

Project no. 238013

MULTIMOD

Multi-scale Computational Modeling of Chemical/Biochemical Systems

Initial Training Network (ITN)



PhD POSITION PAPER

Numerical Solution of Multivariate PBMs

Start date of project: 15 December 2009

Duration: 48 months

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Position N°

18

Host Institution

CERTH

Release 0.1

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1 Introduction

A population balance approach will be employed for the calculation of the dynamic multivariate particle distribution in particulate systems. The population balance models will incorporate the particle morphology effects (i.e., porosity, crystallinity, surface-area etc.) in order to account for the various micro-scale phenomena at the particle level. The research is multidisciplinary as aspects of numerical analysis and computer science (parallel programming) will be applied for the description of classical chemical and biochemical engineering systems such as granulation, polymerization and cell cultures.

2 Present state of the art

Chemical/biochemical particulate processes are often described by univariate, size distributions of particles or cells. This approach assumes that the dynamic evolution of the particle population depends only on a single internal variable (usually particle/cell volume or mass) and that all other properties (e.g., number of radicals, species concentrations, physiological state, age etc.) are evenly distributed among the population. In recent years, it has been recognized that size alone is often not adequate to fully characterize a population and consequently, multivariate population balance models (PBM) have emerged. The functional numerical solution of multivariate PBMs is considered a very challenging task, due the excessive demands in computational requirements. The present advances are driven by the need to develop models for commercial particulate chemical and biological processes that are capable of integrating molecular, micro- and meso-scale phenomena (i.e., molecular kinetics with individual particle and population balance models) to larger scale processes including mixing equipment and fluid flow.

3 Scope

The development of computational tools for the prediction of multivariate particle size distribution (PSD) in biochemical and particulate systems is of prime importance for the design and production of new high-quality products. The present challenges are driven by the need to develop models for commercial chemical and biochemical particulate processes that are capable of integrating nano-, micro- and meso-scale phenomena (i.e., individual particle/cell and population balance models) to larger scale processes including mixing equipment and fluid flow. Furthermore, the functional numerical solution of the multivariate PBE is considered a very challenging task, due the excessive demands in computational requirements.

4 Objectives/Methodologies

A multiscale, multidimensional population balance framework will be developed for commercial particulate chemical and biological processes. Individual tasks will include: (i) Development of different numerical approaches for the solution of multivariate PBEs (e.g., finite-element, sectiobal, high resolution, Monte-Carlo and moment methods) (Month 4-24), (ii) Development of an algorithmic PBM framework that can be integrated with both the larger-scale (i.e. CFD) and smaller-scale (i.e. internal structure, single particle) models

of the process (Month 25-42) and (iii) Application to pharmaceutical granulation, polymerization systems and cell cultures. (Month 32-45).

5 Collaborations/Partners Involved

The numerical modeling framework developed by CERTH will be applied to processes of industrial interest including (a) granulation in pharmaceutical processes (in collaboration with BTS), (b) catalytic polymerization systems (in collaboration with BOREALIS) (c) cell populations (in collaboration with USTR) and (d) emulsion systems (in collaboration with UCBL).

6 Deliverables

D9. Comparative review of multivariate PBE solution techniques.

D10. PBM of catalytic polymerization systems.

7 References

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- [4] Qamar, S., and Warnecke, G., (2007). Solving Population Balance Equations for Two-Component Aggregation by a Finite Volume Scheme. *Chem. Eng. Sci.*, 62, 679-693.
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