Conference Program

Computational Fluid Dynamics in Chemical Reaction Engineering III

25-30 May 2003
Kongresszentrum
Davos, Switzerland

co-sponsored by:
American Institute of Chemical Engineers
U.S. National Science Foundation
Dow Chemical Company
DuPont
Fluent

Conference Co-Chairs
Rodney O. Fox
Iowa State University

J. A. M. Kuipers
University of Twente

ENGINEERING CONFERENCES INTERNATIONAL, INC.
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Notes

- Lunches and dinners will be at the Cresta Sun Hotel.
- All technical sessions will be at the Congress Center.
- All poster sessions will be at the Congress Center.
- No smoking at ECI conference technical or social functions.
- Please turn cellular telephones to vibrate and conduct telephone conversations outside the meeting room.
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Monday, 26 May 2003

7:00 - 8:15  Breakfast (available at the hotels)
            Late Registration at Kongresszentrum  (8:00-8:30)

8:30 - 8:40  **Conference Welcome, Introductions, and Conference Overview**
            Rodney O. Fox
            Iowa State University; Conference Chair
            J. A. M. Kuipers
            University of Twente; Conference Co-Chair
            Herman Bieber
            Engineering Conferences International Conferences Committee

**Day 1: Gas-solid flows: Fluidized-bed and riser reactors**
Session Chairs: Bob P. Hoomans, DSM Research
                Hamid Arastoopour, Illinois Institute of Technology

8:40 - 10:15  **Invited Talks**

*Multi-Fluid CFD Modeling of Fluidized Bed Reactors*
Bjorn Hjertager
Aalborg University

*Applications of DNS and LES for Prediction and Study of Particle-Laden Turbulent Flows*
Kyle Squires
Arizona State University

10:15 - 10:45  Coffee/Tea Break

10:45 - 12:30  **Oral Presentations**

*Comparison of continuum models using the kinetic theory of granular flow with discrete particle models and experiments: extent of mixing induced by bubbles*
G. A. Bokkers
University of Twente

*DQMOM model for gas-solid fluidized bed with aggregation and breakage*
Daniele Marchisio
Iowa State University

*Gas-solid particle flow in horizontal channel: decomposition of the flow and inter-particle collision effects*
Alexander Kartushinsky
Tallinn Technical University

*Experimental and numerical study of gas-solid flow in circulating fluidized beds*
Gorik van Engelandt
Ghent University

*Experimental and computational validation of the simplified scaling rules for fluidized beds*
Ruud van Ommen
Delft University of Technology
Monday, 26 May 2003 (continued)

12:30 – 13:30 Lunch

13:45 - 14:15 **Poster Presentations - Group I**

I-1 *Modeling the injection of liquid reactants into fluidized bed reactors*
Stefan Bruhns
TU Hamburg-Harburg

I-2 *A three-dimensional simulation of gas/particle flow and ozone decomposition in the riser of a circulating fluidized bed*
Kim Granly Hansen
Aalborg University

I-3 *An experimental and numerical study of large scale fluctuations in CFD boiler flow*
Claus Ibsen
Aalborg University

I-4 *CFD simulation of bubbling fluidized beds using alternative Eulerian-Eulerian modeling approaches: sensitivity analysis on the drag model*
Paola Lettieri
University College London

I-5 *Numerical study of effect of design parameters on performance of structured packing using computational fluid dynamics*
Joseph Smith
CDa-acces

I-6 *Analysing the wall collision process of non-spherical particles*
Martin Sommerfeld
Martin-Luther-Universitat

I-7 *Large-eddy simulation of particle-laden turbulent channel flow*
Bert Vreman
University of Twente

I-8 *CFD modeling of combustion and particle behaviour in a rotary dryer*
Peter Witt
CSIRO Minerals

I-9 *Numerical simulation of heterogeneous flow structure in gas-solid fluidization*
Ning Yang
Chinese Academy of Sciences

14:15 – 15:15 **Poster Session – Group I** (with coffee service)

15:15 – 19:00 *ad hoc* Meetings, Networking, Free Time

19:00 - 20:30 Dinner

20:30 - 21:30 Social Hour
Tuesday, 27 May 2003

7:00 - 8:15 Breakfast

**Day 2: Gas-liquid flows: Bubble-column and air-lift reactors**
Session Chairs: Robert F. Mudde, Delft University of Technology
Bernard A. Toseland, Air Products and Chemicals

8:30 - 10:15 Invited Talks

*Bubble Column Flows: Modeling and Experiments*
Milorad Dudukovic
Washington University

*How Realistic Can One Model Bubbly Flows?*
Martin Sommerfeld
Martin-Luther University

10:15 - 10:45 Coffee/Tea Break

10:45 - 12:30 Oral Presentations

*Determination of interfacial forces in gas-liquid systems*
Francesco Bertola
Politecnico di Torino

*Analysis of continuous gas and liquid flow bubble column reactor using CFD modeling: fluid phase hold-ups and mixing characteristics*
Shane Cox
University of New South Wales

*Modelling bioreactors with oxygen transfer and microbial kinetics*
Kumar Dhanasekharan
Fluent Inc.

