MASS AND ENERGY BALANCES AS STATE-SPACE MODELS FOR AEROBIC BATCH FERMENTATIONS

R. Dondo and D. Marqués
Grupo de Control de Procesos
Instituto de Desarrollo Tecnológico para la Industria Química (INTEC)
Guemes 3450 (3000) Santa Fe – Republica Argentina
e-mail: rdondo@ceride.gov.ar

Abstract:
The main aim of this work is the development of mathematical models of aerobic batch fermentations for its use in estimation and control algorithms. Most batch fermentation models are empirical and simple, and do not provide interrelationships between state variables and measurements. In this work such interrelationships are obtained from mass and energy balances of the fermentation components. Since aerobic fermentations with formation of a single metabolite exhibit three degrees of freedom, three independent kinetic equations are necessary to build the state space model. Test results on the batch fermentation of xanthan gum are presented.

1. Introduction

Many publications have applied advanced control to fermentative processes carried out in continuous or fed-batch bioreactors [Wu *et al.* (1985); Takamatsu *et al.* (1985); Lim *et al.* (1986); San and Stephanopoulos (1986); Williams *et al.* (1986); Modak and Lim (1987); Agrawal *et al.* (1989); San and Stephanopoulos (1989); Shi *et al.* (1989); Harmon *et al.* (1989); Diener and Goldschmidt (1994); reviews by Shioya (1992) and by Shimizu (1993)]. The main obstacle for applying advanced process control to batch fermentations is the poor quality of the processes models, the relative low number of measurements, and the scarcely-known interrelationships between states and measured variables.

In batch fermentations, the main system variables can vary widely along the process. Thus, there is an opportunity for driving the manipulated variables in optimal fashion. Some publications examined the problem of determining optimal control trajectories in fermentors, considering different objective functions and control variables. Constantinides *et al.* (1970) presented probably the first paper that proposed the use of optimal control in batch bioreactors. Reuss (1986) presented a review on the use of optimal control in fermentative process, and only few of the reviewed works considered batch operations. In recent years, Asenjo *et al.* (1995) and Lee *et al.* (1999) presented articles on the optimal control of batch reactors, including experimental validations. In spite of the fact that trajectory optimization is a well-known technique, it has not been widely applied to fermentative processes. The reason is that optimal control results are highly dependent on the process model, and many fermentation models do not accurately represent the dynamic behavior.

Erikson *et al.* (1978) is one of the first publications where mass and energy balances have been used for modeling fermentations. The balances were used to derive optimal operating conditions in continuous single-cell production reactors. Roels (1980) generalized the concepts presented by Erikson *et al.* (1978) to other fermentations (aerobic with or without product formation and anaerobic fermentations); and outlined a scheme for building models on the basis of the available kinetic information. The relevance of macroscopic principles for modeling bioengineering systems was also discussed. Heijnen and Roels (1981) developed a slightly more complex scheme, specific to aerobic fermentations. Simple models were proposed for estimating yield coefficients on substrates with different degrees of reduction. The authors analyzed the effect of the temperature on yields and on the maintenance coefficients. Minkevich (1983) modeled the fermentation as a set of partial metabolisms, and used mass and energy balances for interrelating the partial metabolism kinetics. The influence of intracellular characteristics on the rate of physiological processes and on the culture productivity was discussed. Andrews (1989, 1993) presented a similar scheme, but with the aim of estimating macroscopic yields. Andrews (1989) discussed the limitation of yield values for the different product types.

The mentioned works show the relation between the kinetics of the intracellular processes with different levels of complexity but assuming that the intracellular reaction rates and the mass transfer mechanisms between the cells and its environment are in the steady state. Batch fermentations are time-varying processes, and we did not find any publication on the use of balances onto batch processes.

In this work, we derive a time-varying state-space model that is applicable to aerobic batch fermentations. This work is organized as follows. In section 2, state-space equations for batch fermentations are derived from a model that involves five partial metabolisms. Microscopic balances are used to calculate the relations between partial metabolisms and the net consumption of the main components. Also, macroscopic balances are used to calculate the relations between the partial metabolism rates, the variation of main component