STEADY STATE OPTIMIZATION OF THE CYCLOHEXANOL PRODUCTION UNIT

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Abstract

The main objective of this paper is to cover the first stage of a real time optimization project for a cyclohexanol production multiphase reactor. Firstly, the optimization problem is stated and the upper layer of a two layers real time optimization approach is solved off-line. Some equations of the steady state process model show to yield a difficult NLP. The mathematical steady state model is validated with industrial data and it is based on mass, energy and momentum balances. Several simulation results are presented which show that the resulting optimization problem is a complex one. Failure of convergence may occur depending on the code for solving the NLP, but improved operating conditions may be reached.

Keywords

Optimization, Production of Cyclohexanol, Multiphase Reactor.

Introduction

The operation of a chemical plant should supply several requirements of safety, quality, environmental laws and economic tasks. The execution of the economic and operational goals, however, should be made concomitantly with the continuous operation of the plant. Thus, the great challenge for this century beginning is to propose alternatives of solving this problem. For this it is proposed the real time integration of continuous chemical processes, that is considered as an area of point and incipient research. The real time optimization can be performed by two approaches, namely, one layer and two layers. The one layer real time optimization (Figure 1) is built up in such way that the control and the optimization problems are solved together. To make the solutions easier, a common procedure is to use a linear objective function in the controller or to linearize the economical objective function (Gouvêa and Odloak, 1998), since most of such objective functions are nonlinear. However, the inclusion of the linear approximation of the economical objective function in the predictive controller objective function may lead the closed loop system to be unstable, so that a suitable approach is to use the economical nonlinear optimization problem. Moreover it is very sensitive to model mismatch and if the prediction of the optimal steady

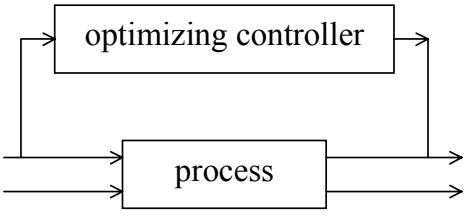

Figure 1. Schematic of the one layer real time optimization

state is performed through a rigorous process model, the dimension of the optimization problem can be too large which may make it difficult to calculate the control actions in a short period of time. Using simplified process models, as e.g. linear identified process models, may not be adequate as important pieces of information can be lost. So, in these cases the more traditional two-layers approach, schematically shown in Figure 2 may be preferred. This

approach may be seen as a hierarchical control structure, in such way that some advanced control algorithm, working as a lower layer, has as a task to keep the process in the set-points defined by an optimization block. Both layers are in somehow completely independent, in the way they define their parameters based on the solutions of each objective function. The dimension of the problem and the fact that some predictive control strategy can be robustly tuned by several available techniques, make this approach to be popular.

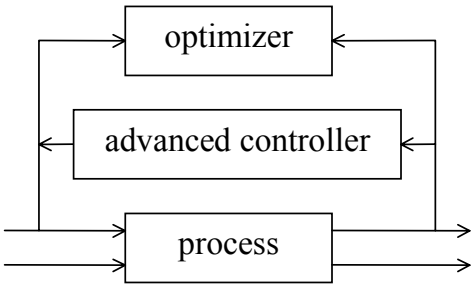

Figure 2. Schematic of the two layers real time optimization

To reach the real time integration initially it should develop the steady state optimization of chemical processes. Because of that, in this work the cyclohexanol production optimization will be presented using a modeling in steady state.

In the next section, the cyclohexanol reactor is briefly described as well as some characteristics that the optimization strategy must have. After that, the optimization problem is solved and finally the work is concluded given direction to further research.

Production of Cyclohexanol

The choice of this process is due to the fact of this substance to be a intermediate for obtation of industrial products of great commercial value as the nylon. The reactor (Figure 3) is composed by tubular modules immersed in a boiler. Some of the modules are constituted by concentric tubes through where the reagents and the coolant flow. Some modules, through where the only reagents flow, are used concentric tubes. The reagent flow from one module to another and the coolant is added to each of the modules. The coolant stream, that comes from the boiler and eventually of a new feeding of condensed (make-up), is divided among the tubular modules, with different flow rates.

