



# MULTI-SCALE COMPUTATIONAL MODELING OF CHEMICAL AND BIOCHEMICAL SYSTEMS (MULTIMOD)



## 3<sup>rd</sup> Workshop & Retreat Meeting

Chalkidiki – Greece: 09-10 May 2013

### AGENDA

#### Thursday, 09 May 2013

09:00 – 11:00 Invited Speaker: “Metabolomics and Network Biology for sensitive monitoring in cell culture engineering”. Dr. Klapa Maria (FORTH/ICE-HT)

#### 11:00 - 11:30 Coffee Break

11:30 – 12:00 **Fellows 1:** “Quantum Chemistry Investigation of Fluorinated Copolymer Systems of Industrial Interest”. E. Mavroudakos, D. Moscatelli (POLIMI)

12:00 – 12:30 **Fellows 2:** “Towards Computer-Aided Screening of Ionic Liquids for or Cellulose Dissolution: A Hybrid Model-Based and Data-Driven Methodology”. D.S. Wicaksono, J. Viell, W. Marquardt (RWTH)

12:30 – 13:00 **Fellows 4:** “Incremental Identification of Solution Polymerization Reaction Kinetics: Case Studies”. N. Kerimoglu, A. Mhamdi, W. Marquardt (RWTH)

13:00 – 13:30 **Fellows 6:** “Mathematical Micro-, Meso- and Macro-scale modelling of heterogeneous catalytic loop reactor for the production of polyolefins”. M. Rezaei. (BOREALIS AND CERTH)

#### 13:30 - 15:00 Lunch

15:00 – 15:30 **Fellows 7:** “Particle Characterization Using VIS-NIR Spectroscopy”. G. Emidio, S. Thennadil, J. Morris (USTR)

15:30 – 16:00 **Fellows 8:** “The Assessment of Iron (II) Binding Sites onto Wool Keratin Via Molecular Dynamics” J.K. Marzinek, Y. Zhao, G. Lian, A. Mantalaris, E.N. Pistikopoulos (UNILEVER).

16:00 – 16:30 **Fellows 9:** “Spectroscopic Monitoring of Emulsions Polymerization Using Kubelka-Munk Theory”. N. F. Dehanov, S. N. Thennadil (USTR)

16:30 – 17:00 **Fellows 10:** “Airflow and Particle Deposition in a Dry Powder Inhaler An Integrated CFD Approach”. J. Milenkovic, A.H. Alexopoulos and C. Kiparissides (CERTH)

17:00 – 17:30 **Fellows 11:** “Closing the Loop From in Silico to in Vivo: Modelling and Optimisation of Bacterial Cell Culture Systems”. A. Tsipa, A. Mantalaris, E.N. Pistikopoulos (ICL)

17:30 – 18:00 **Fellows 12:** “Coupling of Population Balance Modelling to Computational Fluid Dynamics” Per J. BECKER, F. PUEL, N. SHEIBAT-OTHMAN (UCBL)

#### 20:30 Dinner

## Friday, 10 May 2013

09:00 – 10:30 Invited Speaker: "Coordination of mitophagy and the mitochondrial retrograde response during ageing". Prof.N. Tavernarakis (IMBB/FORTH)

**10:30 - 11:00** *Coffee Break*

11:00 – 12:30 Invited Speaker: "Development and Regulation of Advanced Therapy Medicinal Products (ATMPs) for Regenerative Medicine" Prof. A.S. Tsiftoglou (AUTH)

**12:30 - 14:00** *Lunch*

14:00 – 14:30 **Fellows 16:** "Hybrid Modelling of Biotech Processes". N. Egwu (BTS)

14:30 – 15:00 **Fellows 17:** "A Biological Relevant Distributed Cell Cycle Model in GS-NS0". D.G. García Münzer, M. Kostoglou, M.C. Georgiadis, E.N. Pistikopoulos, A. Mantalaris (ICL)

15:00 – 15:30 **Fellows 18:** "Growth Kinetics of a Cute Myeloid Leukemia Cells Cultured in 2D and 3D Enviroments`1". M. Fuentes Garí, R. Misener, S. Brito Dos Santos, A. Mantalaris, E.N. Pistikopoulos (ICL)

15:30 – 16:00 **Fellows 19:** "HydrodeNitrogenation of Pyridine over a Sulphided NiMo/Al<sub>2</sub>O<sub>3</sub> Catalyst: a Kinetic Study". C. Shreedhar (UGENT and BP)

16:00 – 17:00 **Coordinator's Report:** Progress Report on MULTIMOD ITN:

- *Scientific:* workplan; objectives; milestones.
- *Training:* in line with Annex I; secondments; collaborations; complementary training; industry exposure.
- *Management:* Financial Aspects; Reporting; Requirements; Any proposed re-orientations of the networks' activities.
- Actions for the Coming Period