

Program

Computational Fluid Dynamics in Chemical Reaction Engineering IV

June 15-20, 2008

Whistler, British Columbia, Canada

4050 Whistler Way, Whistler, BC, V0N 1B4

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Chinese Academy of Sciences, China

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Sunday, 15 June 2008

16:30 - 18:30	Registration
18:30 - 19:30	Welcome Reception
19:30 - 20:30	Dinner

IMPORTANT ANNOUNCEMENTS

- **Technical Sessions will be held in Mt. Currie North.**
- **Poster Sessions and meals will be held in Mt. Currie South.**
- **Audiotaping, videotaping and photography of presentations are strictly prohibited.**
- **Speakers – Please leave at least 5 minutes for questions and discussion.**
- **Please do not smoke at any conference functions.**
- **Turn your cellular telephones to vibrate or off during technical sessions.**
- **Be sure to make any corrections to your name/contact information on the Master Participant List or confirm that the listing is correct. A corrected copy will be sent to all participants after the conference.**

Monday, 16 June 2008

07:30 - 08:15 Breakfast Buffet

08:20 - 08:30 Conference Welcome, Introductions, and Conference Overview

Opening Remarks:

Dr. Minye Liu, DuPont Engineering Research and Technology

Conference Chair

Day 1: Gas-solid flows

Session Chairs: Madhava Syamlal, NETL, USA

Kuo Chen Tsai, Shell Global Solutions, USA

08:30 - 09:30 Multi-scale simulation of poly-disperse, dense gas-particle flows
J.A.M. Kuipers, University of Twente, Netherlands

09:30 - 10:00 Coffee/Tea Break

10:00 – 11:00 Numerical Simulation of fluid- multi size particle flow systems
Hamid Arastoopour, IIT, USA

11:00 – 11:15 Break

11:15 - 12:30 **Oral Presentations**

Experimental validation of CFD models for polydisperse fluidized powders based on the quadrature methods of moments

Daniele Marchisio, Politecnico di Torino, Italy

Understanding the interactions between hydrodynamics and chemistry in coal gasifier simulations

Sreekanth Pannala, Oak Ridge National Laboratory, USA

Heat transfer in rotating fluidized beds in a static geometry: A CFD study

Nicolas Staudt, Universite Catholique de Louvain, Belgium

12:30 – 14:00 Lunch

14:00 - 16:30 **Poster Session**

Application of the direct quadrature method of moments (DQMOM) to a hollow-cone water spray

Tron Solberg, Aalborg University Esbjerg, Denmark

Circulating fluidized bed (CFB) riser height: the key to difference between apparent and intrinsic flow-regime diagrams

Wei Wang, Institute of Process Engineering, Chinese Academy of Sciences, China

CFD simulation of ozone decomposition in fluidized beds with consideration of sub-grid structures

Wei Wang, Institute of Process Engineering, Chinese Academy of Sciences, China

CFD simulations for a spouted bed reactor based pyrolysis pilot plant

Luis Diaz, Ikerlan Technological Research Centre, Spain

Monday, 16 June 2008 (continued)

Effect of angle of inclination on transport and reaction in finite hollow cylinders
Anthony G. Dixon, Worcester Polytechnic Institute, USA

Numerical proof of concept of a rotating chimney for rotating fluidized beds
Nicolas Staudt, Universite catholique de Louvain, Belgium

A rapid method for determining the pressure distribution of blood flow system in vein using advanced computational fluid dynamics simulation
Siti Aslina Hussain, Universiti Putra Malaysia

CFD simulation of soot filtration in DPFS
S. Bensaid, Politecnico di Torino, Italy

Sediment dynamics using the phase field method
David R. Rector, Pacific Northwest National Laboratory, USA

Numerical simulation of gas-liquid-reactors with bubbly flows using a hybrid multiphase-CFD approach in openfoam (HIRES-TFM)
Holger Marschall, Technical University of Munich, Germany

15:00	Coffee served at Poster Session
16:30 - 19:30	<i>ad hoc</i> meetings, networking, free time
19:30 - 21:00	Dinner
21:00 - 22:00	Social Hour

Tuesday, 17 June 2008

07:30 - 08:15 Breakfast Buffet

Day 2: Bed Reactors

Session Chairs: Patrick Mills, Texas A&M University, USA
Wei Ge, China Academy of Science, China

08:30 - 09:30

Oral Presentations

Verification and validation of CFD simulations of high-re flow and heat transfer in fixed beds

Anthony G. Dixon, Worcester Polytechnic Institute, USA

Preliminary simulation of non-uniform distribution of two-phase flow through parallel channels

Long Fan, the University of British Columbia, Canada

09:30 – 10:00

Coffee/Tea Break

10:00 - 11:00

Oral Presentations

Discriminating characteristics for simulation-based design and scaling of spouted beds

Charles Finney, Oak Ridge National Laboratory, USA

Numerical investigation of catalyst wetting inside trickle bed reactors

A. Koudil, IFP, France

11:00 - 11:15

Stretch Break

11:30 - 12:30

Oral Presentations

Effect of the restitution coefficient on the computed hydrodynamics of a gas solid fluidized bed