The deterministic mathematical model used to describe the reactor is based on the work by Santana (1999) and Toledo et al. (2002). This model considers the peculiarities of tubular modules that compose the reactor. The process model is constituted of conservation laws of mass, energy and momentum. The mass and energy balance are in the form, respectively:

$$\frac{dC}{dz} = f\left(C, T, P, Tr_n, \cdots\right) \tag{1}$$

$$\frac{dT}{dz} = f\left(C, T, P, Tr_n, \cdots\right) \tag{2}$$

where C is concentration, T is temperature, P is pressure and Tr_n is refrigerant temperature in the n-tubular module. Moreover, equations for predicting the heat coefficients must be present as well as a way to describe evaporation that may occur, depending upon the operating conditions. Each of these equations must be applied to each module for both regions, namely, the tubular and annular. Since the reactor is essentially a tubular one, axial dispersion is considered. Thus, the steady state process model presents a set of ordinary differential equations if radial dispersion is neglected, which is, together with the hypothesis that the solid-liquid phase is a single pseudo-homogenized fluid, a reasonable simplification that can be made in order to reduce the complexity of the process model. The mathematical model was validated with industrial data.

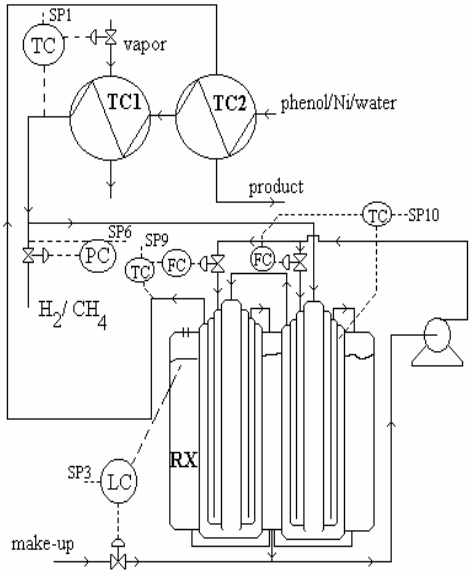

Figure 3. The cyclohexanol reactor

Thus a model describing the process must be able to characterize different phenomena are not easily described. Model mismatch affects the prediction of the steady state operational point which in turn affects the economical objective function.

Optimization Problem

Choice of Variables

Due to the process peculiarities, the economical objective considered is to maximize the production of cyclohexanol while maintaining the phenol concentration at the exit of the reactor below environmental restrictions and the temperature in each tubular module in an allowable value range. There are several manipulated variables that can be used to attain optimal operation reactor. In this stage, the flow rate of each coolant stream is manipulated as well as the temperature of the feed stream and the mass flow rate of phenol. To prove the influence of the flow rates of coolant stream (qr1-qr6) was developed the factorial design as a procedure of sensitivity analysis. This method is based on the selection of a fixed level number to each variable and executes all possible combinations. Each variable is tested at two level, a superior (+) and an inferior (-). In this work it was used a deviation of ±10%, which is in accord to the real operating conditions range. The statistically significant principal effects of the variables on mole fraction of phenol in the liquid phase for a 95% confidence level are presented in Figure 4.

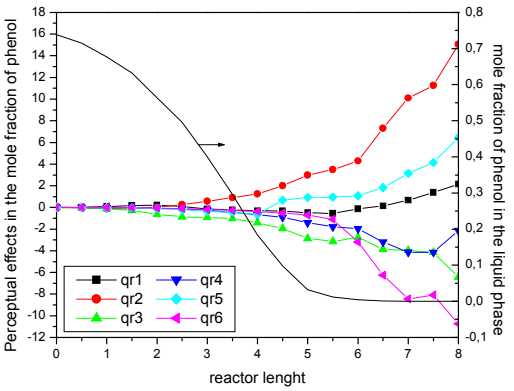

Figure 4. Perceptual effects in the mole fraction of phenol in the liquid phase

It can be seen by this figure that the flow rates of coolant stream (qr1-qr6) have significant principal effects in the mole fraction of phenol in the liquid phase, which is a crucial variable for the process.

Optimization Algorithm

To implement an optimization algorithm based on SQP technique (Successive Quadratic Programming) presented in the literature taking into account economical and equipment operability objectives, the gradient of the objective function and of the restrictions related to the decision variables must be provided. There are some way to make it. One procedure known as the integral approach (Tanartkit and Biegler, 1995) is to integrate the differential equations so that the NLP solver treats them as implicit algebraic non-linear equations. This procedure however may drastically increase the CPU time depending on the NLP solver used. One way to avoid integration is to discretize the differential equations as e.g. proposed by Renfro et al. (1987) among other authors (e.g. Logsdon and Biegler, 1993) who suggest to apply orthogonal collocation. This procedure is known as the discrete approach. In this work the first order derivatives were evaluated numerically by finite differences, which can generated several mismatches in the optimal operational point evaluation and failures of convergence.

To illustrate a model mismatch that can occur, a typical phenol mole fraction profile for the reactor is show in Figure 5. In this system there is a catalyst deactivation which means that the model has to be identified continuously. As can be seen the model mismatch can be considered small but, even so, it is significant to bring difficulties for the process optimizations.

