

Program

Computational Fluid Dynamics in Chemical Reaction Engineering IV

**19-24 June 2005
Il Ciocco Hotel and Conference Center
Barga, Italy**

co-sponsored by:

American Institute of Chemical Engineers

Conference Co-Chairs

Anthony G. Dixon

Worcester Polytechnic Institute

Harry van den Akker

Delft University of Technology

Ahmad Haidari

Fluent Inc.

ECI

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Sunday, 19 June 2005

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

Note: All meals will be served in the dining room except for Thursday's Dinner. Locations for all technical sessions, coffee breaks, and social hours locations will be announced on site. No smoking at ECI conference technical or social functions. Please turn cellular telephones to vibrate and conduct telephone conversations outside the meeting room.

Monday, 20 June 2005

07:30 - 08:15 Breakfast Buffet

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

Anthony G. Dixon, Worcester Polytechnic Institute;
Conference Chair

Harry van den Akker, Delft University of Technology; Co-Chair
Ahmad Haidari, Fluent Inc.; Co-Chair

Herman Bieber, ECI Conferences Committee

Day 1: Gas-solid flows: Fluidized-bed and riser reactors

Session Chairs: Paola Lettieri, University College London
Sankaran Sundaresan, Princeton University

08:30 - 09:30 *CFD Models for Polydisperse Solids Based on the Direct Quadrature Method of Moments,*

Rodney Fox

Iowa State University, USA

09:30 - 10:00 Coffee/Tea Break

10:00 – 11:00 *Multiscale Modeling of Gas-Fluidized Beds,*

Martin van der Hoef

University of Twente, Netherlands

11:00 – 11:15 Break

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

CFD-Modeling of the Multiphase Flow in CFB Reactors with Application in Semi-Dry Flue Gas Cleaning,

Christian Schreithofer

University of Leoben, Austria

CFD Modeling of Flow and Reaction Kinetics in a Fluidized Bed,

Fariborz Taghipour

University of British Columbia, Canada

A Modification of the Gibilaro-Foscolo 'Particle Bed Model'

Luca Mazzei

University College London, United Kingdom

Monday, 20 June 2005 (continued)

Simulating the Dynamics of Spouted Beds Using an Eulerian-Eulerian Model,

Cea Finney

Oak Ridge National Laboratory, USA

Discrete Particle Modeling of Chemical Vapor Deposition in the Fluidized Bed Reactor,

Ernst-Ulrich Hartge

Technical University Hamburg-Harburg, Germany

12:30 – 14:00

Lunch Buffet

14:00 - 15:00

Poster Presentations

Experimental and Numerical Analysis of Circulating Fluidized Beds

Elizabeth Cruz

University of New Brunswick, Canada

Characteristic Speeds From Filtered Continuum Gas-Solid Flow Models

Juray DeWilde

Ghent University, Belgium

Simulations of Bubbling Gas-Solid Fluidized Bed Reactors Using the Two-Fluid Model

Havard Lindborg

Norwegian University of Science and Technology, Norway

Towards the CFD Modelling of Bimodal Gas Fluidized Beds

Olumuyiwa Owoyemi

University College London, United Kingdom

Wall Effects in Fixed and Fluidized Beds

Khairyah AL-Hamad

Kuwait Oil Company, Kuwait

Theoretical Modeling of Oil Rich Gaseous Conversion and Fixed Bed Reactor for Fischer-Tropsch Synthesis

Vadim Ermolaev

Moscow State University of Environmental Engineering, Russia

Monday, 20 June 2005 (continued)

Computational Fluid Dynamics Simulations of Transient Thermal Response in a Packed Bed

Matej Komel

National Institute of Chemistry, Slovenia

Comparison of Near-Wall Modeling Approaches for Fixed Bed CFD

Guillaume Leising

Worcester Polytechnic Institute, USA

CFD Simulations of Fixed Beds of Cylindrical Particles

Ertan Taskin

Worcester Polytechnic Institute, USA

15:00 - 16:30 **Poster Session 1** (with coffee on terrace)

16:30 - 19:30 *ad hoc* Meetings, Networking, Free Time

19:30 - 21:00 Dinner

21:00 - 23:00 Social Time

Tuesday, 21 June 2005

07:30 - 08:15 Breakfast Buffet

Day 2: Gas-liquid flows, liquid-liquid flows

Session Chairs: Kostas Kontomaris , DuPont Central R&D
Ludovic Raynal, Institut Francais du Petrole

08:30 - 09:30 *Modeling Some Multiscale, Multiphysics Phenomena in Multiphase Reactors,*
Faiçal Larachi
Laval University, Canada

