

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.

Successor Program to United Engineering Foundation Conferences

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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