Large eddy simulation of a bubble column reactor using Euler-Lagrange approach
E.I.V. van de Hengel
University of Twente

Lattice-Boltzmann simulation of turbulent transport in the vicinity of bubbles and drops
Kostas Kontomaris
DuPont Central Research and Development

*CFD modeling of bubble columns at Fischer-Tropsch Conditions*
Bente Sannæs
Statoil

12:30 – 13:30 Lunch
13:45 - 14:45  

**Poster Presentations – Group II**

**II-1**  
Influence of different closures on the CFD prediction of the hydrodynamics of bubble column flows  
Muthanna Al-Dahhan  
Washington University

**II-2**  
Local characteristics of flows in airlift photo-bioreactor via CARPT experiments and CFD simulations  
Muthanna Al-Dahhan  
Washington University

**II-3**  
Numerical aspects of bubble column predictions  
Stefano Bove  
Aalborg University

**II-4**  
Flow generated by an aerated rushton impeller: two-phase PIV experiments and numerical simulations  
Niels Deen  
University of Twente

**II-5**  
Bubble column large scale dynamics: structures or no structures?  
Wouter Harteveld  
Delft University of Technology

**II-6**  
Experimental validation of a bubble column reactor with inter-phase mass transfer  
Alfredo Iranzo  
AEA Technology GmbH

**II-7**  
CFD modeling of a co-current gas-liquid downward flow through a packed bed column  
Abdelhakim Koudil  
IFP

**II-8**  
On the comparison between population balance models for CFD simulation of bubble columns  
Daniele Marchisio  
Iowa State University

**II-9**  
Simulation of heavy liquid metals bubbly flows with the computer codes CFX4 and Modefrontier  
Giovanni Mercurio  
ENEA

**II-10**  
Multi-phase applications in liquefied natural gas (LNG) plants  
Vibhor Mehrotra  
Bechtel Corporation

**II-11**  
The effect of bubble-bubble interactions on bubbly flows  
Sarah Monahan  
Iowa State University
II-12 Bubble formation in multiple orifices
Xie Shuyi
National University of Singapore

II-13 Bubble behaviour and interaction in a swarm
Martin Sommerfeld
Martin-Luther University

II-14 Flow pattern visualization in a mimic anaerobic digester using CFD
Mehul Vesvikar
Washington University

II-15 The effects of varying geometrical parameters on laminar mixing in a tank agitated by a paddle agitator via simulations
Zahira Yaakob
Universiti Kebangsaan Malaysia

14:45 – 15:45 Poster Session – Group II (with coffee service)
15:45 – 19:00 ad hoc Meetings, Networking, Free Time
19:00 - 20:30 Dinner
20:30 - 21:30 Social Hour
**Wednesday, 28 May 2003**

7:00 - 8:15  Breakfast

**Day 3: Industrial challenges: Industrial perspective on CFD and discussion of new application areas**
- Session Chairs: Anthony Dixon, Worcester Polytechnic Institute
  - Joseph Smith, ADAPCO Cda-acces

8:30 - 10:15  **Invited Talks**

*Extension of CFD by Process Simulation Methods*
Holger Seguin
Bayer

*Using CFD Models to Understand the Impact of Flow-Field Design on PEM Fuel Cell Performance*
Stephen Fell
Adam Opel AG

10:15 - 10:45  Coffee/Tea Break

10:45 - 12:30  **Oral Presentations and Industrial Round-Table Discussion**

*CFD with detailed chemistry for process engineering*
Marc Heggemann
Sulzet Innotec

*Industrial CFD analysis of gas liquid stirred tank mixers and validation with experimental data*
Mark Liu
Computational Dynamics Ltd.

*Innovative approach for optimizing multiphase reactors*
Pingping Ma
Air Products and Chemicals Inc.

