Program

Computational Fluid Dynamics in Chemical Reaction Engineering IV

June 15-20, 2008
Whistler, British Columbia, Canada
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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 ad hoc 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 Mougin, 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
  Umhack 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