A HYBRID NEURAL MODEL FOR THE PRODUCTION OF SORBITOL AND GLUCONIC ACID USING IMMOBILIZED *Zymomonas mobilis* CELLS

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Abstract— **Only ten years were enough for hybrid neural network-first principle models (HNM) reach a status of a standard industrial tool. This modeling strategy is employed here to represent the production of sorbitol and gluconic acid from glucose and fructose, using permeabilized and immobilized *Zymomonas mobilis* cells. Mass component balances are derived for the substrate concentrations. A multilayered neural network is used to represent the reaction rate. Experimental results were used to develop and validate the model. The HNM allows the elucidation of the phenomena involved in the process. It is observed from the results that the resistance for mass transfer from the liquid to the particles is increased at higher substrate concentrations and that the reaction rate depends on the concentrations of substrate and product in the particles. Additionally, it may be stated that the flexibility of the HNM allows the development of a model that would otherwise be difficult, if based solely on phenomenological principles.**

Keywords— **hybrid modeling methods, neural networks, enzymatic reaction, basket reactor.**

I. INTRODUCTION

The limitations of neural networks (e.g. extrapolation difficulties) naturally led to the development of hybrid models in which they were integrated with other knowledge representations of the process.

A decade ago, Psichogios and Ungar (1992) proposed a hybrid neural network-first principle modeling strategy (HNM) by the insertion of neural networks into phenomenological models to represent parameters of difficult description. Since then, this kind of HNM was adopted for several applications, such as:

- bioreactors (Thompson and Kramer, 1994; Schubert *et al.*, 1994; Fu and Baford, 1996; Van Can *et al.*, 1997; Tholodur and Ramirez, 1996; De Azevedo *et al.*, 1997; Costa *et al.*, 1999; Henriques *et al.*, 1999);
- chemical reactors (Martinez and Wilson, 1998; Molga and Cherbanski, 1999);
- polymerization reactors (Vega *et al.*, 1997; Nascimento *et al.*, 1999);
- metallurgic reactors (Reuter *et al.*, 1993);
- dryers (Cubillos *et al*, 1996; Zbicinski *et al.*, 1996; Mateo *et al.*, 1999);
- flotation plants (Cubillos and Lima, 1997; Gupta *et al.*, 1999);
- pressure vessels (Van Can *et al.*, 1996);
- distillation column (Safavi *et al.*, 1999) etc.

Nowadays, the hybrid neural strategy has evolved into a standard industrial technique (Mogk *et al.*, 2002).

In the present work, modeling is used to aid in the development of a new process: the enzymatic production of sorbitol and gluconic acid using permeabilized and immobilized cells of *Zymomonas mobilis* in a spinning basket reactor.

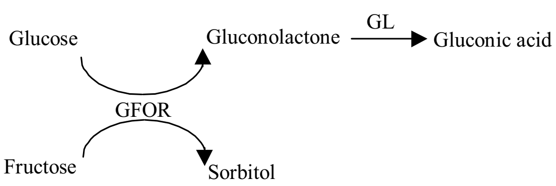
The objective is that the model helps in the understanding of the phenomena that happen in the process and also provides inferences of variables in the particles of immobilized cells.

With that purpose, a hybrid model is introduced here. This model explicitly considers mass transfer of the substrate from the liquid medium to the immobilized cells as well as the reaction rates, under different operational conditions.

It is expected that the resulting model will allow the optimization of the process.

II. METHODS

A. *Zymomonas mobilis*



The enzymatic mechanism for *Zymomonas mobilis* is sketched above. The enzymes GFOR (glucose-fructose oxidoreductase) and GL (gluconolactonase) are present in *Zymomonas mobil*is cells. GFOR is capable of converting glucose and fructose mixtures, oxidizing the first to gluconolactone and simultaneously reducing the