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

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Summary

In this paper we have developed an estimability analysis method to identify the subset of potentially estimable parameters from the proposed experimental data. The emulsion copolymerization model involves 59 unknown parameters. The complete set of parameters cannot be estimated from the experimental measurements available. Thanks to the method developed, 21 parameters were selected and identified. The non estimable parameters were set to nominal values taken from literature. The mathematical model was validated under both batch and fed batch conditions.

Keywords

Estimability analysis, parameter identification, experimental measurements.

Introduction

Emulsion polymerization is an important industrial process used to produce a great variety of polymers for multiple uses (e.g. paints, adhesives, coatings, varnishes…). The complexity of emulsion polymerization systems arising from factors such as their multiphase nature, nonlinear behavior, the large number of parameters involved in the model, and sensitivity to disturbances, induces intense difficulties on modeling and makes the development of optimization procedures of emulsion polymerization reactions a very challenging task.

Accurate estimation of the model parameters is required to obtain reliable predictions of the products properties (polymer and latex). However, due to the mathematical model structure and to a possible lack of measurements, the estimation of some parameters may be impossible. The main limitations to the parameters estimability are their weak effect on the measured outputs and the correlation between these effects. The method developed in this paper consists to assess whether the model parameters will be estimable from existing or proposed experimental data, and determine the subset of the most influential parameters that can be estimated from the data when the complete set of model parameters cannot be estimated.

The mathematical model for the emulsion copolymerization of styrene and butyl acrylate in the presence of n-dodecyl mercaptan as a chain transfer agent has been developed. This model involves 49 parameters among which 21 parameters were selected by the estimabality analysis method. The 28 other parameters were taken from the literature.

The unknown 21 parameters were identified from the experimental measurements available (i.e., the global conversion, number and weight molecular weights, average particles diameter, and styrene residual mass fraction) by using a genetic algorithm. The process model was finally validated by several new experiments carried out in batch and fed-batch conditions.

The resulting validated model is then used for the optimization of the end-use properties of the produced products (polymer and latex).