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Model Reduction Techniques for Dynamic Optimization of Chemical Plants Operation

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Abstract

The application of model reduction techniques in the context of dynamic optimization of chemical plants operation is investigated. The focus is on the derivation and use of reduced models for the design and implementation of optimal dynamic operation in large-scale chemical plants. The recommended procedure is to apply the model reduction to individual units or groups of units, followed by the coupling of these reduced models, to obtain the reduced model of the plant. The procedure is flexible and accurate and leads to a major reduction of the simulation time.

Keywords: model reduction, dynamic optimization, alkylation

1. Introduction

The strong competition in the industrial environment nowadays demands for economical operation of chemical plants. This goal can be achieved in two ways, which do not exclude each other. One approach is to continuously respond to the market conditions through dynamic operation. A second approach is to develop control systems that maintain the steady state or implement the optimal dynamic behaviour. For the first approach, the economical optimality is achieved through dynamic optimization. For the second approach, the development of the plantwide control structures to achieve stable operation is of paramount importance.

However, both approaches presented above require dynamic models of the chemical plant. The quality of the model is crucial for achieving the objective: the model must represent the plant behaviour with good accuracy, but the complexity must be limited because both applications require repeated solution during limited time. Another requirement is that the model is easy to be maintained and adapted to future plant changes.

The order-reduction of the process model could offer a solution. Several linear [1] and nonlinear techniques [2] have been developed and their application to different case studies reported. Although significant reduction of the number of equations is achieved, the benefit is often partial, because the structure of the problem is destroyed, the physical meaning of the model variables is lost and there is little or no decrease of the solution time [3].

In this contribution, the derivation of the optimal control profiles is realised by using a reduced model obtained through the model reduction with process knowledge approach. The procedure takes into account the inherent structure that exists in a chemical plant in the form of units or groups of units that are connected by material and energy streams. This decomposition mirrors the decentralization of the control problem. The recommended procedure is to apply model reduction to individual units, and then to couple together these reduced models. The technique will be applied to a case study: the *iso*-butane alkylation plant.

2. Approaches to dynamic optimization

The objective of the dynamic optimization is to determine, for a dynamic system, a set of decision variable time profiles (pressure, temperature, flowrate, heat duty etc.) that optimise a given performance criterion, subject to specified constraints (safety, environmental and operating constraints).

The dynamic optimization problem of interest in this contribution can be stated as follows:

$$\min_{u(t),t_f} Obj(x(t_f), u(t_f), y(t_f), t_f, p) = \int_0^{t_f} obj(x(t), u(t), y(t), t, p)dt \tag{1}$$

$$s.t. \quad f(x(t), \dot{x}(t), u(t), z(t), p) = 0 \tag{2}$$

$$g(x(t), u(t), z(t), p) = 0 \tag{3}$$

$$x_{min} \leq x(t) \leq x_{max} \tag{4}$$

$$u_{min} \leq u(t) \leq u_{max} \tag{5}$$

$$z_{min} \leq z(t) \leq z_{max} \tag{6}$$

$$x(0) = x_0 \tag{7}$$

In this formulation, $x(t)$ are state (dependent) variables, $u(t)$ are control (independent) variables and $z(t)$ are algebraic variables, while p are time-independent parameters.

The dynamic models of chemical processes are represented by differential-algebraic equations (DAEs). Equation (2) and (3) define such a system. Equations (4), (5) and (6) are the path constraints on the state variables, control variables and algebraic variables respectively, while equation (7) represents the initial condition of the state variables. Obj is a scalar objective function at final time, t_f.

The most common approach to DAE-based optimization problems is the transformation of the infinite-dimensional dynamic problem into a finite-dimensional nonlinear programming problem (NLP) [4]. Two main approaches have been developed in order to make this transformation.

The first one is to decompose the dynamical system into the control and the state spaces. In the next step, only the control variables are discretized and remain as degrees of freedom for the NLP solver [5]. The method is called the sequential approach. The DAE system has to be solved at each NLP iteration. The disadvantages of the approach are: problems of handling path constraints on the state variables, since these variables are not included directly in the NLP solver [5]; the time needed to reach a solution can be very high in case the model of the dynamic system is too complex; difficulties may arise while handling unstable systems [4].

In the second approach, both the state and the control variables are discretized. In this way, a large-scale NLP problem is obtained, but the DAE system is solved only once, at

the optimal point. In this way, the disadvantages of the sequential approach are eliminated, but there is still the issue of handling the problem size [4].
In the recent years, a new approach has been developed for eliminating this disadvantage [5]. This approach is called the quasi-sequential approach and takes the advantages of both the sequential and the simultaneous approaches: since both the control and the state variables are discretized, the path constraints for the state variables can be handled; the DAE system is integrated only once, so the computation becomes more efficient.

