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Multiobjective dynamic optimization of a fed-batch copolymerization reactor

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1 Introduction

Multiobjective optimization problems are encountered in most real-world applications and more recently in chemical processes ([1], [2], [3], [4]). Since such problems involve several objective functions with conflicting nature, the final optimum is not unique but a set of non dominated solutions (the Pareto front) which show a trade-off among the whole objectives. A decision support approach is then used to rank the Pareto solutions according to the decision maker's preferences.

Emulsion polymerization is an important industrial process used to produce a great variety of polymers of multiple uses (e.g. paints, adhesives, coatings, varnishes). Moreover, it has significant advantages over bulk and solution polymerization processes such as heat removal capacity and viscosity control. These advantages result mostly from the multiphase and compartmentalized nature of the emulsion polymerization which allows the production of polymers of high molecular weight at high polymerization rates, delivering a high versatility to product qualities. However, the complexity of emulsion polymerization systems arising from factors such as the multiphase nature, nonlinear behaviour and sensitivity to disturbances induce more intense difficulties on modelling and make the development of optimization procedures of emulsion polymerization reactions a very challenging task.
Molecular weight distribution (MWD), polymer microstructure, glass transition temperature (T_g) and particle size distribution (PSD) and morphology are the main parameters witch strongly govern the end-use properties of the products (latex and polymer).
The present paper deals with a multiobjective dynamic optimization of an emulsion copolymerization fed-batch reactor. The aim is to produce core-shell particles with specific end-use properties by using two criteria subject to a set of tight operational constraints and the mathematical model of the system. The nondominated zone (Pareto's domain) is obtained by using evolutionary algorithm. The ranking is therefore obtained by decision making support.

2 Formulation and results

The process model was developed and validated for the batch and fed-batch emulsion copolymerization of styrene and butyl acrylate in the presence of n-C12 mercaptan as chain trans-

fer agent ([5]). The objective of the model is to predict different variables including overall monomers conversion, number and weight average molecular weights, particle size distribution and residual monomer fractions. The objective of the process is to produce core-shell particles with a specific end-use properties depending on the glass transition temperature profile (Fig.1). The monomers used (styrene and butyl acrylate) in the copolymerization process have different reactivity ratios and there polymers have very different glass transition temperature (-54 $°C$ for butyl acrylate and 100 $°C$ for styrene). The key feature of the optimisation problem is to determine optimal feed rate profiles necessary to control polymerization reactions in order to produce particle with a designed morphology and glass transition temperature. Two objective functions have been selected for the optimization of this process. The first one is to minimize the error between the glass transition temperature and the desired profile. The second objective is to maximize conversion at the end of the process.

$$
\begin{aligned}
Minf = [f_1, f_2] & \\
& f_1 = \frac{1}{t_{fc} - t_0} \int_{t_0}^{t_{fc}} |T_g - T_{g1}|\, dt + \frac{1}{t_{fs} - t_{fc}} \int_{t_{fc}}^{t_{fs}} |T_g - T_{g2}|\, dt \\
& f_2 = -X(t_f) \\
s.t. \quad & \dot{\boldsymbol{x}} = \boldsymbol{f}\left(\boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{p}, t\right) \\
& \frac{1}{t_{fc} - t_0} \int_{t_0}^{t_{fc}} \left(0.9 - X(t)\right)^2 dt \leq \epsilon^2 \\
& \boldsymbol{u}_{inf} \leq \boldsymbol{u}(t) \leq \boldsymbol{u}_{sup}
\end{aligned}
\tag{1}
$$

where T_g is the glass transition temperature at an instant t, T_{g1} the desired glass transition temperature for the core, T_{g2} the desired glass transition temperature for the shell, t_{fc} and t_{fs} the times necessary to feed the core and the shell production respectively, $X(t_f)$ are conversion and the end of the process and $\boldsymbol{u}$ the control vector (feeds and time periods).

