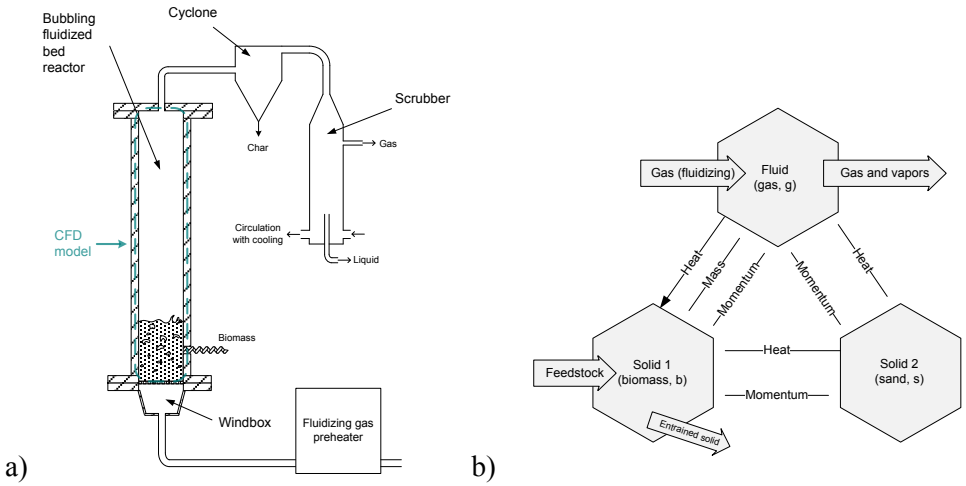

Figure 1: a) The configuration of the experiemental setup with CFD model indicated, b) the framework of the eulerian multiphase model.

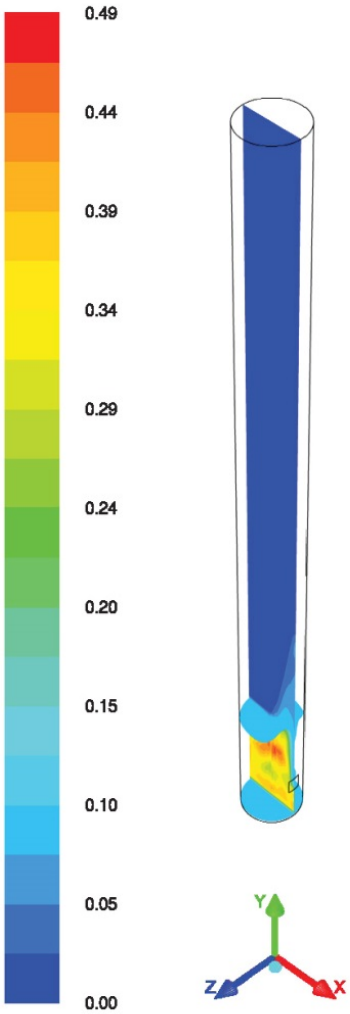

Figure 2: An example of volume fraction of solids inside the reactor.

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LATTICE BOLTZMANN SIMULATIONS APPLIED TO UNDERSTANDING THE STABILITY OF MULTIPHASE FLUID INTERFACES

Gerald G PEREIRA[1]

[1] CSIRO Computational Informatics, Clayton, 3166, AUSTRALIA

Corresponding author's e-mail: Gerald.Pereira@csiro.au

Keywords: Multiphase, Lattice Boltzmann, interface stability, oil and gas

ABSTRACT

Multiphase fluid flow occurs in a multitude of industrial and technological situations ranging from oil and mineral recovery to microfluidic and nanofluidics. In these cases we are interested in modelling the flow of two immiscible phases through a complex geometrical domain. In the past few years, the Lattice Boltzmann method has been developed to model fluid flow, both for single phase and two or more phases. In this study we consider the flow of a less viscous phase into a more viscous fluid (say water into oil) and focus on the stability of the interface. In particular, it is known in this case the interface becomes unstable, leading to fingers of the less viscous phase jetting through the more viscous phase. This has deleterious effects in oil recovery processes, since much oil is bypassed. We use the LB method to model this flow for a variety of fluid rheologies.

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Orr-Sommerfeld stability analysis of two-fluid Couette flow with surfactant

V.P.T.N.C.Srikanth Bojja[1] , Maria Fernandino[1], Roar Skartlien[2]

[1] NTNU Department of Energy and Process Engineering, 7491 Trondheim, NORWAY

[2] Institute for Energy Technology (IFE), Instituttveien18, 2027 Kjeller, NORWAY

Corresponding author's e-mail: srikanth.bojja@ntnu.no

Keywords: Lattice Boltzmann Method, Linear stability, Orr-Sommerfeld, Amphiphilic surfactant.

ABSTRACT

In the present work, the surfactant induced instability of a sheared two fluid system is examined. The linear stability analysis of two fluid Couette system with an amphiphilic surfactant [1] is carried out by developing Orr Sommerfeld type stability equations along with surfactant transport equation and the system of ordinary differential equations are solved by Chebyshev-Tau method [2][3]. Linear stability analysis [4] reveals that the surfactant induces Marangoni instability for perturbations with sufficiently long wavelength.

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EFFECT OF COMPRESSIBILITY IN CFD SIMULATIONS OF AN OSCILLATING WATER COLUMN DEVICE

Arun KAMATH[1] , Hans BIHS[1], Jan Erik OLSEN[2] , Øivind Asgeir ARNTSEN[1]

[1] Department of Civil and Transport Engineering, NTNU, 7491 Trondheim, NORWAY

[2] SINTEF Materials and Chemistry, 7465 Trondheim, NORWAY

Corresponding author's e-mail: arun.kamath@ntnu.no

Keywords: Clean Energy, Oscillating Water Column, OWC, compressibility, CFD

ABSTRACT

An Oscillating Water Column (OWC) device is a wave energy converter that has a chamber with an air column above a water column. The water column in the device is excited by the incident waves and it transfers kinetic energy to the air column. The air is then alternatively driven out and sucked in to the chamber. This motion of the air drives a turbine to generate electrical energy.

The hydrodynamics of an OWC device can be studied in detail using CFD simulations as it provides a large amount of detail regarding the flow field in and around the device. This is essential in order to understand the working of the device and produce an efficient and stable design.

Water is generally modelled as an incompressible fluid in CFD simulations relating to coastal and marine civil engineering problems. In the case of an OWC device, the compressibility of air can be an issue that affects its performance. Sarmento and Falcão (1986) have studied the problem theoretically and Thakker et al. (2003), and Sheng et al. (2013) analysed it numerically. They concluded that air compressibility is a factor that has to be considered in practice. In order to gain more insight into the working of the device, CFD simulations with compressible air and incompressible water are to be carried out in a two-phase model.

It is essential to identify the ratio between the air column height and the water depth in the chamber at which the effect of compressibility is pronounced and has strong consequences on device efficiency. This paper studies the variation of the free surface and the chamber pressure oscillations for different wavelengths while considering air compressibility. This is compared with their behaviour when air is modelled as an incompressible fluid. The difference in the flow rate through the device under the two different conditions is also studied. The ratio of the air column height and the water depth is also varied to identify the condition at which modelling air compressibility becomes an important factor in the simulations.

This study uses a two-dimensional numerical wave tank in a two-phase CFD model that can treat air as a compressible fluid and analyses its effect on the working of the device. The numerical model uses a fifth-order finite difference WENO scheme for convection discretization and a TVD third-order Runge-Kutta method for time discretization. Wave generation and absorption is carried out using the relaxation method. Turbulence modelling is carried out using the k-ω model. The level set method is used to obtain the free surface. This provides a sharp representation of the free surface which is of high importance in the case of an OWC device. The computing performance of the model is improved using parallel processing using the MPI library.

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ABSTRACT NO. (Will be filled in by organizer)

CFD MULTIPHASE SIMULATION OF TWO-FLUID SLOSHING WITH FREE SURFACE MOTION USING THE LEVEL SET METHOD

Hans BIHS[1], Arun KAMATH[1], Øivind Asgeir ARNTSEN[1]

[1] Department of Civil and Transport Engineering, NTNU, 7491 Trondheim, NORWAY

Corresponding author's e-mail: hans.bihs@ntnu.no

Keywords: Multiphase Flow, Sloshing, Level Set Method

ABSTRACT

A numerical model is used to calculate sloshing of two immiscible fluids in a rectangular tank with free surface. The numerical results are compared with experimental data (La Rocca et al., 2005). In the experiments the rectangular tank rotates around the horizontal axis, generating the sloshing of the fluids. Measurements of the interface motion between the lighter and heavier fluid and between the lighter fluid and air exist. The numerical model uses the level set method for the prediction of the interfaces between the different phases. The convective terms of the momentum equation are discretised with the conservative finite-difference version of the fifth-order WENO scheme, while the level set functions are treated with the Hamilton-Jacobi version of the WENO method. For integration in time, the third-order TVD Runge-Kutta scheme is employed. As a result both spatial and temporal numerical discretizations exhibit high numerical accuracy and stability. The pressure is treated with the projection method, and the corresponding Poisson equation is solved with the preconditioned BiCGStab method. The model is fully parallelized based upon the domain decomposition strategy and the MPI library.

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CFD SIMULATION OF THE TWO-PHASE FLOW OF DIFFERENT MIXTURES IN A CLOSED SYSTEM FLOW WHEEL

José F. ROCA R.[1*], **João N.E. CARNEIRO**[1], **José E.S. OLIVEIRA**[1], **Sjur MO**[2], **Martin FOSSEN**[3], **Stein T. JOHANSEN**[2]

[1]Instituto SINTEF do Brasil, 22251-050 Rio de Janeiro, BRAZIL

[2]SINTEF Materials and Chemistry, 7465 Trondheim, NORWAY

[3]SINTEF Petroleum Research, 7465 Trondheim, NORWAY

[*] E-mail: jose.roca@sintefbrasil.org.br

ABSTRACT

The objective of this work is to study the behaviour of mixtures involving air/water and oil/water at low pressures and oil/ high CO_2-content gas at high pressures in a closed system 'Wheel Flow Loop'. Such apparatus has been used in different contexts before, e.g. to evaluate the mixture apparent viscosity of different emulsions or the hydrate behaviour under realistic conditions of pressure and temperature. Typically, torque and velocity measurements are used to estimate the overall wall shear stresses. In a few cases, there exists the possibility to visualize the interface between phases through a (sapphire) window. Furthermore, secondary flow present in such curved configurations may have an effect on pressure loss depending on ratio of pipe diameter and curvature radius and flow regime. Consequently, more detailed information on the flow and phase distribution in the wheel is very relevant to understand the underlying physics in the wheel and aid data interpretation.

In this paper, two-phase flow in the Wheel Flow Loop geometry is simulated numerically, by means of a classic Volume of Fluid (VOF) approach and a kind of coupled "VOF" / Eulerian-Eulerian approach. Numerical results have been compared with experimental data obtained in the SINTEF Multiphase Flow Laboratory at Tiller in Norway for different mixtures showing reasonable agreement. Torque/velocity output data has received special attention.

Experiments have evidenced hysteretic behaviour when an increasing-decreasing stepwise rotation velocity is imposed to the wheel. Both this phenomenon and the carry-over starting point have been successfully reproduced by the CFD calculations. Finally, 3D calculations of the flow using the commercial tool ANSYS FLUENT have been critically compared with a Quasi-3D (Q3D) approach.

Keywords: Wheel flow loop, CO_2-rich mixture, two-phase flow, Quasi-3D.

