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Robust analysis of hybrid dynamical systems for 1, 3-propanediol transport mechanisms in microbial continuous fermentation

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ABSTRACT

A better understanding of the biological phenomena observed in cells requires the creation and analysis of mathematical models of cellular metabolism and physiology. In the study of the glycerol continuous bioconversion to 1, 3-propanediol by *Klebsiella pneumoniae*, there are some uncertain factors such as the mechanism about the transports of substances across cell membrane. In this paper, a nonlinear hybrid system which describes the intracellular reductive pathway is presented, according to the possible transport mechanisms of 1, 3-propanediol across cell membrane. The existence, uniqueness, and continuity of the solutions for the nonlinear hybrid system are discussed. It is difficult to measure the concentrations of intracellular substances; so, a quantitative robustness analysis method is proposed. Taking the robustness of intracellular substance concentrations as the performance index, an identification model is proposed, which is subjected to the constraint of nonlinear hybrid dynamical system. Finally, an algorithm procedure is constructed to solve the parameter identification model, and the most possible transport mechanism of 1, 3-propanediol and the optimal parameters of the corresponding system are also given.

1. Introduction

1, 3-Propanediol (1, 3-PD) is an important chemical substance which can be used as a solvent, antifreezing agent or fine chemical engineering substance, especially as a monomer for polyesters, polyethers and polyurethanes. As a result, its microbial production has recently paid much attention due to its low cost, high production and no pollution, etc. [1]. Glycerol bioconversion to 1, 3-PD by *Klebsiella pneumoniae* has been widely investigated since 1980s due to its high productivity.

In 1995, Zeng and Decker [2] proposed a five-dimensional dynamical system of glycerol fermentations, in which the concentrations of biomass, glycerol and products (1, 3-PD, acetate and ethanol) in reactor were considered. Xiu et al. [3] improved the model so that it could well describe the operating conditions in a relatively wide range. Gao et al., Wang et al. and Ye et al. provided further investigations on the five-dimensional dynamical system, including parameter identification, optimal control and dynamical behavior analysis [4–6].

In 2008, Sun et al. [7] first proposed a nonlinear dynamical system involving concentration changes of three intracellular substances (glycerol, 1, 3-PD and 3-hydroxypropionaldehyde (3-HPA)) and two key enzymes (1, 3-PD oxydoreductase (PDOR) and glycerol dehydratase (GDHt)) in glycerol fermentation to 1, 3-PD by *Klebsiella pneumoniae*. The intermediate substance (3-HPA) is not only the product of enzyme catalysis of GDHt but also the substrate of enzyme PDOR. 3-HPA can inhibit the growth of cells and the activity of GDHt [8]. In the model proposed by Y.Q. Sun et al., it is assumed that 1, 3-PD

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