BIODEGRADATION KINETICS OF BENZENE AND TOLUENE AS SINGLE AND MIXED SUBSTRATE: ESTIMATION OF BIOKINETICS PARAMETERS BY APPLYING PARTICLE SWARM OPTIMIZATION

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***Abstract*— This paper aims to describe the microbial biodegradation kinetics of benzene and toluene as single and mixed substrates. Particle Swarm Optimization (PSO) is used as the parameter identification procedure. Initially, the Monod and Andrews models were used. To predict the interactions between the substrates, more sophisticated models of inhibition and the SKIP model were applied. The development of the changes on the competitive inhibition model was also described. The models were evaluated using experimental data on *Pseudomonas putida* F1 activity found in the literature. Simulation results showed that the best description of the biodegradation process of a pure substrate can be achieved by the Andrews model and in the case of a mixture by the modified competitive inhibition model. These results were expected because both substrates are catabolized by the same metabolic pathway through *Pseudomonas putida* F1. The SKIP model also captured the substrate interactions well. The performance of PSO was excellent and the methodology developed in this work can be considered as very efficient.**

***Keywords*— benzene, competitive inhibition, Particle Swarm Optimization, toluene.**

I. INTRODUCTION

The mono-aromatics hydrocarbons benzene and toluene are found in oil derivatives and are widely used in chemical industries as raw materials for synthesis of other products (Phelps and Young, 2001). The benzene is involved in the production of rubber, plastics, pesticides and inks. The toluene is an important commercial chemical product generally used as a dilution agent of inks and as a solvent in the production of resins, glues and oils.

These composites are considered dangerous substances to the human health mainly for being depressors of the central nervous system. Besides, they cause damages to the respiratory, gastrointestinal and reproductive systems. Benzene is proved to be a carcinogenic and mutagen substance (Fernandes *et al*., 2002), being able to cause leukemia. Hence, the extreme toxicity of benzene and toluene and their frequent presence in industrial discharges and fuel spilling as environmental contaminants have accelerated the research efforts to develop the green biodegradation technologies based on the last achievements of system modeling and optimization. The key knowledge for the biodegradation process optimization of toxic compounds must be searched about the kinetics of the microbial growth and the relationship between the substrates in the system.

Several papers showed that microbial metabolism of a compound in a mixture can be strongly influenced by the presence of other compounds in the mixture (Reardon *et al*., 2000; Deeb *et al*., 2001; Brandt *et al*., 2004). In order to understand synergetic and/or antagonistic interactions (Jo *et al*., 2007) of the substrates in the mixture it is necessary to consider the metabolic pathway of each compound for the microorganism. According to Harder and Dijkhuizen (1982) homologous and heterologous compounds are those that use the same and different metabolic pathways, respectively. The presence of other compounds in a mixture of homologous substrates can result in positive effects due to the increased microbial growth and the induction of degradative enzymes. Nevertheless negative effects such as competitive inhibition have been also reported (Chang *et al*., 1993; Oh *et al*., 1994; Bielefeldt and Stensel, 1999; Reardon *et al*., 2000; Lin *et al*., 2007), decreasing the biodegradation substrate rates in the mixture.

Hamed *et al*. (2003) studied the biodegradation of benzene and toluene, individually and in a mixture, by using *Pseudomonas putida* F1 strain. The authors experimentally investigated the interactions among the substrates in the mixture. However, their efforts did not extend beyond the formalization of these phenomena in mathematical models.

The main objective of this paper is to evaluate the kinetics of microbial biodegradation of benzene and toluene through different hypothesis on microbial degradation activity and by validating them through the use of experimental data published in the literature. This goal was achieved by applying Particle Swarm Optimization during the parameters identification procedure.

II. MATHEMATICAL MODEL

A. Microbial Kinetics of Compounds Utilization

The modeling strategy was built by gradually increasing complexity on the kinetic hypothesis related to the biodegradation process in the population level. Specific growth rates described by the Monod (Eq. 1) and An-