NOMENCLATURE

Greek Symbols

ℓ	Turbulent length scale, [m]
λ	Friction factor, $[-]$
μ	Dynamic viscosity, $[\mathrm{Pa}\cdot\mathrm{s}]$
ρ	Mass density, $[\mathrm{kg/m^3}]$
θ	Polar coordinate (angle), $[^\circ]$
τ^{wall}	Wall shear stress, [Pa]

Latin Symbols

a	Pipe radius, [m]
A^{wall}	Wall area, $[\mathrm{m}^2]$
d	Pipe diameter, [m]
De	Dean number ($\mathrm{De} = \mathrm{Re}\sqrt{\frac{a}{R}}$), $[-]$
GOR	Gas-oil ratio, $[\mathrm{m^3/m^3}]$
k	Turbulent kinetic energy, $[\mathrm{m^2/s^2}]$
LSI	Large Scale Interface
N_X	Number of x-cells, $[-]$
N_Y	Number of y-cells, $[-]$
$Q3D$	Quasi-3D
r	Polar coordinate (radius), [m]
R	Wheel radius, [m]
Re	Reynolds number ($\mathrm{Re} = \frac{\rho U_0^{\mathrm{wall}} d}{\mu}$), $[-]$
$\mathrm{Re_c}$	Critical Reynolds number, $[-]$
t	Time, [s]
T	Torque, $[\mathrm{N}\cdot\mathrm{m}]$
U^{wall}	Wall velocity of the wheel, $[\mathrm{m/s}]$
x	Streamwise coordinate, [m]
y	Transversal coordinate, [m]

Sub/superscripts

i	x-index (streamwise)
j	y-index (transversal)

INTRODUCTION

During oil production gas, oil and water may flow simultaneously in pipes, forming complex mixtures which are often difficult to characterize under realistic conditions. A closed system wheel flow loop has been used by different authors (e.g. Johnsen et al., 2001) as an approach to estimate the apparent viscosity of mixtures under different water cuts and realistic pressure - temperature conditions. The idea behind such setting is that the wheel may, in some respect, resemble a pressurized infinite loop. Recently, mixtures with high CO_2 content have received special attention due to current pre-salt scenarios in Brazil (Almeida et al., 2010). The presence of CO_2 in unusual amounts may compromise mechanical integrity due to pipeline corrosion while influencing other issues related to flow assurance such as excessive Joule - Thomson cooling, wax deposition, inorganic scaling, among others. Experiments for such mixtures in flowing systems are very expensive and rarely found. Thus, the wheel setup has been also evaluated here for systems containing significant CO_2 content.

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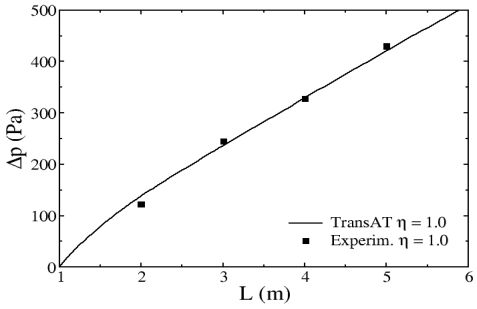
Modelling of particle transport and bed-formation in pipelines

C. Narayanan, D. Lakehal
ASCOMP GmbH, Technoparkstr. 1, Zurich, CH 8005, Switzerland
lakehal@ascomp.ch

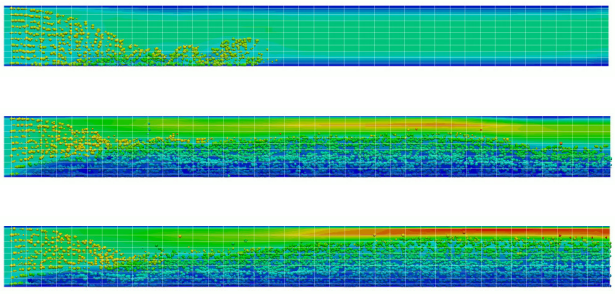
ABSTRACT

The transport of black powder in pipelines (released due to pigging for example) is a critical question in long term pipeline maintenance due to its toxicity. In general, particle transport in pipelines could occur in different regimes such as dilute flows to high mass-loading conditions, to conditions where particle beds form in the pipeline. The modelling of particle transport, therefore, needs a comprehensive approach that can handle all the different regimes. A range of complex phenomena have to be accounted for, such as turbulence of the carrier phase, particle-turbulence interaction, particle-wall interactions including effect of surface roughness, particle-particle interactions, particle agglomeration, deposition, saltation and re-suspension. As such only the modelling of particle transport in the dilute regime for small particles can be reliably modelled under the assumption of one-way coupling. The generalization of particle transport modelling to conditions of two-way coupling, dense suspensions, bed-formation etc. have to be validated carefully against experimental results.

The current study will present a hierarchical modelling framework for the particle transport regimes mentioned above including validation and application of the model to select industrially relevant flows (pressure drop in particle laden flows in pipes, and particle bed-formation and prediction of critical velocity of transport in pipes). The modelling will focus on statistical representation of particle-particle interactions close to the close-packing limit (collision stress) and particle-wall interactions including the effect of statistical roughness. In terms of turbulence modelling, unsteady simulations will be used given the limitations of the RANS approach; Large eddy simulation (LES) and Very Large Eddy Simulation (VLES) methods will be emphasized, which have the ability to provide sufficient flow unsteadiness needed to lift up the particles and move the deposited bed. The results were obtained with the CMFD code TransAT (e.g. in Figures below). The main issues and limitations will be discussed in the paper.



Pressure drop in a pipe with wall roughness gradient of 1.5°, for a mass-loading of 1.0.



Formation of a particle bed in a channel; background contours axial velocity, particles colored by particle axial velocity

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QUASI-3D MODELLING OF TWO-PHASE FLOWS IN PIPES

Alexander VIKHANSKY[1]

[1] CD-adapco, Didcot, UK

Corresponding author's e-mail: alexander.vichansky@cd-adapco.com

Keywords: multiphase pipeline transport; free surface flow; pipe flow.

ABSTRACT

Traditionally the pipe flow simulators are based on 1D models, where the essential physics such as inter-phase drag and flow regimes are modelled using empirical correlations. Three decades or so of intensive R&D activity in the field imply that the 1D models reach maximum of their predictive capacity. On the other hand, the growing power of modern computers allows an engineer to perform more CPU time-consuming calculations either on his own computer or on a remote server. Although the full 3D modelling of a multiphase flow in an industrial pipeline belongs to a distant future, there is a growing interest to the so-called quasi-3D (Q3D) models where parameters of the flow are averaged along the horizontal chord of the pipe. These models allow for (an approximate) resolution of the gas-liquid interface and therefore, the transition from the stratified to bubbly flow is computed rather than modelled.

Development of a dedicated Q3D software tool is an ambitious task; in the present work we demonstrate that an existing commercial 3D software can be used for the same purpose. The advantage of our approach is obvious: there are lot of physical models e.g., RANS turbulence, phase transition, VOF, which are already available for a general user. We show that the standard version of STAR-CCM+ enables one to perform transient two-phase Q3D simulations on a desktop PC within few days – an action, which would require weeks of a multiprocessor cluster if done in a full 3D mode.

We use a special, but simple, meshing technique and a minor alteration of the standard parameters of the k-ε turbulence model in order to model dispersed and stratified two-phase flows. Particles and bubbly flows in horizontal pipes are modelled in Q3D and full 3D modes and the results are compared with available experimental data. The predicted and measured distribution of the dispersed phase across the pipe section are in reasonable agreement. The transient air-water slug flow in a 37m – long 7cm – diameter pipe is modelled under different flow rates of the phases. Our main focus is on the frequency of the slugs, which is also in a good agreement with the experimental data.

SAMPLE RESULTS

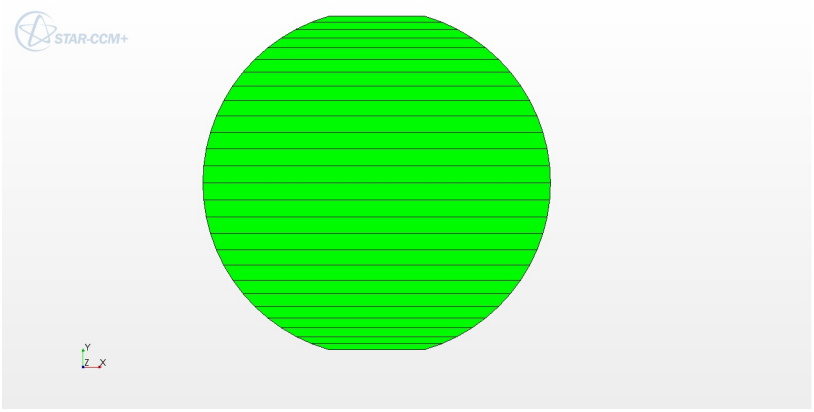

Fig. 1 Q3D mesh.

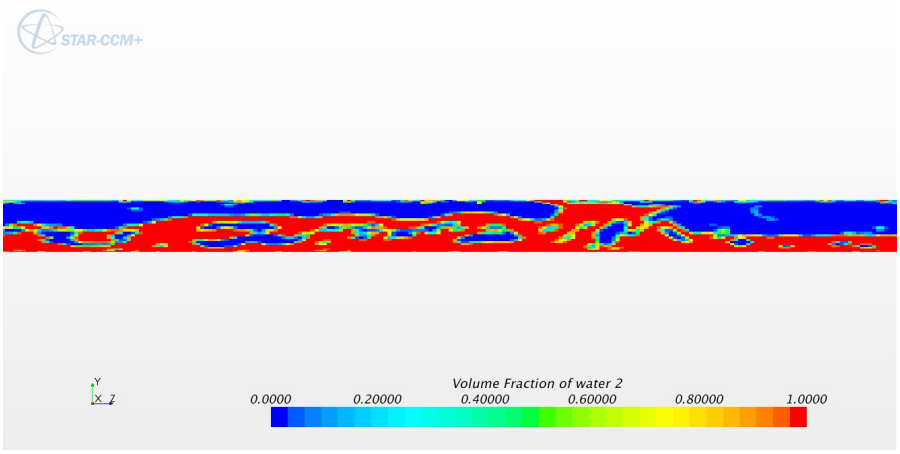

Fig. 2 Volume fraction of water.

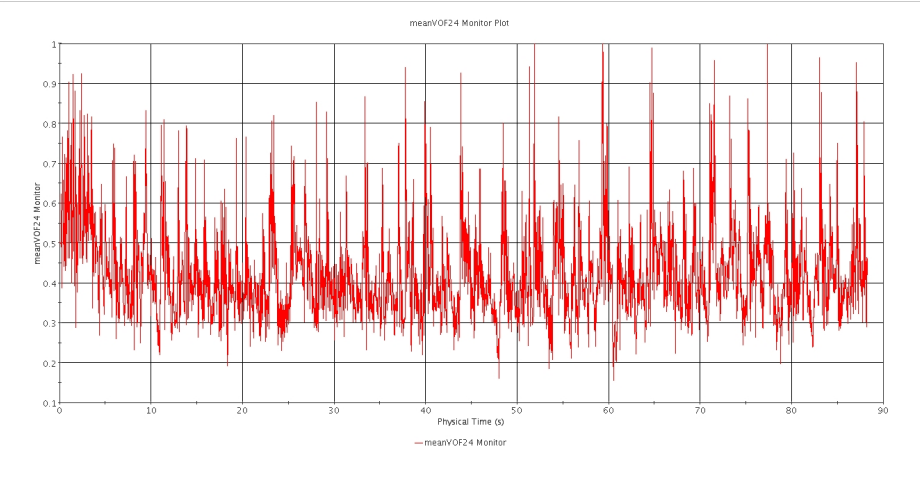

Fig. 3 VOF time monitor.