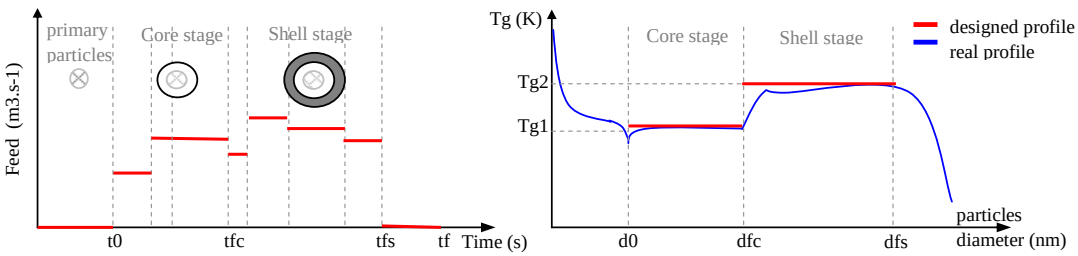

Fig. 1. optimal feed rates and glass transition temperature profiles

The set of the non dominated solutions (the Pareto front) was obtained by an evolutionary algorithm. A decision support approach (MAUT : Multiple Attribute Utility Theory) is then used to rank the Pareto solutions according to the decision maker's preferences. Finally, the resulting optimal solution is implemented to the real system (Fig.2)

3 Conclusions

In this work, multiobjective dynamic optimization problem has been addressed to determine optimal feed profiles necessary to produce core-shell latex particles with specific end use properties. This has been achieved by tracking a designed glass temperature profile while maximizing the final conversion. The non-dominated solutions were obtained and ranked by using MAUT strategy. The simulations of the best solution showed a good agreement with the desired profiles.

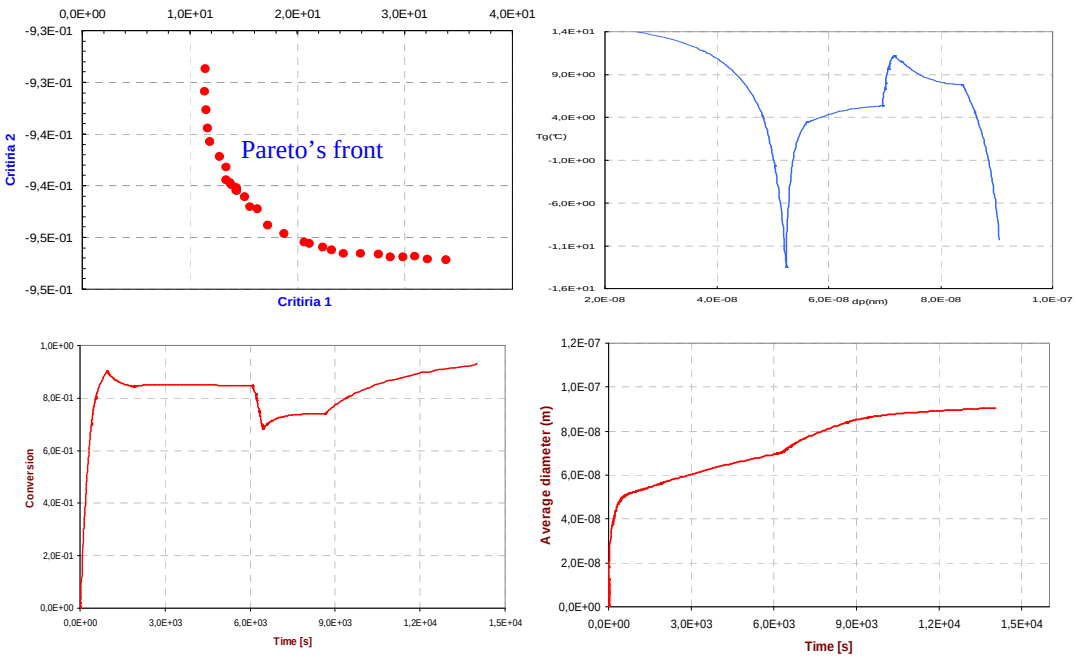

Fig. 2. Pareto's front and the main results related to the optimum solution (glass temperature profile, the overall conversion and the average particles diameter)

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