Complex Systems Challenges in BioEngineering Modelling and Simulation

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Abstract

Introducao: Bioengineering has a considerable potential for the use of complex systems (CS) in modelling and simulation. Biological systems are built on functional elements, where the large variety of existing chemical and physical properties allow them to present a vast diversity at any scale level. Furthermore, the composites and control structures that build-up from the different levels, tend to form self-organised and regulated mechanisms, all of which are capable to provide adaptation and redundancy of systems that support life. Therefore, CS modeling of cells and colonies is an important challenge in the post-genome era of Biotechnology.

Legacy technology The authors first approach to the use of CS was applied to the study of quality and safety of refrigerated foods during their life cycle. Some of the tested concepts (e.g. elements, composites, structures, agents and scenarios) constitute today a 'legacy technology' for bioengineering process simulation, and therefore, examples of simulations are presented. This approach has however a 'limit of scale' due to the use of the finite element method (the building block), being therefore, better suited for describing macroscale phenomena, such as heat/mass transfer, fluid flow, simple chemical reactions, Michaelis-Menten enzyme mechanics or Monod microbiological growth; and not for simulating the cell and colonies at the mesoscale. Thus, one of the main challenges for bioengineering is to develop strategies that enable the description of systems from the mesoscale to the macroscale.

BioReactor engineering: Mesoscale to macroscale! Simulation tools are now being developed to assist during process prototyping. These include, describing cell dynamics (cycle and metabolism), cell to cell communications and colony dynamics (quorum sensing) inside bioreactors. Such tools present a huge potential to be used in networks, cellular automata (individual based models - artificial life) and information theory for mining relationships, as well as, other pattern recognition techniques that provide information to build mesoscale models and link them to macroscale events. Currently as a *'work in progress'*, the authors present some of their strategies, as well as, theoretical and experimental CS challenges of modelling and simulating the flocculating yeast (*S. cerevisiae*) growth during fed-batch fermentations.