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ABSTRACT NO. (Will be filled in by organizer)

Simulation of two-phase viscous oil flow

Stein Tore JOHANSEN[1], Sjur MO[1], Jørn KJØLAAS[2], Christian BREKKEN[2] and Ivar ESKERUD SMITH[2]

[1]SINTEF Materials and Chemistry, 7465 Trondheim, NORWAY

[2]SINTEF Petroleum, 7465 Trondheim, NORWAY

Corresponding author's e-mail: Stein.T.Johansen@sintef.no

Keywords: Two phase pipe flow, viscous fluid, turbulence, laminar-turbulence transition, Quasi-3D modelling

ABSTRACT

Multiphase flows of heavy oils and other fluids with high apparent viscosity is a particular industrial challenge. Main challenges here is that interfacial waves, atomization at the large scale gas–liquid interface as well and bubble entrainment and separation all are significantly modified by high fluid viscosity. In addition the viscous liquid may behave as laminar while gas and other low viscosity liquids show turbulent behaviour. Accordingly, correct modelling of the turbulence, including correct transitional behaviour between turbulent and laminar flow becomes of great importance.

In this paper we have investigated two phase flows of gas at a rather high density ($\rho = 45$ kg/m^3) and a viscous oil ($\mu = 0.09$ Pa $\cdot$ s). Experiments have been performed at the SINTEF Multiphase Flow Laboratory at Tiller, Trondheim. The experimental section was horizontal and 3" in diameter, and pressure drop, liquid hold-up time series and video-documentation (see Figure 1) of the flow was recorded.

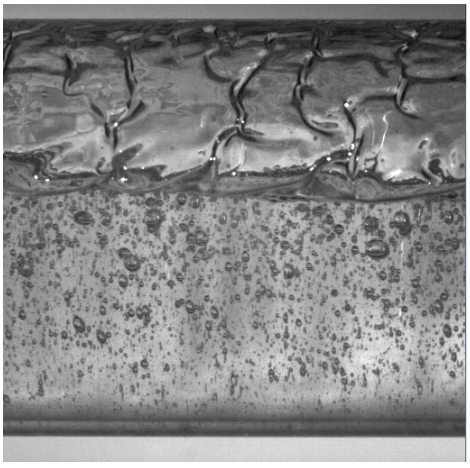

Figure 1 Illustration of viscous two phase flow (flow direction to the left).

The experiments have been analysed and simulated by the Quasi 3D flow model which has been developed in the LedaFlow development project. The results show that flow regimes are well predicted, as well as liquid fractions (hold-up) and pressure drops. Furthermore, some cases have been identified where the Quasi 3D concept is challenged and where the full 3D effects need special attention and modelling. A representative time series is seen in Figure 2,

showing good qualitative and quantitative agreement with the experiments. The corresponding flow structure is seen in Figure 3.

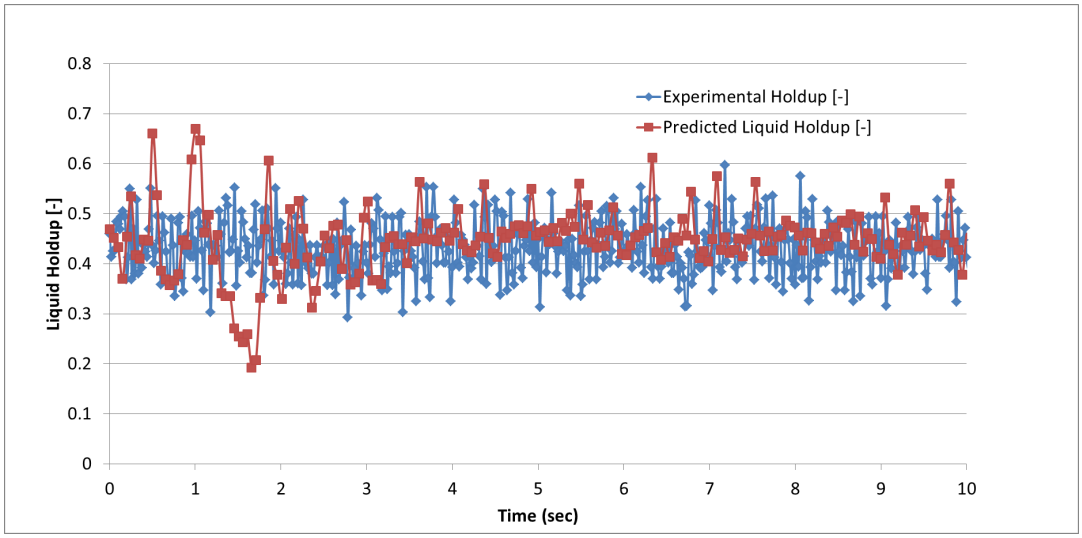

Figure 2 Excerpts of predicted versus experimental time series of liquid holdup (U_{sg} = 4.0 m/s and U_{sl}=0.9 m/s)

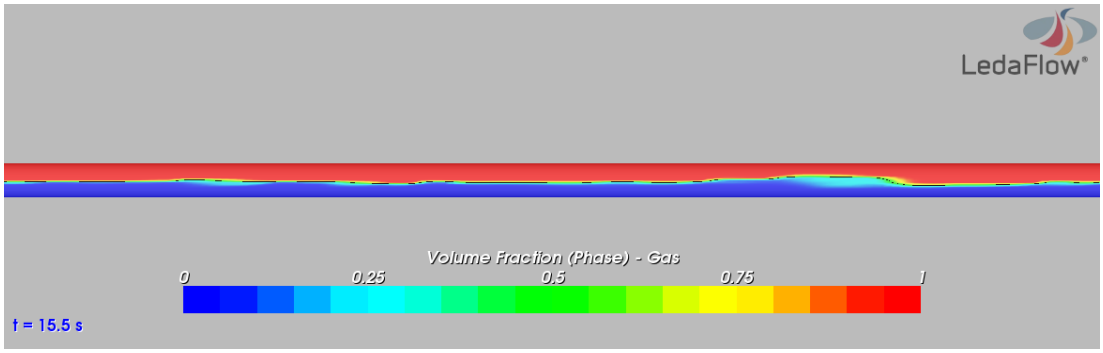

Figure 3 Snap shot of predicted gas fraction for the flow shown in Figure 2. Turquoise colour around the wave crest indicates entrained gas bubbles. Flow direction is to the right.

In the paper we describe the experiments in more details, discuss the general challenges on viscous flow modelling, present the special features of our Quasi-3D flow model and compare predictions to the experimental results. Finally we discuss the perspectives of multidimensional modelling as a virtual laboratory for multiphase pipe flows comprising viscous liquids.

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ADDING ARGON INJECTION THROUGH THE DPM+VOF TECHNIQUE TO AN ADVANCED MULTIPHYSICS AND MULTISCALE MODEL FOR CONTINUOUS CASTING OF STEEL

Pavel Ernesto RAMIREZ LOPEZ[1], Pooria Nazem JALALI[1], Ulf SJÖSTRÖM[1] and Christer NILSSON[2]

[1] Swerea MEFOS AB, Box 812, SE-971 25, Luleå, SWEDEN
[2] SSAB EMEA, SE-971 88, Luleå, SWEDEN

Corresponding author's e-mail: pavel.ramirez.lopez@swerea.se

Keywords: Bubble and droplet dynamics, Argon injection, Discrete Phase Modelling, Volume of Fluid, solidification, metal flow, heat transfer, Lagrangian methods, Free surface flow, Multiphase heat and mass transfer, Multilevel/multiscale, Casting and solidification.

ABSTRACT

An advanced numerical model able to predict transiently the multiphase flow, heat transfer and solidification in a Continuous Casting mould based on the Volume of Fluid Method (VOF) [1,2] in combination with the tracking of bubble trajectories during argon injection through the Discrete Phase Model (DPM) developed by Cloete et al.[3] is presented.

The presented methodology allows studying the effect of Argon injection on process stability; particularly, it investigates the influence of argon injection on steel/slag flow dynamics, powder consumption, solidification and shell growth. Thus, different injection parameters such as bubble diameter and gas flow rate were combined with specific casting practices to emulate industrial cases. As a result, the model makes possible the identification of stable or unstable flows within the mould as a function of argon injection rates under a variety of casting conditions (casting speed, nozzle submergence depth, etc.).

Application to the industrial practice in a European Research Fund for Coal and Steel project is an ongoing task and preliminary results are illustrated [4]. These results are fully applicable to explain the effect of gas injection on the behaviour of mould level fluctuations and shell growth conditions in the mould. Moreover, the predicted flow behaviour and bubble trajectories demonstrate good agreement with observed level fluctuations, standing waves and gas departure positions observed on a physical model based on liquid metal and industrial observations.

Ultimately, the increased process knowledge is used to optimize gas injection to provide a smooth and even distribution along the mould that benefits process stability. The robustness of the model combined with physical model observations make possible the description of phenomena difficult to observe in the caster, but critical for its performance and quality of the final product.

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GOVERNING PHYSICS OF SHALLOW AND DEEP SUBSEA GAS RELEASE

Jan Erik OLSEN & Paal Skjetne
SINTEF Materials and Chemistry, 7465 Trondheim, NORWAY

Corresponding author's e-mail: Jan.E.Olsen@sintef.no

Keywords: marine environment, HSE, bubble dynamics

ABSTRACT

Surfacing gas from ruptured subsea gas pipelines and gas well blowouts poses a threat to offshore operators. Quantitative estimates of surface concentrations are essential for all safety assessments. An Eulerian-Lagrangian CFD model has been developed to study large scale bubble plumes from subsea gas release. The model incorporates forces and effects from buoyancy, gas expansion, drag, turbulent dispersion and gas dissolution. Validation against experiments conducted in a 7 meter deep pool show good consistency between experiments and model.

The model is applied to release scenarios from depths of 30 and 300 meters which represent shallow and deep subsea gas release respectively. The dominating physics is identified, and the difference in behavior between a shallow and deep release is discussed.

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MODELING OF BUBBLY FLOWS WITH FREE SURFACE

Deepak JAIN, J.A.M. KUIPERS, Niels G. DEEN*
Department of Chemical Engineering and Chemistry, Eindhoven University of Technology,
5600 MB Eindhoven, THE NETHERLANDS

Corresponding author's e-mail: N.G.Deen@TUe.nl

Keywords: Bubble column reactor, discrete bubble model, volume of fluid method, free surface, computational fluid dynamics

ABSTRACT

Bubbly flows are quite prevalent in nature and are often accompanied with a free surface of the fluid phase. Also in many processes in the chemical, biochemical and metallurgical industries, such flows have established their use. Therefore, to design and operate bubble column reactors, a thorough understanding of column hydrodynamics is needed. However, even after several decades of research, the understanding is still limited to empirical approaches dominating the design and optimization of these units. In recent times, with the advent of computational fluid dynamics (CFD) and high speed digital computers, multiphase flow simulation is rapidly gaining interest. A particular challenge here is the existence of a wide range of time and length scales which have to be accounted for. Moreover in bubbly flow simulations, very often the free surface is not accounted for and an artificial boundary condition is used to avoid problems at the outflow boundary. In this work, we propose a hybrid method where the free surface is modelled using a volume of fluid (VOF) method whereas the individual bubbles are tracked using the discrete bubble model (DBM) while accounting for all relevant forces acting on them.

In other words, two well established CFD methods (VOF & DBM) are fused to form a novel hybrid model. We actually consider in our model a multi-phase system with three distinct phases, the gas phase, the liquid phase and the bubble phase. It should be noted here that, although the physical properties of gas and bubble phase are the same, the treatment in the model differs a lot. The gas and liquid phases are treated as continuous phases and are solved on a Eulerian grid. The surface between the gas and liquid phase is solved using a colour function which denotes the fractional amount of liquid in that particular grid cell. The bubbles are described in a Lagrangian framework using Newton's second law of motion. Four-way coupling is embedded to take care of bubble-bubble, bubble wall and bubble-liquid interactions.

