Modeling Uncertainty Analysis in Distributed Systems

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Motivation:

The design of bioreactors is a challenging task because of the simultaneity of transport and reaction phenomena (i.e. cell metabolism, fluid flow and/or heat conduction) inherent to the processes. The high degree of uncertainty when working with living organisms in addition to process operational uncertainties (e.g. daily fluctuations in feed, variations in production levels) and physical property uncertainties adds complexity to this already challenging design problem. Recent progress in both theoretical approaches as well as computer power have renewed the interest of many researchers for rigorous mathematical techniques to handle process design in the presence of these uncertainties (e.g. Grossmann and Co-workers, 1981-1990; Pistikopoulos, 1990 – 2000). In this presentation, we will develop a consistent framework for designing distributed systems in two or three dimensions with full consideration of parameter and model uncertainty. We will illustrate the mathematical programming framework to determine the associated optimal design parameters under material properties and model uncertainty. Our case studies will clearly show advantages of the uncertainty approach over the traditional nominal design of the distributed systems. The advantages of the novel approach for the design of bioreactors with maximum flexibility against uncertain parameter variations will be demonstrated.

Introduction:

Bioreactors in general and fermentation-reactors (or fermenters) in particular, work on the same basic premise -- a product is obtained by the mass culture of a microorganism. In this presentation we shall focus our attention on the mathematical modeling of batch and continuous processes in fermenters. The entire range of fermentation processes can be classified broadly into the following four major groups based on the type of products they produce:

- Biomass
- Microbial enzymes
- Microbial metabolites
- Modify a compound that is added to the fermentation

A typical fermentation process operates in three stages: the pre-mixing stage, the actual fermentation stage and the effluent-treatment stage. The fermentation stage is modeled in terms of a number of variables (e.g. biomass concentration, substrate concentration) and parameters (e.g. growth rate of the biomass, yield of the biomass). There is a lot of literature about the effective modeling of batch and continuous fermentation reactors. Lee and Huang (2000) described a detailed modeling framework of batch fermentation for ethanol production.

Bizukojc and Ledakowicz (2003) discussed a morphologically structured model for the growth and accumulation of citric acid. These models make use of process/model parameters (e.g. the growth rate of microbes, the feed rate of substrate etc.) that are assumed to be known and are treated as constants. Oftentimes, these parameters have associated with them some amount of uncertainty which is inevitable considering the method of their determination. As is obvious, this culminates in uncertain profiles of the variables of concern and that may not be desirable. It is therefore necessary to analyze the effect of uncertainty of parameters on the predictive-capabilities of the relevant model with mathematical rigor.

Methodology:

We will incorporate flexibility index concepts with the transport phenomena i.e. diffusion and convection equations of distributed systems in the presence of parameter and model uncertainties. Our approach assesses the distributed system by solving the transport equations with the help of the discretization scheme i.e. finite volume method and the curvilinear coordinate transformation for complex geometry. First and second order sensitivity maps are applied to improve convergence and robustness of the proposed algorithm. The sparse solver technology will help us to reduce the computational burden in this large scale transport design problem.

In particular we will argue for the product purity concern, ensuring operability and risk management under uncertainty. Furthermore, we will present guidelines for designing the distributed system. Alongside robustness against uncertainties, we advocate multi-objective metrics unifying non-commensurate performance targets such as expected return, acceptable levels of risk. We will also discuss computational difficulties encountered in this large scale distributed system and how to circumvent them.

Significance:

In this presentation we highlight how rigorous uncertainty analysis and transport equations with the detailed bio-reaction mechanism can allow design engineers and plant managers to select the reactors with high performance. Simultaneous consideration of design and uncertainty at the conceptual stage offers higher flexibility and lower expected cost at the operating stage. We will demonstrate with the help of dynamic transport simulations that the traditional approach of nominal design with an over-design to handle uncertainty offers inferior cost performance as compared to our design approach.

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