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Optimal temperature control of an industrial batch reactor with regard to swelling

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Abstract

The contribution of this work deals with the optimization of the temperature profile of a three-phase batch reaction with regard to swelling phenomena. The optimization procedure is carried out in the form of an optimal control problem. The system is modeled using a dynamic first-principles model for the reaction which is linked to a hydrodynamic model.

Keywords batch reactor swelling, optimal control, dynamic, hydrodynamic model

1. Introduction

Reactor swelling phenomena can produce significant productivity losses if this is not considered during process operation. Reactor swelling occurs when the vessel content level rises due to a gas or vapor stream that passes through the liquid. The vapor or gas stream can have different sources: gas is injected in liquid phase of the reactor where a reaction has to be carried out; or it occurs when the reaction produces a vapor phase product which travels to the reactor surface. In this work it is shown that using a reaction and a hydrodynamic model the operation improvement of an industrial size reactor using optimal control is possible.

2. Problem Statement

In the beginning of the process operation, until the complete dissolution of component A, the reactor system consists of three phases: solid, liquid and gas. Four equilibrium reactions in series take place in the liquid phase and a catalyst is used in solubilized form. A solvent is not used in the reaction step of this process. The reaction scheme is as follows:

$$A_s \rightleftharpoons A_l \quad (1)$$

$$A_l + B \rightleftharpoons C + D \quad (2)$$

$$B + C \rightleftharpoons E + D \quad (3)$$

$$B + E \rightleftharpoons F + D \quad (4)$$

$$B + F \rightleftharpoons P + D \quad (5)$$

where A_s and A_l represent component A in solid and liquid phase, respectively. Raw materials are component A and B; components C, E, F are intermediates and D is the gaseous by-product and P is the desired product. The production of component D creates a vapor flow that travels to the reactor mass surface and produces a certain void fraction in the liquid mass. The extent of the void fraction is dependent on the vapor hold-up in liquid phase which is dependent on the vapor flow rate and implicitly on the reaction rate of product D. In this work an optimum temperature profile is calculated which will not rise the reactor content level above a maximum value.

2.1. Methodology

In order to carry out the proposed reactor operation optimization, process models are developed and validated. The reactor model used for optimization has two parts: a first principles part that describes the production rate of component D and a hydrodynamic model which calculates the level of reactor content based on the vapor flow rate.

2.2. The reaction kinetics model

The reaction is modeled using an irreversible reaction model due to the fact that component D hold-up in liquid phase is not significant. The kinetic model is described by Simon et al. [1]. The goal of the optimization is to calculate the safest optimal temperature profile with regard to swelling. This can be achieved

by two ways: the equilibrium reaction is modeled as irreversible reactions; therefore the formation rate of product *D* is the maximum at any time. This assumption is not too far from the reality and therefore is acceptable. The second way is to choose the most conservative hydrodynamic model, which will predict the highest volume rise for a certain gas flow rate. For this three hydrodynamic models are tested: the bubbly, churn-turbulent [2] and the Kataoka-Ishii model [3].

2.2.1. The hydrodynamic models

In order to describe the effect of liquid swelling the pool void fraction α is calculated using a hydrodynamic model. The swelled height *H* [m] in terms of the average pool void fraction and the height of the resting liquid H_0 [m] is given by Eq. (6):

$$H = \frac{H_0}{1-\alpha} \tag{6}$$

Unfortunately specially designed experiments were not carried out in order to verify the hydrodynamic models. However, plant data of component D evacuation rate from the reactor was available. The volumetric accumulation rate of component D was used to calculate the swelling height of the reaction vessel during normal operation. This calculation was carried out by converting the volumetric accumulation rate into vapor velocity using the liquid density, the reactor area, pressure and temperature. The vapor rate was used to calculate the reactor height during the process operation. The calculated levels are in the range of the expected reactor level values therefore it is concluded that the hydrodynamic model can be used for modeling the swelling phenomena. It was concluded that the bubbly model calculates the highest reactor level; therefore it is the most conservative and it will be used in the reactor temperature optimization.
The connection between the chemical reactor model and the hydrodynamic model is made by the formation rate of component *D*. Using the ideal gas law this molar rate is converted into volumetric flow rate and by division with the reactor area is converted into gas velocity. Using the hydrodynamic model and the calculated gas velocity the void fraction α and the swelled reactor level *H* is calculated.