3. Model reduction for dynamic optimization

As seen in the previous chapter, all the approaches used to solve the dynamic optimization problem integrate, at some point, the dynamical system of the chemical process. In order to obtain more efficiently the values of the optimum profile of the control variable, a suitable model of the system should be developed. That means that the complexity of the model should be limited, but, in the same time, the model should represent the plant behaviour with good accuracy. The best way to obtain such a model is by using the model reduction techniques. However, the use of a classical model reduction approach is not always able to lead to a solution [6]. And very often, the physical structure of the problem is destroyed. Thus, the procedure has to be performed taking into account the process knowledge (units, components, species etc.).
In the following chapter, the application of the model reduction with process knowledge for the dynamic optimization will be presented. This will be done by means of a case study: the *iso*-butane alkylation plant.

3.1. The iso-butane alkylation plant

The alkylation of *iso*-butane is a widely used method for producing high-octane blending component for gasoline. For the purpose of this study, the following reactions capture the overall chemistry:

$$C_4H_8 + i - C_4H_{10} \rightarrow i - C_8H_{18} \tag{8}$$

$$C_4H_8 + i - C_8H_{18} \rightarrow C_{12}H_{26} \tag{9}$$

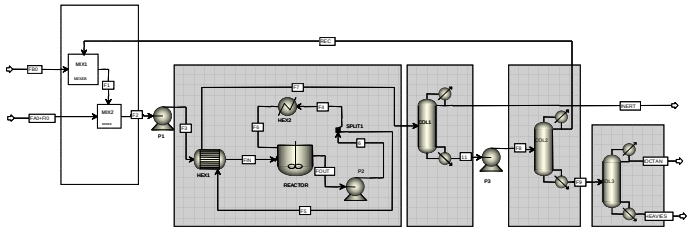

Figure 1. The *iso*-butane alkylation plant.

The reactions are exothermic and occur in liquid phase. The secondary reaction (9) has large activation energy, therefore high selectivity is favoured by low temperatures. The cooling is achieved in an external heat-exchanger. The second reaction is suppressed by keeping the concentration of butene low. Therefore, a large excess of *iso*-butane is fed to the reactor. From the reactor effluent, the light impurities, reactants, products and heavy products are separated by distillation and removed or recycled.

The plantwide control structure (Figure 2) is the same as the one determined to have a stable behaviour in [6]: the flowrate of the fresh butene is specified, while the *iso*-butane is introduced by inventory control.

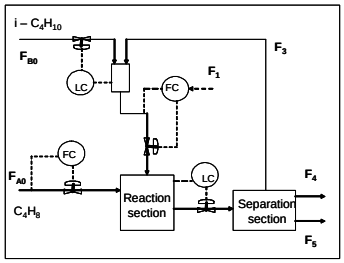

Figure 2. The proposed plantwide control structure for the *iso*-butane alkylation plant.

Local control is also present: the reactor is operated at constant volume and temperature, while for the distillation columns, the levels, pressure, and top and level compositions are controlled.

The objective of the dynamic optimization problem should be stated before the model reduction is performed, in order to choose the right variables to be kept in the reduced model. The objective of the dynamic optimization problem will be stated as follows:

Increase the plant production by 20% with minimal energy consumption in the distillation columns.

It should be mentioned that this focus on energy may lead to a long transition period.

3.2. Reduced model

The full nonlinear model is developed using Aspen Dynamics. For obtaining the reduced model, the same procedure presented in [6] is used. However, in this case the reduced model will be developed using gProms.

First of all, the plant flowsheet is split into units / group of units. The splitting it is done in units to which local control is applied: the reactor (plus the heat exchangers around it), the distillation columns, mixing vessels, pumps. Since the mixers and the pumps are considered instantaneous (no dynamics) they are not interesting for the model reduction. Further, the units are individually reduced.

Since the reactor has a strong nonlinear behaviour, the model simplification is used. A dynamic model is written using gProms, consisting of five component balances, and considering constant temperature and physical properties.