Our new hybrid model is verified against the benchmark PIV experiments reported by Deen et al. (2001). Additional validation is performed using the bubble PIV data published by Lau et al. (2013). The model results are in good agreement with the experimental findings. Results from free surface modelling can, for instance, be used to improve the ladle stirring in steel making process where slag formation on the top plays an important role.

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SIMULATION RESULTS

Below are presented the snapshots obtained from the simulation of the hybrid volume of fluid-discrete bubble method.

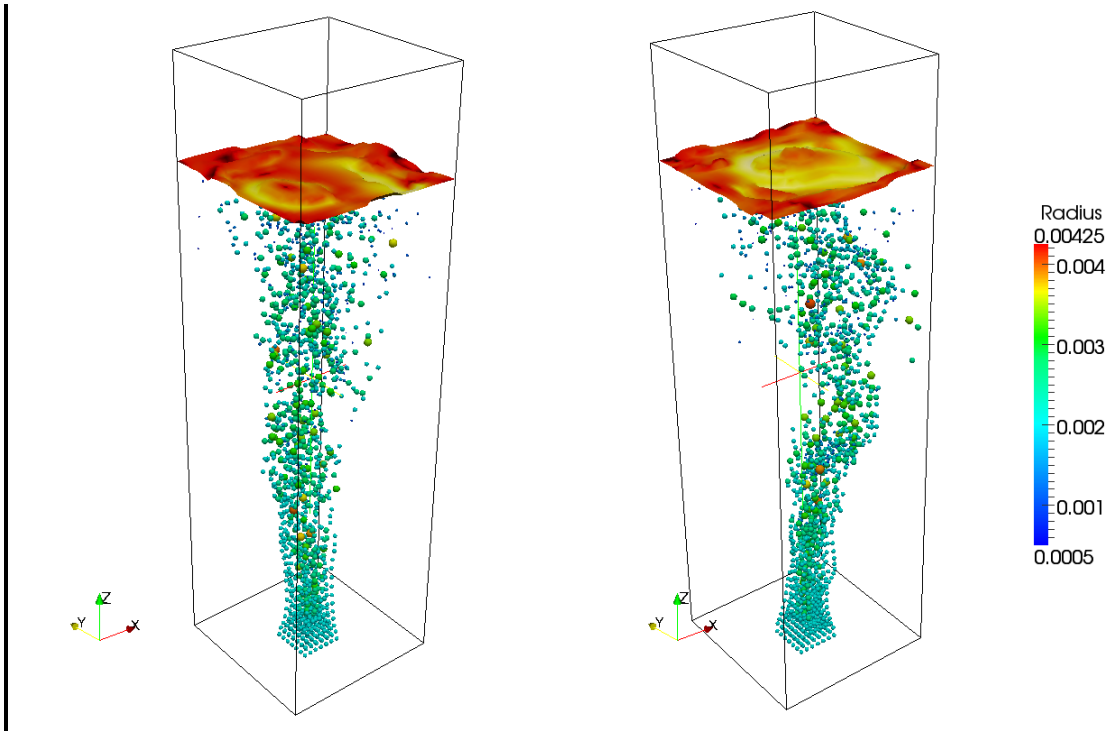

Figure 1: Simulation snapshot for air-water system in a square bubble column at t = 50 s and t= 100 s. The air bubbles are injected in an initially quiescent liquid at discrete positions through the bottom boundary corresponding to a superficial velocity of 0.5 cm/s. The bubbles leave the free surface eventually as they rise through the liquid. The perturbations due to bubbles can be seen influencing the topology of the free surface. The colours of the bubbles in the figure represent the distribution of the radius.

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ANALYSIS OF PARTICLE DEPOSITION FROM TURBULENT LIQUID-FLOW ONTO SMOOTH CHANNEL WALLS

Magali DUPUY*, Arunvady XAYASENH, Hervé DUVAL
Laboratory of Chemical Engineering and Materials, 92295 Châtenay-Malabry, FRANCE

Corresponding author's e-mail: magali.dupuy@ecp.fr

Keywords: Fouling/clogging, metal refining, turbulent deposition, Lagrangian methods.

ABSTRACT

In this study, we analyse the motion of hydrosol particles in the near-wall shear layer of a turbulent channel flow. Since we are concerned with hydrosol, the fluid phase is a liquid and the solid to fluid density ratio is of the order of 1 (whereas aerosols are characterized by a large density ratio, *i.e.*, about 10^3). The channel walls are supposed to be smooth enough for the flow regime to be hydraulically smooth. The liquid flow-field is described using the kinematic model proposed by Fan and Ahmadi (1995). It is a simplified stationary representation of the vortices close to the solid wall, based on experimental observations and numerical results (Cleaver and Yates (1975), Corino and Brodkey (1969), Smith and Metzler (1983)). We expect that the main features of hydrosol deposition can be captured from this crude description of the near-wall turbulence structure.
Lagrangian particle tracking is performed in order to determine the particle limiting trajectory and estimate the particle deposition velocity (defined as the ratio of the deposited particle flux to the particle bulk concentration). The particle dynamic equation may include the buoyancy, the drag, the pressure gradient, the added mass and the lift forces. The particles are non-Brownian. The drag force is modelled by the Stokes steady drag assuming that the particle Reynolds number is lower than 0.1. Faxen corrections as well as wall correction factors may be added in order to take into account flow inhomogeneity at the particle scale and the hydrodynamic interactions between the particle and the wall. Since the hydrodynamic interactions diverge close to the wall (preventing the particles from depositing), we consider that the roughness elements, which cover the wall surface, can make contact at a finite particle to wall separation (distinct from the particle to roughness element separation).
Numerical simulations were performed for friction velocity ranging from 3mm.s^{-1} to 15mm.s^{-1}, dimensionless particle diameter from 0.03 to 1.36 (in wall units), particle to liquid density ratio from 1 to 1.4 and dimensionless wall roughness height from 5×10^{-4} to 0.027.
The results show that the inertia effects are very weak except for the lift force in specific cases. For nonbuoyant particles, direct interception is the main deposition mechanism. The numerical results collapse well onto a curve. Therefore a law giving the deposition velocity as a function of the different parameters is proposed. For buoyant particles the deposition is controlled by sedimentation for the smallest values of friction velocity. When friction velocity increases, the direct interception contribution increases as well, and may prevail on sedimentation. In the latter case, we could not establish a simple law which account for our numerical results.

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Modelling Pulverised Fuel Transport for Industrial Applications

Allan LOVE[1*], Donald GIDDINGS[1], Henry POWER[1]

[1] Division of Energy and Sustainability, University of Nottingham, Nottingham, UK

Corresponding author's e-mail: enxail@nottingham.ac.uk

Keywords: Multiphase, Industrial Modelling, Lagrangian, Particle, Energy

ABSTRACT

The flow of pulverised fuel in a power plant is one example of gas-particle flows in the energy and process industries. Computational Fluid Dynamics is increasingly deployed to predict the behaviour of such flows. Despite wide use, traditional modelling approaches are often inadequate for solving industrial problems. An example is the concentration of particles within a coal burner's fuel feed due to particle inertia and inter-particle collisions. To address this a number of two-phase flow models have been investigated and their applicability and accuracy assessed by comparison with experiments in the literature for horizontal and vertical pipes (Tsuji 1982, 1984), and pipe bends (Huber 1994 and Akilli 2001) with a relatively high mass loading of the discrete phase. The physics investigated includes: particle-wall collisions, particle-particle collisions, structure dependent drag and volume fraction effects. Models have been implemented in the commercial CFD software ANSYS FLUENT R14.5 for the Discrete Phase Model. The results show a significant improvement over industry best practice and provide an indication as to the key physics and the effects of scale on confined gas-particle flows. This paper will provide an overview of the CFD models developed for application to pulverised fuel flows and discuss the gap between academic development and industrial adoption of advanced CFD models.

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SAMPLE RESULTS

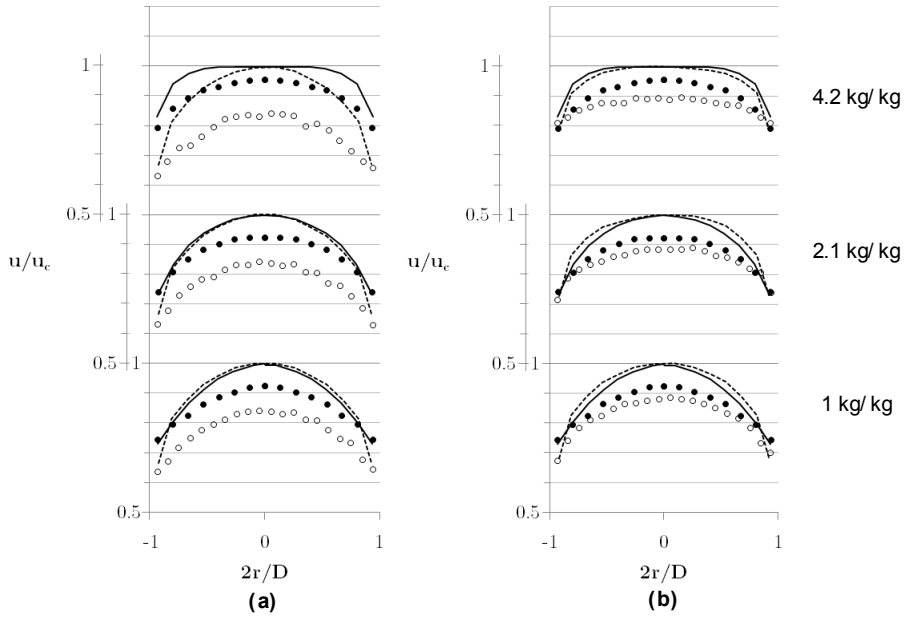

Figure 1: Normalised air and particle velocities for the vertical pipe (D=0.0305m) of Tsuji (1984) at mass loadings of 1, 2.1 and 4.2 kg/kg. (a) Discrete Particle Model (DPM) (b) DPM including wall, particle collision and drag models. — Experimental gas velocity, ● Experimental particle velocity, - - - Model gas velocity, ○ Model particle velocity.

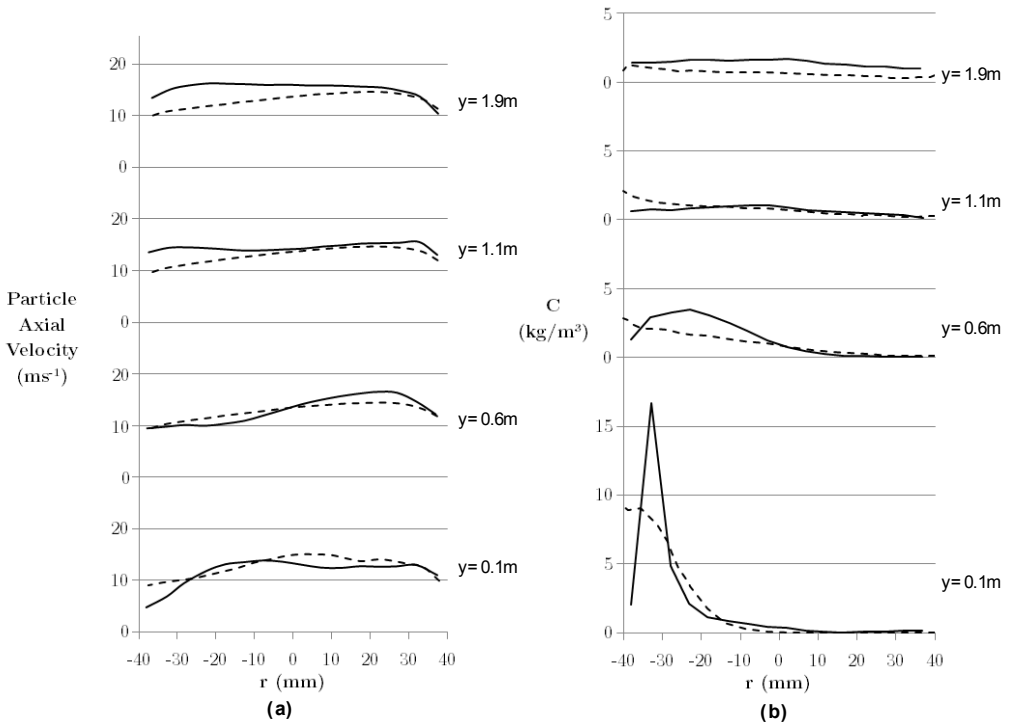

Figure 2: Particle velocity (a) and concentration (b) for the vertical pipe section (D=0.08m) of Huber (1994) at axial locations of 0.1, 0.6, 1.1 and 1.9m for the Discrete Phase Model including wall and particle collisions. — Experimental, - - - Model.