*Use of VOF CFD simulations for gas-liquid flow through structured packing characterization*
Ludovic Raynal
Institut Francais du Petrole

12:30 - 13:30  Lunch (for those not on the Optional Excursion)

**Optional Excursion to Engadine Valley/Three-Mountain Pass** (departs 12:30, box lunches provided)

13:30 - 20:00  *ad hoc* Meetings, Networking, Free Time (for those not on the Optional Excursion)

20:00 - 22:00  Conference Banquet
Thursday, 29 May 2003

7:00 - 8:15 Breakfast

Day 4: Single and multiphase chemically reacting flows: CFD with detailed chemistry, fine-particle formation, or other processes sensitive to reactive mixing
Session Chairs: Jerzy Baldyga, Warsaw University of Technology
Kuochen Tsai, Dow Chemical

8:30 - 10:15 Invited Talks

CFD Modeling of Precipitation Systems
Laurent Falk
ENSIC-LSGC

Computations of Reactive Flows with Detailed Chemistry
Stephen B. Pope
Cornell University

10:15 - 10:45 Coffee/Tea Break

10:45 - 12:30 Oral Presentations

Reactive chaotic mixing inside twisted curved pipes
Cecile Boesinger
LaTEP

Comparison between different CFD modeling approaches for non-premixed turbulent flames with and without swirl
Alessandro Zucca
Politecnico di Torino

Effect of turbulence modulation, dispersion of evaporating droplets and swirl intensity on turbulent spray combustion processes
Mahmoud Maneshkarimi
Technical University of Darmstadt

Aggregation of colloidal particles in turbulent flow in narrow pipes
Miroslav Soos
ETH Zurich

CFD analysis and optimization of shell side reactor flow
Jan Vierendeels
Ghent University

12:30 – 13:30 Lunch

13:45 - 14:45 Poster Presentations – Group III

III-1 Reactive mixing in stirred tanks
Jerzy Baldyga
Warsaw University of Technology
III-2 Formation of agglomerate particles: application of CFD and population balance for the prediction of size distribution
L. Blanc
Lab. de Genie Chimique

III-3 CFD studies of reaction and heat transfer near the wall of a fixed bed
Anthony Dixon
Worcester Polytechnic Institute

III-4 Modeling and simulation of nanoparticle formation and growth in shear flows
Sean Garrick
University of Minnesota

III-5 Influence of particle properties on the yield and selectivity of fast heterogeneously catalyzed reaction
Johannes Khinast
Rutgers University

III-6 Numerical simulation of a chemically reacting gas-liquid flow: CFD modeling of a cool flame vaporizer
Dionysis Kolaitis
National Technical University of Athens

III-7 Numerical simulation of transfer and reaction processes in ethylene pyrolyzer
Xingying Lan
State Key Lab of Heavy Oil Processing

III-8 Modeling turbulent species mixing in HEV static mixers with LES models
Minye Liu
DuPont Company

III-9 Investigations of turbulent mixing in different environments
Mikael Mortensen
Chalmers University of Technology

III-10 Effects of buoyancy and forcing on transitioning and turbulent lifted flames
Joseph Nichols
University of Washington

III-11 CFD studies of reactions at the microscale
D. G. Norton
University of Delaware

III-12 Hybrid finite-volume/PDF method for the simulation of industrially relevant flows
Venkatramanan Raman
Stanford University

III-13 CFD modeling for runaway prevention in chemical reactors
Leszek Rudniak
Warsaw University of Technology
Thursday, 27 May 2003 (continued)

**III-14** Effects of mixing on parallel chemical reactions in a double feeds semi-batch stirred-tank reactor process
Lars Vicum
ETH Zurich

**III-15** CFD study of nano-particle formation by reactive precipitation
Liguang Wang
Iowa State University

**III-16** CFD studies on transitions in flow structure and shear rate distribution from Couette flow reactors to stirred tanks
Hua Wu
ETH Zurich

14:45 – 15:45 Poster Session – Group III (with coffee service)
15:45 – 19:00 ad hoc Meetings, Networking, Free Time
19:00 - 20:30 Dinner
20:30 - 22:00 Social Hour
Friday, 30 May 2003

7:00 - 8:15 Breakfast

Day 5: Interphase transfer, non-Newtonian and liquid-solid flows
Session Chairs: Nitin Kolhapure, DuPont
               Minye Liu, DuPont

8:30 - 9:20 Invited Talk

Recent Advances in DNS of Turbulent Viscoelastic Channel Flows: Understanding Polymer-Induced Drag Reduction
Antony Beris
University of Delaware

9:20 - 9:50 Coffee/Tea Break

9:50 - 12:00 Oral Presentations

Solids distribution in stirred tanks and CFD
Arthur Etchells
DuPont

CFD simulation of dense solid-liquid stirred suspensions
Giorgio Micale
University of Palermo

LES-DPM simulation of vaporization phenomena in a CFB riser
Gilles Flamant
CNRS-IMP

Heat transfer with azimuthal dependence in gas-solid pipe flows: capabilities of an Eulerian-Lagrangian model
Valerie Chagras
University Henri Poincare

Wall-to-bed heat transfer modeling of a gas-solid bubbling fluidized bed
D.J. Patil
University of Twente

12:00 - 13:00 Lunch and departure