09:30 - 10:00 Coffee/Tea Break

10:00 - 11:00 *Breaking, Merging and Splashing Bubbles: the Art of Fluid Interface CFD,*
Prof. Stéphane Zaleski
Université Pierre et Marie Curie , France

11:00 - 11:15 Break

Oral Presentations

Parallelization of an Euler-Lagrange Model Using a Mixed Domain Decomposition and a Mirror Domain Technique: Application to Dispersed Gas Liquid Two Phase Flow,
Dadan Darmana
University of Twente, Netherlands

Lattice Boltzmann Simulations of Drop Coalescence and Chemical Mixing,
Xinli Jia
Clarkson University, USA

Experimental and Numerical Study of Mass Transfer in Single Droplets,
Alexander Pawelski
TU-Berlin, Germany

Mass Transfer, Mixing and Chemical Reactions in Deformable Bubble Swarms,
Johannes G. Khinast
Rutgers University, USA

Tuesday, 21 June 2005 (continued)

12:30 – 14:00 Lunch

14:00 - 15:00 **Poster Presentations**

Validation of Bubble Column CFD Model Formulation for Uniform and Non-Uniform Flow Conditions

Sarah Monahan

Iowa State University, USA

Modeling of Two-Phase Plume Formation

Baizin Chen

National Institute of Advanced Industrial Science and Technology, Japan

Computational Fluid Dynamics Simulations of a Bubble Column With a Discrete Population of Bubbles

Abdelhakim Koudil

Institut Francais du Petrole, France

Direct Numerical Simulation of Deformable Bubbles in Wall-Bounded Shear Flows

Fabricio S. Sousa

University of São Paulo, Brazil

CFD Simulation of Turbulent Drop Breakage and Coalescence in a Kenics Static Mixer: Predicted Drop Sizes Compared to Experimental Data

Zdzislaw Jaworski

Technical University of Szczecin, Poland

CFD Study of Large-Scale Aerobic E. Coli Fermentations: Effects of Imperfect Mixing on Process Yield

Jo Maertens

Ghent University, Belgium

Advances In CFD in Modeling Solution Crystallization

Ahmad H. Haidari

Fluent Inc., USA

Simulation of Catalytic Converter With Dynamic Feed Flow

Samy L. Mukadi

University of Alberta, Canada

Tuesday, 21 June 2005 (continued)

Study of Liquid Viscosity Influence on Liquid Holdup in Trickle-Bed Reactors With Structured Packings Via CFD Calculations

Ludovic Raynal

Instut Francais du Petrole , France

Simulation of Single and Simultaneous Injection of Oil and Coke Oven Gas Into the Blast Furnace

Sabine Slaby

Christian Doppler Laboratory for Chemical Engineering at High Temperatures, Vienna, Austria

Simulation of Flow and Chemical Reactions in a Claus Sulfur Converter

Habib Zughbi

King Fahd University of Petroleum & Minerals , Saudi Arabia

15:00 - 16:30 **Poster Session 2** (with coffee on terrace)

16:30 - 19:30 *ad hoc* Meetings, Networking, Free Time

19:30 - 21:00 Dinner

21:00 - 23:00 Social Time

Wednesday, 22 June 2005

07:30 - 08:15 Breakfast Buffet

Day 3: Industrial challenges: Industrial perspective
On CFD and discussion of new application areas

Session Chairs: Minye Liu, DuPont Engineering Technology
Pingping Ma, Air Products and Chemicals Inc.

08:30 - 09:15 *Evolution of CFD as a Tool for Chemical Engineering,*
Richard LaRoche
Fluent Inc., USA

09:15 - 10:00 *CFD: Perspectives of a Commodity Chemical Company,*
Glenn Price
Nova Chemicals, Canada

10:00 - 10:30 Coffee/Tea Break

10:30 - 12:15 **Oral Presentations**

*Integration and Verification of a SO₂-Chemisorption Model for
Computational Spray-Tower Analysis,*
Martin Demuth
University of Leoben, Austria

Can We Use CFD to Predict Mixing Time in Stirred Tanks?
Minye Liu
DuPont Engineering Technology, USA

*Reactor Design Optimization Based on 3D CFD Modeling of
Nitrides Deposition in MOCVD Vertical Rotating Disc Reactors,*
Bojan Mitrovic
Veeco TurboDisc Operations, USA

*CFD Modeling of Trickle Bed Reactors: A Case of Hydro-
processing Reactor,*
Vivek V. Ranade
National Chemical Laboratory, India

12:30 - 14:00 Lunch (for those not on the Optional Excursion)

Optional Excursion to Lucca (departs 12:30, box lunches provided)

Wednesday, 22 June 2005 (continued)