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Numerical study of the gas-particle flow in a conveying line: accounting for wall-friction and wall-roughness

Afsaneh SOLEIMANI[1,2*], Simon SCHNEIDERBAUER[1,2], Stefan PIRKER[1,2]

[1] Christian Doppler Laboratory on Particulate Flow Modeling, Johannes Kepler University, Linz, Austria

[2] Department of particulate Flow Modelling, Johannes Kepler University, Linz, Austria
Afsaneh.Soleimani@jku.at

Keywords: Pneumatic conveying, gas-particle flow, wall-friction, wall-roughness, numerical modeling, boundary condition.

ABSTRACT

In many industrial processes, powdery dust (like coal or cement) has to be conveyed from a feeding vessel towards its processing point. The associated gas-particle flow should be studied carefully in order to optimize the design and operation efficiency of such an industrial system. In these processes, the movement of the conveyed particles is strongly affected by the wall-friction and wall-roughness of the conveying line. Therefore, wall boundary conditions for the solids wall shear stresses and the granular temperature, i.e. the transfer of momentum and energy, play an important role in the behavior of the particles in a typical pneumatic conveying line, when using kinetic theory based two-fluid models (TFM). The present study is a preliminary step towards the improvement of the numerical modeling of gas-particle flow by considering the effect of wall-friction and wall-roughness in the framework of TFM. For this purpose, in a first step, the boundary conditions of Johnson-Jackson are included in the twoPhaseEulerFoam solver of OpenFOAM-2.2.x in order to consider the wall-friction effect on the movement of particles. A straight conveying line using Johnson-Jackson boundary conditions is simulated. The results show that the particles' velocity at the wall is in better agreement with the experimental results (of Sommerfeld and Kussin, 2004), compared to the results of the original solver neglecting wall-friction. However, the model is valid only for a specific adjusted value of the specularity coefficient. Thus, a new boundary condition which incorporates sliding and non-sliding collisions (proposed by Schneiderbauer et al., 2012) is included in the solver. The velocity profiles of the particles, using the latter boundary condition, are compared to that of Johnson-Jackson case and the experimental results. It appears that the boundary conditions of Schneiderbauer et al. yield better agreement with experimental data since these are more general. But still the vertical velocity profile of the particles is not symmetric as observed from the experiment because of the effect of gravity. Wall-roughness appears to be an important factor for the transfer of tangential momentum in vertical direction. Wall-roughness and shadow effect (Sommerfeld and Huber, 1999) are studied in order to propose a new way for including these phenomena in TFM simulations. Finally, the proposed model is implemented in twoPhaseEulerFoam, and particle's velocity profiles are compared to the last results and the experiment. The results show that wall roughness has a strong effect on rebound and redispersion of the particles and accordingly changes the particles' concentration in the section of conveying line significantly. Including wall roughness in the solver, results in more symmetric profiles of particles' velocity and a better agreement with the experimental data.

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Numerical and Experimental Study on Airborne Wear Particles from Wheel-Rail Contacts

Hailong Liu[1] , Lage Jonsson[1,2], Pär Jönsson[1]

[1] KTH, Royal Institute of Technology, SE-100 44 Stockholm, Sweden

[2] FOI, Swedish Defence Research Agency, Division of CBRN Defence and Security, SE-901 82 Umeå, Sweden

Corresponding author's e-mail: hailongl@kth.se

Keywords: Deposition, Concentration and Size Distribution, CFD, Wear particles

ABSTRACT

Particles generated from wear during wheel-rail contacts are one significant contributor to the amount of inhaled airborne nano-sized particles which affect human health in urban environments. It is therefore of interest to investigate the characteristics of these particles. The main idea of this paper is to construct a correlation such as the total generation rate can be estimated between, on one hand experiments where a pin-on-disc machine which situated in a sealed chamber was used to generate particles which were measured at the outlet of the chamber, and, on the other hand, CFD simulations regarding the concentration and size distribution of these wear particles inside the chamber. Four different revolution speeds were applied during the tests. Then, the concentration and size of airborne wear particles were measured online during testing by three particle measurement instruments. In addition, airborne wear particles were collected on filters during the tests and afterward analyzed using SEM. Meanwhile, for the numerical part, a model of the pin-on-disc machine was built together with a sealed box by using the commercial software PHOENICS. The experimental results showed that particles are mostly distributed around 0.01μm and 0.1 μm in diameter. In addition, the SEM images revealed the topography of ultrafine, fine and coarse airborne particles. Also, EDS determinations showed that the chemical composition of these particles is similar and that it mainly contains iron, copper, silicon. The calculations show that the movement of deposited particles differs with varying revolution speeds. Moreover, a deposition velocity is introduced to describe particle loss in the interior of the chamber. Deposition was found to take place at some certain areas. Thus, for part of generated particles it can be deduced that they will stay in the sealed chamber during the tests. This means the loss in the chamber should be accounted for in the determination of the total particle generation rate, as well as the particle size distribution.

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Fully Coupled Multiphase Simulation of a bottom-spray Wurster Coater using a hybrid CPU/GPU CFD/DEM Approach

Eva SIEGMANN[1], Charles RADEKE[1], Johannes G. KHINAST[1,2]

[1] Research Center Pharmaceutical Engineering GmbH, Inffeldg. 13/2, 8010 Graz, AUSTRIA

[2] Institute for Process and Particle Engineering, Graz University of Technology, Inffeldg. 13/3, 8010 Graz, AUSTRIA

Corresponding author's e-mail: eva.siegmann@tugraz.at

Keywords: Discrete element modeling, CFD-DEM, Fluidized bed, Granular flow, Multiphase, Spraying, Coating

ABSTRACT

Where most of the DEM simulations focus on dry material handling, some highly important applications involve liquid chemical sprays. Here, granular material is functionalized by chemical means in order to vitalize surfactant reactions or to realize coating on tablets. Effects like dissolution and wet agglomeration or partial sticking of wet particles needs to be modelled in tandem with the force driven particle interactions. Moreover, in coupled simulations different physical effects like heat transfer and mass transfer between liquid phase and solid phase need to be considered properly. Chemical engineering processes are often lasts for several minutes to hours to finish up. The simulation of such processes is a challenge as well as the huge amount of particles.

Using an in-house DEM code, we simulate a lab-scale Wurster coater with one million particles for at least 60 seconds. The Wurster coater is a bottom spray granulator with a draft tube inside the bed. The tube creates a circulating flow pattern. Air streams into the granulator through a plate at the bottom, which consists of regions with different porosities. The plate has larger orifices below the Wurster tube and therefore the fluidization gas enters at higher velocity below the tube. Whilst processing, air induces a circulation regime of the particles through the Wurster tube. Liquid suspension is sprayed continuously by a bottom spray nozzle. The particles grow according to their residence time in the spray zone.

We use the commercial AVL Fire® solver for the fluid phase and our in-house GPU DEM code XPS for the modelling of the solid phase. Particles are slightly polydisperse. The spray nozzle is modelled by a ray threading technique, which simulates a conical wet fog. The particles are able to wear a film of variable thickness and their mass varies along with the film coating. By statistical means, we monitor residence time distribution and size distribution of the particles.

Efficient simulations of coupled multiphase flow in the million particle range can be achieved by using hybrid CPU/GPU computing on a deskside workstation. The optimization of a coating process demonstrates the strength of tailored simulation tools for chemical and pharmaceutical engineering. The advantage of our CFD-DEM hybrid CPU/GPU simulation method is, that the codes run inside a single workstation but on separate computing platforms. We are able, to do simulations for up to 25 million particles.

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SAMPLE RESULTS

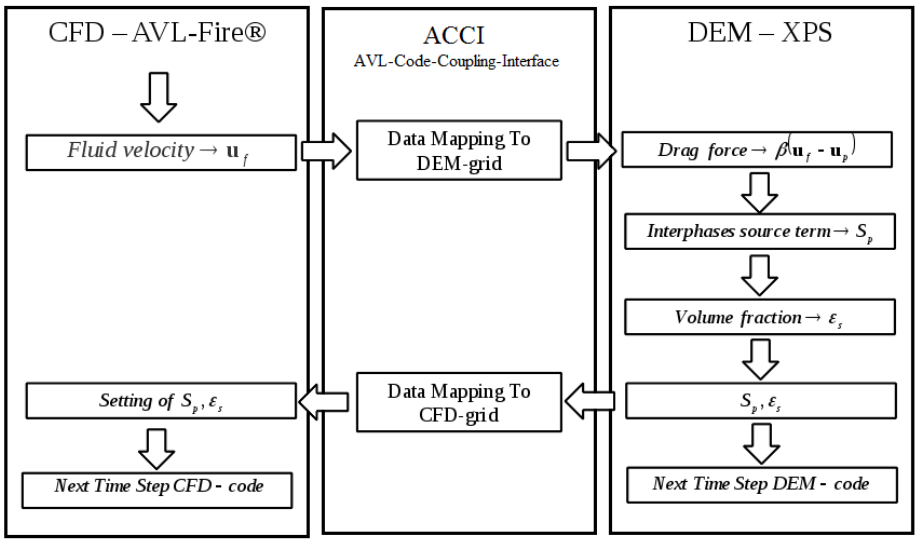

Figure 1: DEM-CFD Coupling Methodology (CFD@CPUs + DEM@GPUs).

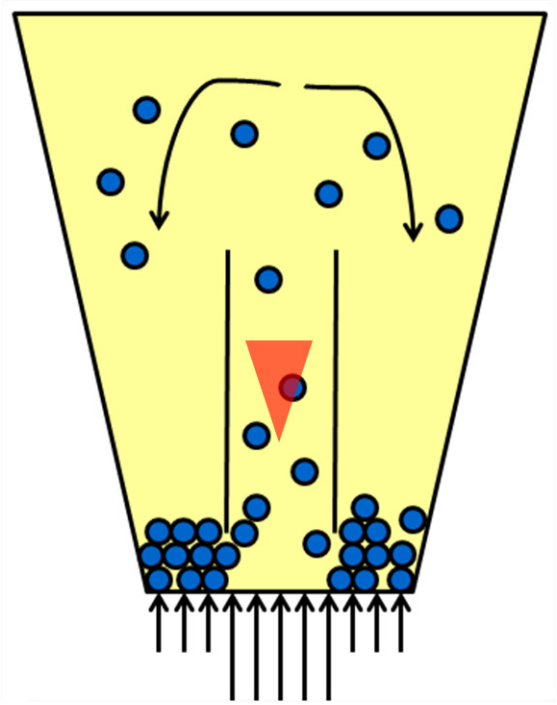

Figure 2: Sketch of a Wurster coater. Air enters through the bottom, the tube inside creates a circulating flow pattern. The spray zone inside the draft tube is marked red.