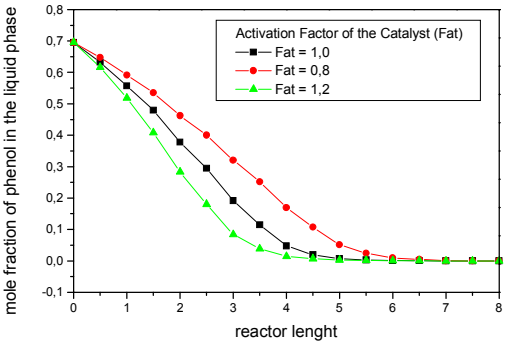

Figure 5. Effect of catalyst deactivation in the mole fraction of phenol in the liquid phase

Results

The constraints of the optimization problem are given in Table 1. Table 2 shows the values used for the coolant temperature, the temperature in the boiler and the composition of the feed. The temperature values are normalized.

Table 3 shows the optimal point obtained (case 1 of Table 3) when applying the SQP of Schittkowski (1985) to the nominal point, which the decision variables are normalized. The values in this table were obtained after 69 interactions. Moreover a line search failure occurred and violation on the Karush-Kuhn-Tucker condition is about 380, i.e., convergence did not occur to a minimum stationary point. So here it can be seen that obtaining an optimal operational point is not that easy.

Table 1. Process constraints.

	qr_i	T_1	T_2	T_3	T_4	T_5
Upper bound	200	0.778	0.778	0.778	0.778	0.778
Lower bound	4000	1.167	1.250	1.389	1.500	1.444
	T_6	T_7	T_8	F_{phenol}	$x_{c,phenol}$	T_{feed}
Upper bound	0.778	0.778	0.778	4000	1	0.778
Lower bound	1.333	1.167	1.111	7500	0.9993	1.033

In order to evaluate if the upper bound on the flow rate of phenol could be achieved it was performed several simulations in which the constraints were tighter than those in Table 2 and were relaxed to those values of Table 2. An intermediate starting point was generated which is also shown in Table 3 (case 2) together with the optimal point (case 3) predicted for this starting point. Note that a significant increase in the production can be achieved. However, this last point (case 3) does also not correspond to a minimum stationary point of the NLP. Moreover, a significant violation on the temperature profile constraint is observed. Here the maximum number of iterations of the SQP algorithm was arbitrarily set to 40 iterations.

Table 2. Constant values used for the optimization problem.

$T_{rf,0}$	Ts,ca	$\frac{Ni}{phenol}$	$\frac{H_2}{phenol}$
0.556	0.933	0.05456	0.0699
$\frac{H_2O}{phenol}$	$\frac{cyclohexane}{phenol}$	$\frac{cyclohexanol}{phenol}$	$\frac{CH_4}{phenol}$
0.0357	0.007292	0.1846	0.002263

Table 3. Optimal operational point predicted.

Case	$T_{al,1}$	$F_{rf,1}$	$F_{rf,2}$	$F_{rf,3}$
1	0.878	0	0	0.002
2	0.769	0.013	0.195	0.456
3	0.878	0	0	0
$F_{rf,4}$	$F_{rf,5}$	$F_{rf,6}$	F_{phenol}	Objective function
0.091	0	0.998	0.797	0.795
0.751	0	1	0.342	0.614*
0	0.017	1	0.950	0.871**

* is the starting point considered for **

Conclusions

In this paper it was analyzed the off-line solution of the upper layer of a typical real time optimization strategy applied to the maximization of cyclohexanol production. A steady state rigorous model was used to describe the process. The model was used to solve an optimization problem of maximizing the production of cyclohexanol while maintaining the concentration of phenol strictly below environmental specifications and while controlling the temperature profile along the reactor in order to avoid deactivation of the catalyst. The optimization problem is a NLP problem possessing differential equations and non-linear algebraic equations and thus exhibits a highly non-convex behavior. In spite of this, when the optimization problem is solved off-line, better operational points can be easily established. However the NLP code used for the simulations could fail to produce a minimum stationary solution of the NLP. This is because it makes use of convex approximations of the Hessian matrix of the Lagrangian function of the NLP. Therefore, since a real time implementation is sought, some further research must be performed. First the estimator for updating the model parameters should be established. Moreover non-convex SQP codes should be preferred (Gouvêa and Odloak, 1998, Lucia et al., 1997) or alternatively modifications in the real time optimization strategy may be introduced in order to enhance its robustness. For the former, discretization of the model must be performed and for the latter conditions must be introduced in order to validate the solution of the optimization layer. Furthermore, for the establishment of the real time optimization strategy dynamic simulations must be performed. Disturbances must be simulated and a criterion for the establishment of steady state must be chosen.

Acknowledgments

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