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| 14:00 - 17:30 | <i>ad hoc</i> Meetings, Networking, Free Time (for those not on the Optional Excursion) |
| 17:00 – 17:30 | Afternoon Coffee |
| 17:30 – 19:30 | “Hot topics”
Selected topics will be discussed; each led by a speaker for 10-15 minutes followed by 15-20 min. discussion. Time will be left open for other issues in CFD brought up by attendees.
Lattice Boltzmann Methods: Harry van den Akker (Delft Univ.)
CFD in Industrial Combustion: Jimmy Li (Air Products & Chemicals)
Multiphase Flow Modeling: Bjorn Hjertager (Aalborg Univ.) |
| 19:30 – 21:00 | Dinner |
| 21:00 – 23:00 | Social Time |

Thursday, 23 June 2005

07:30 - 08:15 Breakfast Buffet

Day 4: Single and multiphase chemically reacting flows: CFD with detailed chemistry, fine-particle formation, or other processes sensitive to reactive mixing

Session Chairs: Rodney Fox, Iowa State University

Dirk Roekaerts, Delft University of Technology

08:30 - 09:30 *DNS and LES of Turbulent Combustion,*
Luc Vervisch
LMNF-INSA, CORIA, France

09:30 - 10:00 Coffee/Tea Break

10:00 - 11:00 *Multiscale CFD Simulations of Portable Microchemical Devices for Hydrogen Production,*
Dion Vlachos
University of Delaware, USA

11:00 - 11:15 Break

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

CFD Modelling of Turbulent Mass Transfer in a Mixing Channel,
Torn Solberg
Aalborg University, Denmark

CFD Modeling of Precipitation of Nano-Particles in Confined Impinging Jet Reactor,
Danielle Marchisio
Politecnico di Torino, Italy

Comparative Study of Transported Scalar PDF and Velocity-Scalar PDF Approaches to Delft Flame III,
Dirk Roekaerts
Delft University of Technology, Netherlands

Aggregation and Breakage of Nanoparticle Dispersions in Heterogeneous Turbulent Flows,
Miroslav Soos
Swiss Federal Institute of Technology, Zürich

12:30 - 14:00 Lunch Buffet

Thursday, 23 June 2005 (continued)

14:00 - 15:00

Poster Presentations

Implementation of Bivariate Population Balance Equations in CFD Codes for Modelling Nanoparticle Formation in Turbulent Flames

Alessandro Zucca
Politecnico di Torino, Italy

CFD Modelling of Fast Chemical Reaction in Turbulent Liquid Flows

Bjorn H. Hjertager
Aalborg University, Denmark

Assessment of Gel Formation Conditions in Turbulent Jets

Miroslav Soos
Swiss Federal Institute of Technology, Zürich

CFD Modeling Of Rotary Cement Kilns: Influence Of Characteristics Of Coal Combustion On Clinker Composition, V.

Vivek Ranade
National Chemical Laboratory, India

Simulation of Photo-Reactors in Eulerian and Lagrangian Frameworks

Fariborz Taghipour
University of British Columbia, Canada

15:00 - 16:30

Poster Session 3 (with coffee on terrace)

16:30 - 19:30

ad hoc Meetings, Networking, Free Time

19:30 - 20:00

Bus up Mountain

20:00 - 22:30

Dinner (Banquet) "Rustic Italian Dinner on the Mountain"

Friday, 24 June 2005

07:30 - 08:15 Breakfast Buffet

**Day 5: Liquid-solid flows; Non-Newtonian and laminar flows:
Polymer reactors and processes with complex fluids,
micro/nano-reactors**

Session Chairs: Johannes Khinast, Rutgers University
Daniele Marchisio, Politecnico di Torino

08:30 - 09:30 *Chemical Reactions in Chaotic Flows – Recent Progress and
Future Directions,*
Fernando Muzzio
Rutgers University, USA

09:30 - 10:00 Coffee/Tea Break

10:00 - 11:00 *Simulations of Solid-Liquid Suspensions: From Dilute to Dense,*
Jos Derksen
Delft University of Technology, Netherlands

11:00 - 11:15 Break

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

*Numerical Simulation of a Solubility Process in a Stirred Tank
Reactor,*
Jos Derksen
TU Delft, Netherlands

*The Influence of the Density Difference on the Mixing Process
in Mechanically Agitated Reactor,*
Hristo V. Hristov
Research Centre Rossendorf, Germany

*Modelling of Packed Bed Membrane Reactors for Autothermal H₂
Production,*
Charudatta S. Patil
University of Twente, Netherlands

*Hydrodynamics of Unbaffled Vessels Stirred with Eccentric
Impellers,*
Giusi Montante
DICMA - University of Bologna, Italy

Friday, 24 June 2005 (continued)

12:30 - 14:00 Lunch

14:00 - 14:30 Summary and Conference Adjournment; Departure (bus to Pisa)