Blake Chandrasekaran, University of Calgary, Canada

Comparison of CFB downers and risers via CFD and reactor modeling

Patrick L. Mills, Texas A&M University-Kingsville, USA

12:30 – 14:00

Lunch

14:00 - 16:30

Poster Session - Discussion

15:00

Coffee served at Poster Session

16:30 - 19:30

ad hoc meetings, networking, free time

19:30 -

Dinner on your own

Wednesday, 18 June 2008

07:30 - 08:15 Breakfast Buffet

Day 3: Industrial Applications

Session Chairs: Pingping Ma, Air Products and Chemicals, USA

Paul Gillis, Dow Chemicals, USA

08:30 - 09:30 Strategies for CFD applications in chemical and oil and gas industries
Kuo Chen Tsai, Shell Global Solutions, USA

09:30 – 10:00 Coffee/Tea Break

10:00 - 11:00 The challenges of combustion CFD modelling
Pierre Q. Gauthier, Rolls-Royce Canada

11:00 - 12:30 Oral Presentations

Numerical simulation of mold filling processes with polyurethane foams: modeling and industrial application

Christian Winkler, University of Stuttgart, Germany

Modeling flow and residence time distribution in a multiple-cell reactor with weir overflow between cells and flow recycling for each cell

Hua Bai, The Dow Chemical Company, USA

Modeling mixing of species with different viscosity in a non-symmetric impinging jet mixer with LES

Minye Liu, DuPont Company, USA

12:30 - 14:00 Lunch

14:00 - 17:30 *ad hoc* Meetings, Networking, free time

17:00 – 17:30 Afternoon Coffee

17:30 – 19:30 Oral Presentations

CFD for large industry at Air Liquide

Guillaume Mougins, Air Liquide, France

Particle deposition in monolithic catalysts

Michael Lykke Heiredal, Technical University of Denmark, Denmark

Computational fluid dynamics model of viscous emulsion breakup

Laura J Dietsche, The Dow Chemical Company, USA

Detailed analysis of the impact of stirring parameters on fluid flow

Umhacker R., MCI - Process Engineering, Austria

19:30 – 21:00 Dinner

21:00 – 22:00 Social Hour

Thursday, 19 June 2008

07:30 - 08:15 Breakfast Buffet

Day 4: Chemically Reacting Flows and Particulates

Session Chairs: Anthony Dixon, Worcester Polytechnic Institute, USA

Daniele Marchisio, Politecnico di Torino, Italy

08:30 - 09:30 CFD modeling of particulate processes
Jerzy Baldyga, Warsaw University of Technology, Poland

09:30 - 10:00 Coffee/Tea Break

10:00 – 11:00 Using Manifold Methods to Achieve Predictivity from Large Eddy
Simulations (LES)
Philip Smith, University of Utah, USA

11:00 - 11:15 Stretch Break

11:15 - 12:30 **Oral Presentations**

Modeling of polymerization reactors by coupling of CFD and reaction kinetics
Andreas Daiss, BASF SE, Germany

MP-PIC calculations of catalytic and non-catalytic chemistry
Sibashis Banerjee, Millennium Inorganic Chemicals, USA

A simulation model for the separation of dispersed liquid-liquid systems in
hydrocyclones based on the coupling of CFD and population balances
Steffen Schuetz, University of Stuttgart, Germany

12:30 – 14:00 Lunch Buffet

14:00 - 16:00 **Oral Presentations**

Modeling of nano-particles precipitation in a confined impinging jets reactor by
means of computational fluid dynamics
Emmanuela Gavi, Politecnico di Torino, Italy

Development of a cfd-based model for the simulation of immobilized
photocatalytic reactors
J.E. Duran, The University of British Columbia, Canada

CFD insights into structured wall microchannel reactors: application to methanol
partial oxidation
Soumitra R. Deshmukh, Velocys Inc., USA

Cavitation modelling and chemical changes
Leonardo Traversoni, Universidad Autonoma Metropolitana, Mexico

16:00 - 19:00 *ad hoc* Meetings, networking, free time

19:00 - 19:30 Reception

19:30 - 22:00 Conference Dinner

Friday, 20 June 2008

07:30 - 08:15 Breakfast Buffet

Day 5: Methods for Multiphase Flows

Session Chairs: A. Koudil, IFP, France
Minye Liu, DuPont Company, USA

08:30 - 10:00 **Oral Presentations**

Modelling the bubble size distribution in gas-liquid reactors with QMOM implemented with a new correction algorithm
Miriam Petitti, Politecnico di Torino, Italy

A comprehensive modeling strategy for gas-sparged, agitated vessels
Jay Sanyal, Ansys/Fluent Inc., USA

CFD simulations in a large-scale aerated reactor with multiple impellers
Özgür Günyol, Delft University of Technology, Netherlands

10:00 - 10:30 Coffee/Tea Break

10:30 - 12:30 **Oral Presentations**

Numerical simulation of gas-liquid-reactors with bubbly flows using a hybrid multiphase-CFD approach in openfoam (HIRES-TFM)
Holger Marschall, Technical University of Munich, Germany

Numerical simulation of reactive mass transfer in gas-liquid flow on structured packing using volume of fluid method
Yacine Haroun, Institut de Mecanique des Fluides de Toulouse / IFP, France

Direct numerical simulation of gas-solid suspension using macro-scale particle methods
Wei Ge, Institute of Process Engineering, Chinese Academy of Sciences, China

A simulation method to determine the transport behaviour of macroscopic particles
Martin Schilling, University of Stuttgart, Germany

12:30 - 14:00 Lunch

14:00 - 14:30 Summary and Conference Adjournment; Departure