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EFFECT OF THE WIND TURBINE WAKE IN LARGE OFFSHORE WIND FARMS

Mihaela Popescu, Balram Panjwani, Jon Samseth, Ernst Meese

SINTEF Material and Chemistry, Trondheim, Norway

Corresponding author's e-mail: E-mail: mihaela.popescu@sintef.no

Keywords: CFD, wind turbine, actuator line approach

ABSTRACT

The aim of this paper is to evaluate the wake effect on the performance of a wind farm using two approaches: CFD (OffWindSolver) and an engineering model (OffWindEng). The CFD solver is developed within the OpenFoam architecture. The unsteady PisoFoam solver is extended to account for wind turbines, where each turbine is modeled as a sink term in the momentum equation. Turbine modeling is based on actuator line concept derived from the SOWFA code, where each blade of the turbine is represented as a line of points. The second approach is a simplified explicit model of the wake (engineering model), which includes: the cumulative impact of multiple shadowing, the effects of wind direction, and the wind speed time delay. Results from the two approaches are applied to the Lillgrund wind turbine farm to illustrate the importance of wind turbine spacing. The maximum loss is 50% relative to the designed farm production, which occurs when the wind direction is 221.6^0 - when all turbines operating in the lee of other wind turbines experience total shading. The loss is relatively high, which is not surprising, for such a dense wind farm configuration as Lillgrund

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A MODELING STRATEGY FOR LARGE-SCALE MECHANICAL DRAFT AIR-COOLED SYSTEMS

CJ Meyer

Department of Mechanical and Mechatronic Engineering, University of Stellenbosch, Stellenbosch, 7600, SOUTH AFRICA

Corresponding author's e-mail: cjmeyer@sun.ac.za

Keywords: axial flow fan, heat exchanger, numerical model

ABSTRACT

Large-scale mechanical draft air-cooled systems are used in arid regions where water for cooling purposes is unavailable. These systems can consist of as many as 288 axial flow fans with diameters in excess of 10 meters and are sensitive to a range of environmental and operating conditions with wind and cross-flows having the most detrimental effect on operation.

The large scale of these systems often limits or prohibits experimental investigation. A numerical analysis strategy, employing equivalent models for the operation of the axial flow fans and heat exchangers, is presented and validated. The models are implemented in OpenFOAM® and a strategy is introduced where the characteristics of the software is exploited to ensure parallel computation.

The numerical strategy is subsequently employed to calculate the detailed flow and temperature fields of an existing air-cooled condenser (ACC) used at a power station.

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A BASELINE MODEL FOR MONODISPERSE BUBBLY FLOWS

Roland Rzehak[1] , Eckhard Krepper[1] , Thomas Ziegenhein[1] , Dirk Lucas[1]

[1] Helmholtz-Zentrum Dresden - Rossendorf, P.O. Box 510119, 01314 Dresden, Germany

Corresponding author's e-mail: r.rzehak@hzdr.de

Keywords: Dispersed gas-liquid multiphase flow, Euler-Euler two-fluid model, closure relations, CFD simulation, model validation.

ABSTRACT

CFD simulations of dispersed bubbly flow on the scale of technical equipment are feasible within the Eulerian two-fluid framework of interpenetrating continua. However, accurate numerical predictions rely on suitable closure models. A large body of work using different closure relations of varying degree of sophistication exists, but no complete, reliable, and robust formulation has been achieved so far.

An attempt has been made to collect the best available description for the aspects known to be relevant for adiabatic monodisperse bubbly flows (Rzehak and Krepper 2013), where closure is required for (i) the exchange of momentum between liquid and gas phases, and (ii) the effects of the dispersed bubbles on the turbulence of the liquid carrier phase. Apart from interest in its own right, results obtained for this restricted problem also provide a good starting point for the investigation of more complex situations including bubble coalescence and breakup, heat and mass transport, and possibly phase change or chemical reactions.

Predictive simulation requires a model that works without any adjustments within a certain domain of applicability. The purpose of the present contribution therefore is to validate this baseline model for a number of experimental data sets taken from the literature. These comprise flow in round pipes of different diameters as well as flat and round bubble columns. Reasonable agreement is obtained for all data with the exact same model. Restriction to situations where a fixed distribution of bubble sizes may be imposed excludes the additional complexity of modelling bubble coalescence and breakup processes and thus facilitates a step-by-step validation procedure. Expanding the range of applicability as well as the achieved accuracy is a continuously ongoing development effort.

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SAMPLE RESULTS

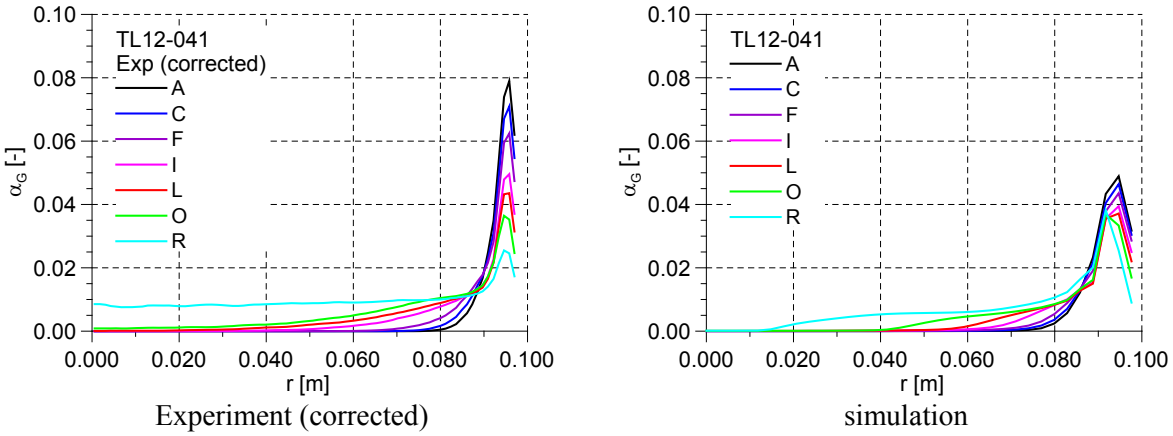

Figure 1: Results on void fraction in developing flow in a DN200 pipe at liquid and gas superficial velocities of J_L=1.017m/s and J_G=0.0096 m/s, data from Lucas et al. (2010).

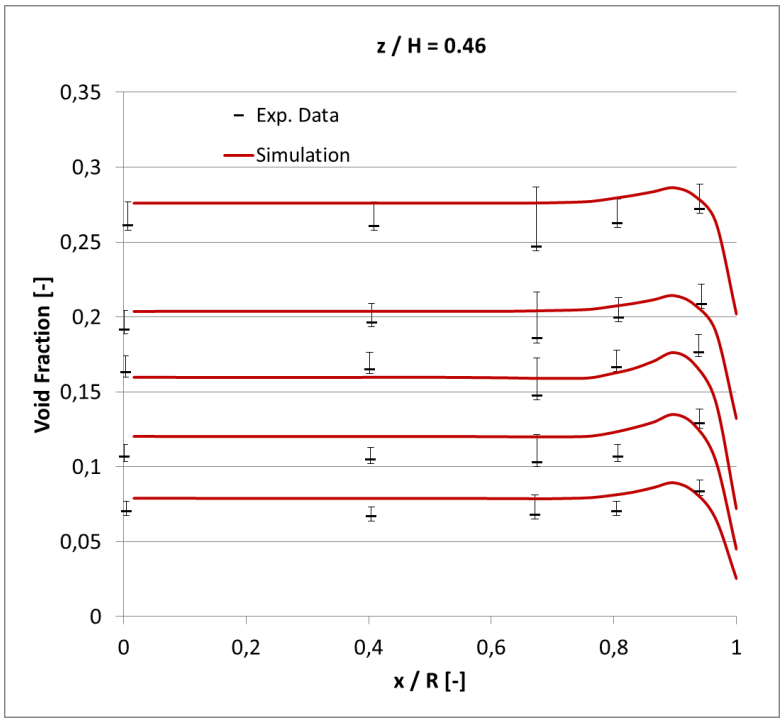

Figure 2: Results on void fraction as a function of gas superficial velocity in a round bubble column, data from Mudde et al. (2009).

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MONODISPERSE BUBBLY FLOWS WITH ANSYS CFX AND OpenFOAM: A COMPARISON

Sebastian H.L. Kriebitzsch[1], Roland Rzehak[1] , Dirk Lucas[1]

[1] Helmholtz-Zentrum Dresden - Rossendorf, P.O. Box 510119, 01314 Dresden, Germany

Corresponding author's e-mail: s.kriebitzsch@hzdr.de

Keywords: Dispersed gas-liquid multiphase flow, two-fluid model, model validation, closure relations.

ABSTRACT

CFD simulations of the multiphase flow in technical equipment can provide a detailed insight into the local flow field and hence potentially be a valuable optimisation and design tool. Such simulations are feasible within the framework of interpenetrating continua, the so-called two-fluid modelling. Within this framework the interfacial transfer processes need to be modelled by suitable closure relations, many of which have been provided in major commercial CFD codes for years. Recently there is an in increasing interest in open source CFD packages and in particular OpenFOAM has become widely known.

Based on previous experience with ANSYS CFX (e.g. Rzehak and Krepper, 2013) a set of closure relations applicable for adiabatic bubbly flow has been implemented in OpenFOAM. Great effort has been made to match all details of the models so that the same results may be expected and residual differences should be only due to different numerical procedures.

In this work we compare simulation results for dispersed gas-liquid pipe flow with experimental data given by Liu (1998) as well as in-house data obtained with the MTLoop facility described in Lucas et.al. (2005). Overall, the experimental data are reasonably well predicted and the predictions are competitive with the results computed with ANSYS CFX. However some differences in the results obtained with OpenFOAM and CFX can be observed, especially in the turbulent quantities in the near wall region.