2.2.2. The optimal control problem

The optimization of the batch reactor with regard to swelling can be regarded as to determine the temperature profile which will not cause the level to rise over a

maximum value. The objective function is to maximize the component *B* depletion or to minimize the content of component *B* at final time and the control variable is the temperature. The inequality path constraint is incorporated by penalizing the objective function. The optimal control optimization problem is formulated in Eq. (7-10):

$$Obj \overset{!}{=} Min[nB(t_f) + \\ + C * \left(\sum_{k=1}^{NS} \int_{t_{k-1}}^{t_k} \left[\max(0, c_k^{in}(n(t), dn(t), y(t), T(t), v_{\mathrm{Re}ac}, t)) \right] dt \right)] \tag{7}$$

Subject to:

$$G(Rdae(dn, n, T, v_{\mathrm{Re}ac}, c_{\mathrm{Re}ac}^{Model}), Hydro(dn, T, P, v_{\mathrm{Re}ac}, c_{Hydro}^{Model}), t_f, t) = 0 \tag{8}$$

$$Y(H_{\max} - H_r(t), t_f, t) \geq 0 \tag{9}$$

$$U(T_{\max} - T(t), t_f, t) \geq 0 \tag{10}$$

where *nB* is the component *B* mol number, t_f is the final time, *C* is a large scalar, *t* is time, NS is number of stages, c_k^{in} is the inequality constraint, *dn* is the accumulation or consumption rate of all components (state derivative vector), n is the mol number of all components (state vector), T is the optimizer proposed temperature. In addition there are upper and lower bounds on the state (n), design ($v_{\mathrm{Re}ac}$) and control (*T*) variables. *G* contains the set of dynamic equations and the set of equality constraints formulated in the form of algebraic equations, *Rdae* is the DAE solubilisation and kinetic model, v_{Reac} is the vector of reaction mass specific constants, $c_{\mathrm{Re}ac}^{Model}$ is the vector of reaction model specific parameters, *Hydro* is the hydrodynamic model, c_{Hydro}^{Model} is the vector of hydrodynamic model specific constants and parameters, *Y* is the inequality path constraint, H_{max} and $H_r(t)$ are the maximum level and calculated reactor content level, respectively. *U* is the constraint on the control variable, T_{max} is the maximum temperature. The final time was chosen when it was considered that swelling cannot pose any problems. The solution of the

optimization problem (the temperature profile values) lies on the path constraint and is bounded by the maximum reactor content level value.
The solution of the optimal control problem in this work is based on the control vector parameterization using a piecewise-constant approximation over equally spaced intervals for the temperature. This optimization method is described by Edgar and Himmelblau [4].

2.3. Results& discussions

In Figure 1 the calculated optimal temperature profile and the resulting reactor level is shown. From implementation point of view it is important that the optimal profile is as simple as possible, therefore the optimization was carried out using fewer number of constant temperature intervals, as well.

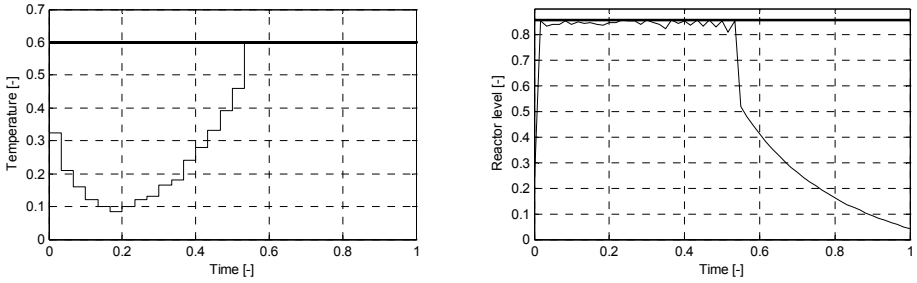

Figure 1 The optimal temperature profile with 20 time intervals (left) and the calculated reactor content height (right). Bold straight lines represent upper control variable and path constraints, respectively.

Additionally the impact on the optimal temperature profile and reaction rate of the liquid surface tension value was analyzed, by running an optimization scenario with half of the original surface tension.

The end point performances compared with the current industrial performance are compared in Table 1.

Table 1 End point values of component B mass for the industrial and calculated optimal temperature profiles

	Number of control intervals					
	20	12	3	2		
				Original surface tension	Reduced surface tension	Industry
Component B end point value improvement %	36	35	33	30	17	0

3. Conclusions

In this work we presented the calculation of the optimal temperature profile for a batch reactor operated under swelling conditions using optimal control. For this we developed a chemical reaction model which was linked with a hydrodynamic model. The resulting temperature profile was simplified in order to allow a simpler implementation. It is concluded that even the simplest optimal temperature profile shows a 30% improvement compared to the current operation.

References

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