

# **ESTIMABILITY ANALYSIS AND PARAMETER IDENTIFICATION FOR A BATCH EMULSION COPOLYMERIZATION REACTOR IN THE PRESENCE OF A CHAIN TRANSFER AGENT**

B. Benyahia , M.A. Latifi , C. Fonteix , F. Pla  
Laboratoire des Réactions et Génie des procédés, UPR 3349 CNRS,  
ENSIC INPL, Nancy-Université 1 rue Grandville, BP 20451, 54001 Nancy Cedex, France  
Tel : ++(33) 3 83 17 52 34, Fax : ++(33) 3 83 17 53 26  
Email addresses : {brahim.benyahia,[latifi](mailto:latifi@ensic.inpl-nancy.fr),[fonteix](mailto:fonteix@ensic.inpl-nancy.fr),[pla](mailto:pla@ensic.inpl-nancy.fr)}@ensic.inpl-nancy.fr

This paper deals with the development of a mathematical model for the emulsion copolymerization of styrene and butyl-acrylate in the presence of n-dodecyl mercaptan as a chain transfer agent.

The model consisted of a system of differential algebraic equations issued from population balance. It involves 49 unknown kinetic and thermodynamic parameters, many of them being impossible to be accurately estimated, due to a lack of experimental data.

So, considering that the main limitations to the parameters estimability are their weak effect on the measured out-puts and the correlation between these effects, a method based on the calculation of a sensitivity matrix was developed and allowed to determine a subset of the 21 most influential parameters.

A stochastic optimization, followed by the determination of the corresponding confidence intervals, allowed then, using a genetic algorithm, to identify these parameters. The 28 non estimable parameters were taken from the literature.

The model was then validated through additional experiments carried out in batch and fedbatch reactors.

Moreover, the results clearly showed that the model was able to predict the time-evolution of overall conversion, amounts of each residual monomers, number and weight average molar masses of the resulting copolymers and average diameters of the latex particles for different experimental conditions.

Finally, the model was successfully used for the optimization of the morphology and the glass transition temperature of the final products.