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SAMPLE RESULTS

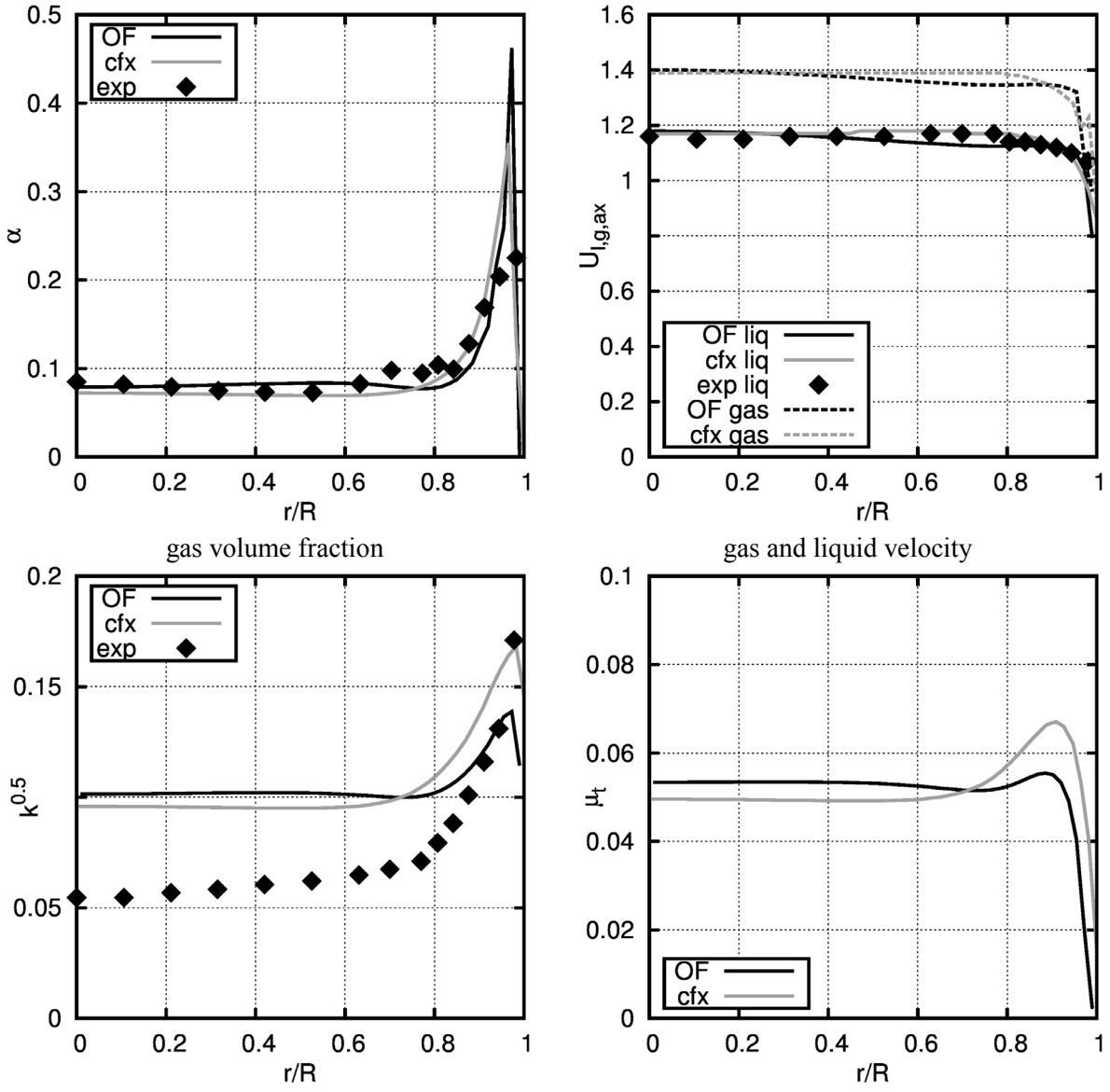

Figure 1: Results for bubbly pipe flow obtained with CFX and OpenFOAM using the baseline model (Rzehak and Krepper, 2013) and the experimental results of Liu (1998) for liquid superficial velocity J_l=1m/s and gas superficial velocity J_g=0.1 m/s.

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EXPERIMENTAL STUDIES OF BUBBLY FLOW IN A MICRO-STRUCTURED BUBBLE COLUMN REACTOR USING DIGITAL IMAGE ANALYSIS

Krushnathej THIRUVALLUVAN SUJATHA, J.A.M. KUIPERS, Niels G. DEEN*

[1] Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, P.O. Box 513, 5600MB Eindhoven, The Netherlands
Corresponding author's e-mail: N.G.Deen@tue.nl

Keywords: Digital Image Analysis, Micro-Structured Bubble Column, wire-mesh, bubble cutting

ABSTRACT

Bubble columns are frequently encountered in the chemical industry for gas-liquid operations. In-spite of their widespread use, bubble columns possesses some disadvantages which affect their performance. To overcome the problems of a conventional bubble column, a novel micro-structured bubble column (MSBC) reactor is proposed. Micro-structuring was realized by using a static mesh of thin wires. Wires serve the purpose of cutting the bubbles leading to a higher contact area and interface dynamics, which both depend upon the wire mesh geometry. The wire mesh can also be coated with a catalyst to perform heterogeneous catalysed reactions. The MSBC reactor is suitable for fast reactions limited by gas-limited mass transfer rates, as it enhances the interfacial area available for mass transfer and also reduces the liquid back mixing leading to formation of compartments. Several experimental techniques are available to study gas-liquid flows: photographic imaging, particle image velocimetry, X-ray tomography, wire mesh sensors, etc.

The scope of this research is to gain a better understanding of the interactions between the bubbles and the wire-mesh (i.e. break-up/by-passing of bubbles). Bubble break-up is predominantly controlled by the geometry of the wire-mesh. The objective of the present work is to obtain a broad set of experimental data to understand the impact of wire-mesh on the hydrodynamics of two phase flow in an air-water system. These data will subsequently be used for the validation of a discrete bubble model (DBM) simulations. For more details on DBM, the reader is referred to the work of Jain et al. (2013).

Experiments are performed for different flow configurations, by varying gas/liquid superficial velocities and also for different wire-mesh lay-outs. The open area of the wire mesh is characterised by the mesh opening, pitch and wire diameter. Experiments are done with woven wire meshes with open area exceeding 60%. An advanced digital image analysis (DIA) technique developed by Lau et al. (2013) is used to determine the bubble size distribution and the gas holdup in the column. The gas and liquid velocities are determined using Particle Image Velocimetry (PIV).

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SAMPLE RESULTS

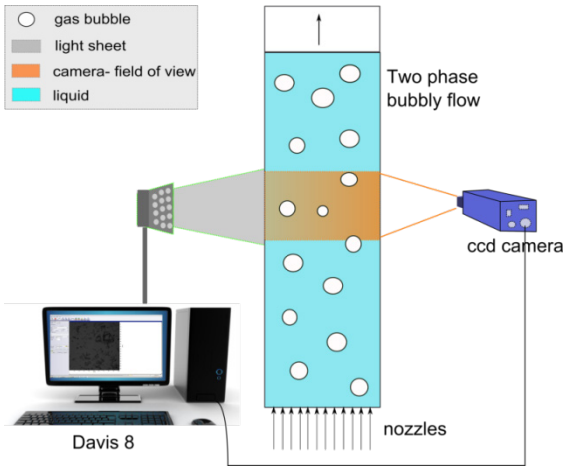

Fig 1: Schematic diagram of Digital Image Analysis – Image Acquisition.

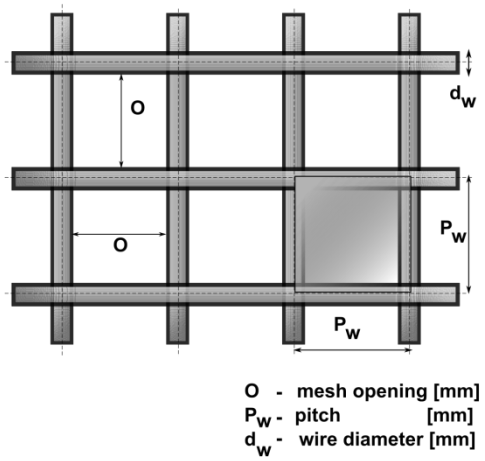

Fig 2: Wire mesh dimensions.

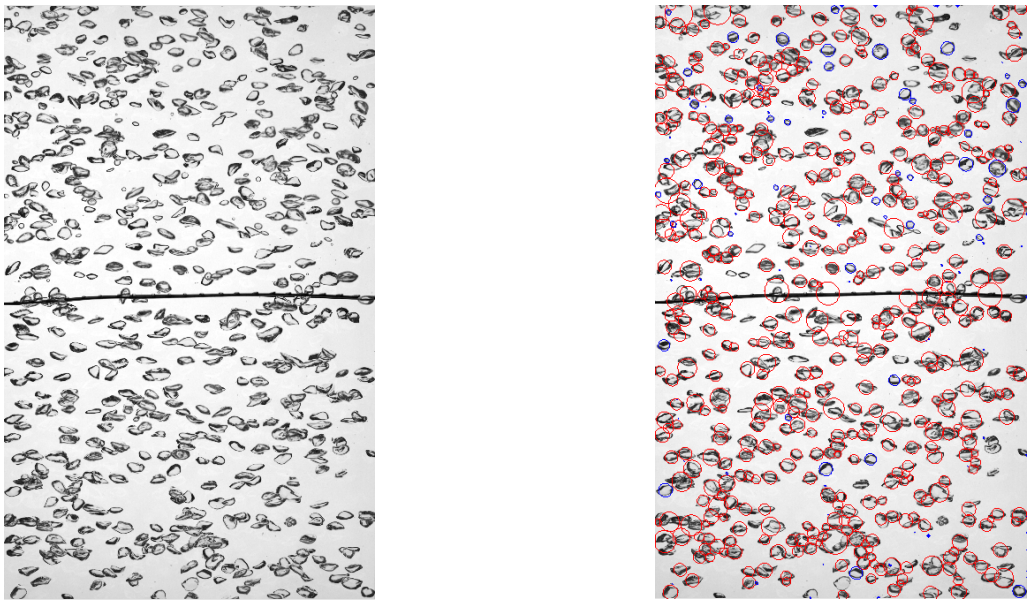

Fig 3: Bubble cutting by wire mesh at superficial gas velocity of $1.5*10^{-2}$ m/s for mesh opening $5.5*10^{-3}$ m. a) raw image obtained from camera b) image with detected bubbles using DIA. Bubbles with overlap/cluster are red and solitary bubbles are blue.

Mesh	*Wire thickness (mm)*	*Opening (mm)*	*Open area (%)*	*Binding*	*Material*
4	0.800	5.500	76	plain	AISI 304
6	0.55	3.683	76	plain	AISI 304
6	0.900	3.333	62	plain	AISI 304
8	0.500	2.675	71	plain	AISI 304
10	0.310	2.200	75	plain	AISI 304
12	0.310	1.806	73	plain	AISI 304
18	0.220	1.191	71	plain	AISI 304

Table 1: Overview of different types of wire mesh used for experiments.

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Two dimensional numerical simulation of bubble dynamics in a vertical Hele-Shaw cell

Xue Wang[1*], Bart Klaasen[1], Bart Blanpain[1], Frederik Verhaeghe[2]

[1] KU Leuven Department of Metallurgy and Materials Engineering, 3001 Leuven, BELGIUM

[2] Umicore Research & Development, 2250 Olen, BELGIUM

Corresponding author's e-mail: xue.wang@mtm.kuleuven.be

Keywords: CFD, volume of fluid method, bubble dynamics, Hele-Shaw cell.

ABSTRACT

A Hele-Shaw cell is a device that consists of two flat parallel plates separated by a small gap. A study of bubble dynamics in a vertical Hele-Shaw cell is relevant to various applications as it contributes to a better understanding of bubble flow in porous media and confined media. However, to the knowledge of the authors, the relation between the gap thickness and the bubble dynamics has not yet been investigated for High-Reynolds flow. In the present paper, a volume of fluid (VOF) method is coupled with a continuum surface force (CSF) model and a wall friction model (porous media viscous resistance model) to investigate this relation. Based on the experimental validation, the main flow properties including shape, path, terminal velocity and pressure distribution are evaluated for different thicknesses, with a focus on the onset of shape and path instability. At the end, the evolution of governing non-dimensional numbers *Re*, *Eo* and $Re(h/d)2$ is discussed.

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A VALIDATED CFD APPROACH TO PREDICT OIL-WATER SEPARATION EFFICIENCY IN THREE-PHASE SEPARATORS

Lanre OSHINOWO, Ehab ELSAADAWY and Regis VILAGINES*
Saudi Aramco Research and Development Center, Dhahran, SAUDI ARABIA

Corresponding author's email: oshinoom@aramco.com

Keywords: Emulsion, gravity separation, three-phase, separator, oil, multiphase, population balance.

