

# 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

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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.

**Sunday, 25 May 2003**

17:00 - 19:00	Registration
19:00 - 19:30	Welcome Reception
19:30 - 21:00	Dinner
21:00 - 22:00	Reception

**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

**Tuesday, 27 May 2003** (continued)

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 Modelfrontier*  
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

**Tuesday, 27 May 2003** (continued)

- 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

**Thursday, 29 May 2003** (continued)

- 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