For the distillation columns, linear model-order reduction will be used. The linear model is obtained in Aspen Dynamics. Some modifications to the previous study have been done to the linear models, in order to have the reboiler duty and the reflux ratio as input or output variables of the linear models. This is needed to have access to those variables in the reduced model, for the purpose of the dynamic optimization. A balanced realization of the linear models is performed in Matlab. The obtained balanced models are then reduced. The reduced models of the distillation columns are further implemented in gProms. When all the reduced models of the individual units are available, these models are further connected in order to obtain the full reduced model of the alkylation plant. The outcome of the model reduction procedure is presented in Table 1, together with some performances of the reduced model.

Table 1. The model reduction of the *iso*-butane alkylation plant

Unit	Model reduction technique	Full nonlinear model	Reduced model
CSTR	Model simplification	15 states	**5** states
COL1	Model order-reduction	188 states	**25** states
COL2	Model order-reduction	194 states	**29** states
COL3	Model order-reduction	169 states	**17** states
Simulation time		150 seconds	**2 seconds**

3.3. Dynamic optimization

After the reduced model is obtained, the dynamic optimization problem (equations (1) – (7)) is implemented in gProms. The single shooting method is used.

The objective function to be minimised is the sum of the reboiler duties in the distillation columns. Two control variables are considered: the flowrate of the fresh feed of butene (F_{A0}) and the flowrate of the first mixer's outlet stream (F_1), which are also the variables on flow control in the plantwide control structure (Figure 2).

After the 20% increase in the production is achieved, the optimizer is asked to ensure a new steady state is reached and the production is kept constant for a while. The two control variables are discretized into 25 time intervals. The size of the first 20 intervals is free, while for the last 5 it is fixed.

A selectivity constraint is imposed, in order to maintain the formation of the secondary products at a low value. All the constraints are introduced as inequality type constraints.

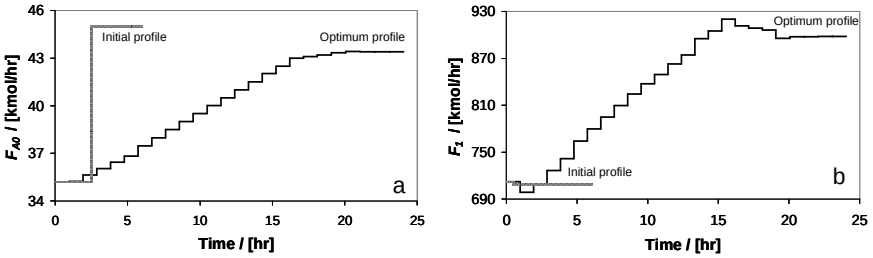

Figure 3. The optimum control profiles for: a) the component A fresh feed flowrate; b) the recycle flowrate.

The optimum profiles of the control variables (Figure 3) are obtained after several time-consuming, trial-and-error iterations. The solution was obtained after a number of about 150 manual iterations, not taking into account the iterations performed by the solver. In each manual iteration, the initial profile was modified by the user, while the solver is trying to optimize this profile. The advantage of having a reduced model at this point is obvious.

Further, the optimum profiles were implemented into Aspen Dynamics. The agreement between the responses of the nonlinear and reduced model is excellent (Figure 4). The difference between the reduced and the nonlinear model response is less than 2.3% at the end of the time span.

However, the transition time is quite long, as expected when the objective was set. From an initial guess of 6 hours, the optimum solution led to a transition time of about 24 hours. To determine the cause of this behaviour, a study of the system's time constant

should be performed. This should be done before implementing the optimization, in order to get a better initial guess, and reduce the optimization time.

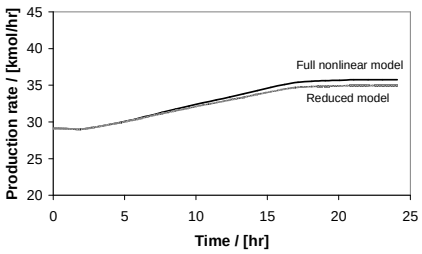

Figure 4. Comparisons between the responses of the full and reduced model after the optimum control profiles are implemented.

4. Conclusions

This paper proposes and demonstrates the advantage of exploiting the inherent structure that exists in a chemical plant for developing reduced models to be used during the dynamic optimization of chemical plants operation. The recommended procedure is to apply model reduction to individual units of the plant, and then to couple together these reduced models. The procedure is flexible, allowing different reduction techniques to be applied for different individual units, and the units to be chosen considering the future use of the reduced model. The solution time is significantly reduced, which makes the model easier to be applied for the purpose of our study. Another advantage of the procedure is the modularity of the reduced model, which can be very useful in the case of future plant changes, or even for when the reduced model is used for a different application. In these cases, instead of having to obtain a new reduced model of the whole plant, only the reduced model of the new unit would be changed.

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