ABSTRACT

A gas-oil-water horizontal gravity separator vessel is modeled with an Eulerian multiphase approach coupled with the population balance model. Previous studies in the literature on the computational fluid dynamics (CFD) modeling of three-phase separators have characterized the dispersed phase with a single droplet size. Describing the droplet size distribution during the separation process is a critical requirement to developing a realistic model to predict separator performance under varying flow rate, water fraction, and phase properties. The evolving droplet size distribution in the dispersed water phase is addressed in this work by solving the population balance equation with the inhomogeneous discrete method incorporating kernels for droplet coalescence. Here, the secondary phase is divided into multiple velocity groups and a number of bins describe the droplet distribution within each velocity group. A transient Eulerian multiphase approach is coupled with the population balance to predict the separation of gas, oil and water phases in a pilot scale three-phase high-pressure horizontal gravity separator for different inlet conditions of liquid flow rate, liquid fraction and water fraction. An overflow wire controls the total liquid level in the separator while the water outlet boundary pressure adjusts automatically in response to an oil-water interface level set point using a Proportional-Integral-Derivative control algorithm. An initial droplet size distribution at the separator inlet is specified based on the estimated mean and maximum stable droplet size, and a Rosin-Rammler distribution. The separator efficiency, determined from the difference in water content in the inlet liquid and outlet oil streams, increases with residence time in the separator, or correspondingly, with a decrease in the inlet flow rate, and increases with the inlet water faction. Excellent agreement is obtained in comparing the experimentally determined separation efficiency with the CFD results for the different flow rates and the inlet water content.

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TOWARDS MODELLING OF MINERAL FLOTATION IMPLEMENTED IN OpenFOAM(R)

Gerhard HOLZINGER[1*], **Gijsbert WIERINK**[1], **Stefan PIRKER**[1]

[1] JKU Department of Particulate Flow Modelling, 4040 Linz, AUSTRIA

Corresponding author's e-mail: gerhard.holzinger@jku.at

Keywords: Flotation, Flotation modelling, Separation, Stirred Tanks

ABSTRACT

The process of flotation is widely used in many fields, e.g. mineral processing, wastepaper deinking or wastewater treatment. The aim of this work is to implement a method for simulating the macroscopic flotation process within the CFD framework of OpenFOAM.

The flotation apparatus is modelled with an Eulerian two-phase model (air and slurry). As in many cases the amount of removed solids is small compared to the total amount of solids, the faction of particles subjected to the flotation process itself is considered a passive scalar phase. Departing from the transport equations for two passive scalars governing equations are derived for the free and attached particle phases, following [Bloom and Heindel, 2003; Koh and Schwarz, 2006]. Flotation models known from literature are included in these equations as source and sink terms. The flotation model is implemented in a modular fashion in order to provide the flexibility and extensibility to use any model available in literature.

Due to the modular nature of the model a whole range of flotation processes can be simulated. A simple air-lift loop reactor is used as proof-of-concept simulation case. For validation a cylindrical stirred tank was simulated. The stirred tank is equipped with a Rushton impeller due to the vast amount of available literature dealing with this set-up [Deglon and Meyer, 2006]. The stirred tank simulation is validated against single-phase [Wu and Patterson, 1989] and two-phase results. Furthermore, the general flotation behaviour is compared with literature dealing with flotation is stirred tanks with a Rushton impeller [Pyke, Fornasiero and Ralston, 2003].

Including flotation modelling into a CFD code allows for studying the impact of the hydro dynamical processes inside a flotation apparatus on the flotation performance. This might provide a tool to improve the design of flotation machines. Due to the small additional computational cost added by the passive scalar equations this model can also be applied to industrial scale flotation equipment.

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RESULTS

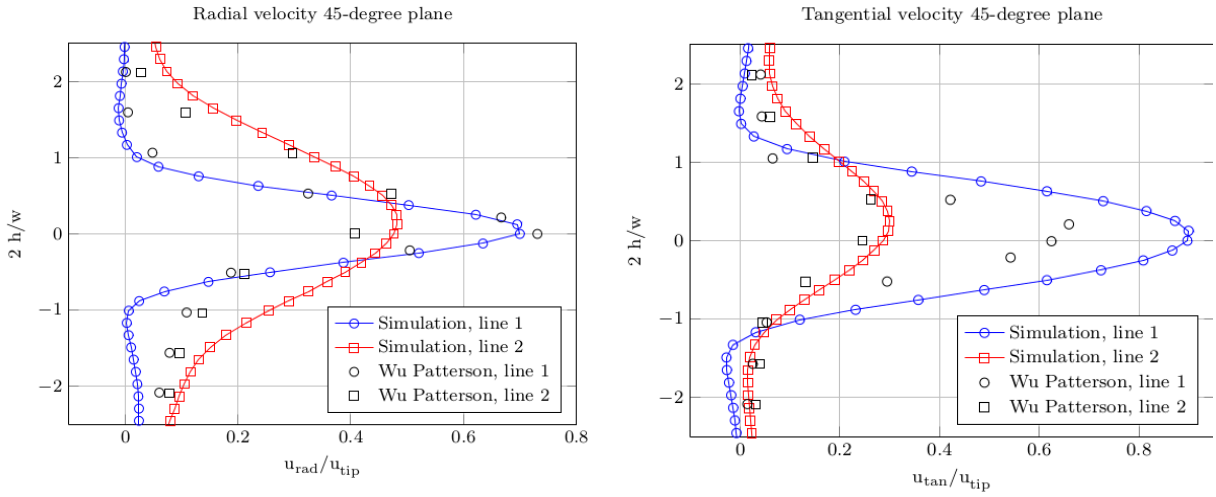

Figure 1: Velocity profiles along vertical lines at r/T = 0.185 and r/T = 0.285.Single phase simulation data compared with LDA measurement data from [Wu and Patterson, 1989].

The derivation of the flotation model follows the derivation in [Bloom and Heindel, 2003] and [Koh and Schwarz, 2006]. Equation (1) shows the governing equations for the number density of the free and attached particles. These equations are rearranged into equations for the particle volume fraction before they are implemented in OpenFOAM. The flotation rate constants k_1 and k_2 (2) are determined by models known from literature.

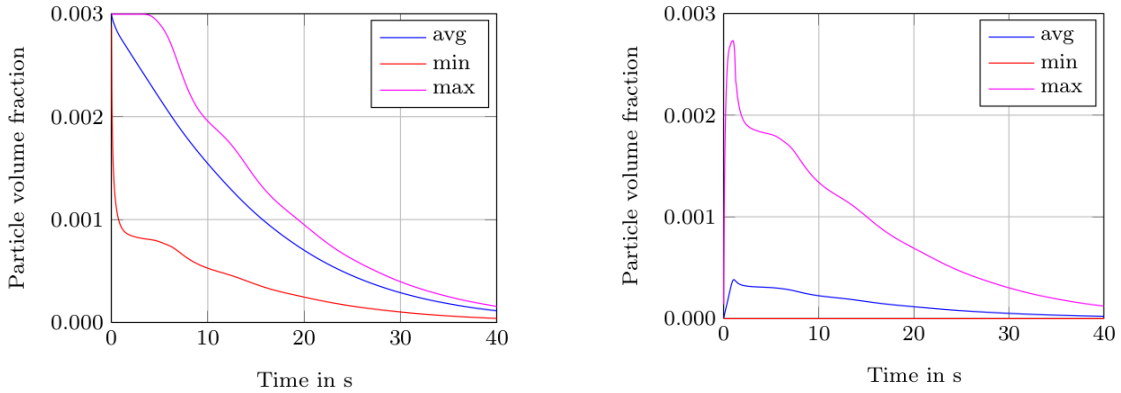

Figure 2: Evolution of the volume fraction of free and attached particles from the air-lift reactor proof-of-concept simulation case. The curves show the minimum, maximum and average volume fraction.

$$\frac{dn_f}{dt} = -k_1(1-\beta)n_B n_f + k_2 \beta n_B$$
$$\frac{dn_a}{dt} = k_1(1-\beta)n_B n_f - k_2 \beta n_B \quad (1)$$

$$k_1 = ZE_c E_a E_s$$
$$k_2 = Z'E_c \quad (2)$$

10th International Conference on CFD in Oil & Gas, Metallurgical and Process Industries
SINTEF, Trondheim, Norway
17-19 June 2014

LAGRANGIAN AND EULERIAN SIMULATIONS OF INCLUSION BEHAVIOUR IN LIQUID METAL PROCESSING

Jean-Pierre BELLOT[1] , Vincent DESCOTES[12], Alain JARDY[1]

[1] Institut Jean Lamour, UMR 7198, CNRS ('LabEx DAMAS'), Université de Lorraine, 54011Nancy, France.
[2] Aperam Alloys Imphy, Centre de Recherche P. Chevenard, BP1, 58160 Imphy,France.

Corresponding author's e-mail: jean-pierre.bellot@ijl.nancy-universite.fr

Keywords: Metal Refining, Process Metallurgy, Lagrangian methods, Population balance methods.

ABSTRACT

The control of metal cleanliness has always been an issue of great concern for the metallurgists since the inclusions directly influence the mechanical properties of the alloys. In most of the metallurgical routes a refining treatment of the molten alloy has been introduced in particular with the aim of improving the metal cleanliness, which means a better control of the particle amount (or the occurrence ratio for very rare exogenous inclusions), the particle size and morphology and finally their composition.

The multiphase CFD provides nowadays efficient techniques for simulating particle behaviour in liquid metal and controlling inclusion cleanliness. When the stirring power and the inclusion phase concentration are high enough[1] the collision process is encouraged which cannot be directly simulated due to the high ratio between reactor and inclusion sizes. In that case the Eulerian approach coupling the solution of the PBE and the CFD of the liquid metal phase is more and more adopted[2,3]. In the opposite situation where aggregation can be neglected, the inclusions can then be considered as isolated particles, and a Lagrangian approach for solving the fundamental dynamic equation emerged as an attractive alternative for tracking turbulent trajectories of inertial inclusions.

In this paper, three examples of numerical modelling of particle behaviour (transportation and growth in the metallic bath) achieved at Institut Jean Lamour are discussed. They illustrate the application of the Lagrangian technique (for isolated exogenous inclusion in titanium bath) and the Eulerian technique without or with aggregation process; applied to the precipitation and growth of inclusions at the solidification front of a Maraging steel, and to endogenous inclusions in molten steel bath of a gas-stirred ladle, respectively. The numerical techniques (modelling, equations and solving methods) are presented in the paper and useful references are reported. Examples of results of inclusion histories illustrate the possibility for effectively controlling inclusion number (or occurrence) and size. These studies, which were performed in close collaboration with our industrial partners, are representative of our on-going research work, aiming to improve the refining of ferrous and non-ferrous alloys and controlling the removal of defects in the solidified products.

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EFFECT OF GEOMETRIC OPTIMIZATION OF HYDROCYCLONES

Nurul HASAN
CEO, Don Computing, 39/385 Bourke St, Melbourne, VIC 3000, Australia

Corresponding author's e-mail: drnhasan@doncomputing.com

Keywords: efficiency of hydrocyclone, hydrocyclone, optimization.

ABSTRACT

Numerous studies have been carried out in order to optimize the performance and particle classification efficiency. A hydrocyclone has five main parts including: cylindrical part, cone part, inlet, vortex finder, underflow, and overflow. There are several important factors in hydrocyclone performance, geometry including vortex finder diameter, vortex finder length, vortex finder thickness, spigot diameter, inlet geometry, inlet diameter, number of inlets, conical angle, and etc. This involves huge list of tests, but FRIENDSHIP-SYSTEMS and Flow-3D combination made the effort easier. Increasing the number of inlets, installing conical top plates on hydrocyclones and modifying the cone angle can also play an important role in efficiency improvement of hydrocylones, and can reduce the hydrocyclone cut size up to 12%. The shape and size of a hydrocyclone has a direct influence on the internal flow structure of the continuous phase and thereby, the separation of particulate phase. In inter condition was fixed and all the parameters are changed to find the optimum separation setting.

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