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On the application of model reduction to plantwide control

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Abstract

The derivation and applicability of reduced-order models for selection and assessment of plantwide control structures is studied. The paper demonstrates the advantage of exploiting the intrinsic structure of a chemical plant, which mirrors the decentralization of the control problem. The recommended procedure is to apply model reduction to individual units, followed by coupling these reduced-order models. This procedure is flexible and accurate, and leads to major reduction of the simulation time. The importance of retaining the model nonlinearity is highlighted.

Keywords: model reduction, plantwide control, nonlinear behaviour, alkylation

1. Introduction

In today's competitive environment, high economical performance of chemical plants is achieved by cost-effective steady state integrated design and by continuously responding to the market conditions through dynamic operation. The desired policy of operation is accomplished by control systems that maintain the steady state or implement the optimal dynamic behaviour. Both the design of plantwide control structures and the dynamic optimization require dynamic models of the chemical plant. To achieve the objectives, the model quality is crucial: predicting the behaviour with good accuracy; limited complexity to allow repeated solution during a restricted time; easy maintenance and adaptation to future plant changes.

Reduction of the model order [1] might offer a solution. Several linear [2] and nonlinear techniques [3] have been developed and their application to different case studies reported. Although significant reduction of the number of equations can be 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 [1].
In this paper, a new approach is proposed, taking advantage of 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 these reduced-order models. This procedure is flexible as the reduction algorithm and accuracy can vary from unit to unit, is able to retain the nonlinearity of the original plant, and preserves the significance of important model variables. The effectiveness of the approach is proven by means of a case study.

2. Order reduction of chemical plant models

Reduction of balanced linear models is easy to apply and the accuracy of the reduced models is guaranteed by theoretical results [2]. In the following, we will present the main steps of a classical approach, discussing the difficulties that are likely to be encountered and possible solutions.
The rigorous model. The starting point of model-based approach to plantwide control is a dynamic model of the plant, which is routinely available as rigorous dynamic simulation obtained using a commercial package. The basic control of inventory at unit level is included. Some model reduction is already present, such as the local thermodynamics and the instantaneous models of valves, pumps, mixers or heat-exchangers. The plant model contains thousands of differential and algebraic equations, with initial conditions derived from a nominal operating point. Sometimes, the numerical solution fails. Locating the cause and finding a remedy is a tough and time-demanding task.
The linear model. State-of-the-art dynamic simulators can be used to obtain a linear model in state-space formulation. The stability of the plant can be assessed by calculating the eigenvalues of the linearization, but the origin of instability might be difficult to identify. We stress that the behaviour of many chemical units is strongly nonlinear, showing high parametric sensitivity or state multiplicity. These effects are enhanced by coupling the units through heat-integration or material recycles. The linear models are reliable near the linearization point, but their accuracy is poor for large disturbances.
The balanced model. In the next step, a linear transformation of the state variables is applied, to produce a model where all the states are equally contributing to the input-output behaviour. Balancing of stable systems is straightforward. If the system is unstable, the stable part is isolated, balanced, and added back to the unstable part of the model. For very large models, the

algorithm often fails due to the ill-conditioning of the Lyapunov equation solved while calculating the gramians.

The reduced-order model. Small Hankel singular values in the balanced realization indicate state variables with little contribution to the input-output behaviour. The reduced-order model is obtained by equating to zero these variables (truncation) or their time-derivatives (rezidualization). Truncation is more accurate in representing the initial part of the dynamic response, but rezidualization preserves the steady state gain. If the dynamics of the systems is essentially high order, no significant reduction can be achieved.

Design of the plantwide control brings some particularities. Although the goal is a control structure for the whole plant, many control loops are local to certain units. For example, instabilities arising from heat-integration are solved by manipulating local heat duties; in distillation, composition of product streams is controlled by reflux rate or reboiler duty. From a plant-wide viewpoint, the design of the control structure is mainly concerned with the inventory of reactants, products, impurities and by-products [4]. The solution is much simpler by excluding the local control loops from the analysis.

The proposed approach consists of a) identification of units or groups of integrated units to which local control is applied; b) application of tailored reduction techniques to individual units or groups of integrated units; c) obtaining the reduced-order of the full plant. In the following, the effectiveness of the approach will be proven by means of a case study.

3. Case-study: plantwide control of *iso*-butane – butane alkylation plant

The alkylation of *iso*-butane with butene is a widely used method for producing high-octane blending component for gasoline. For our purposes, the following reactions capture the essence of the overall chemistry:

$$C_4H_8 + i-C_4H_{10} \rightarrow i-C_8H_{18} \quad (1)$$

$$C_4H_8 + i-C_8H_{18} \rightarrow C_{12}H_{26} \quad (2)$$

The reactions are exothermic and occur in liquid phase. The secondary reaction (2) has large activation energy; therefore high selectivity is favored by low temperatures. Cooling is achieved in an external heat-exchanger. The use of coolant is minimized by a feed-effluent heat exchanger. The second reaction is also suppressed by keeping the concentration of butene low. Therefore, a large excess of iso-butane is fed to the reactor. From reactor effluent, the light impurities, reactants, products and heavy byproducts are separated by distillation and removed or recycled. Figure 1 shows the flowsheet of the plant.

The rigorous model. Steady state and dynamic simulations were built in AspenPlus and AspenDynamics, respectively. The dynamic model includes the basic inventory control (pressures and levels), but no quality control. This

"open-loop" plant is unstable: the reactor's temperature drops fast and all flow rates dramatically increase. Soon, one level control loop reaches its limits, and overflow occurs. The heat-integration around the chemical reactor seems to be the cause. Therefore, a temperature controller is provided. This does not solve the problem, as the plant is still unstable.

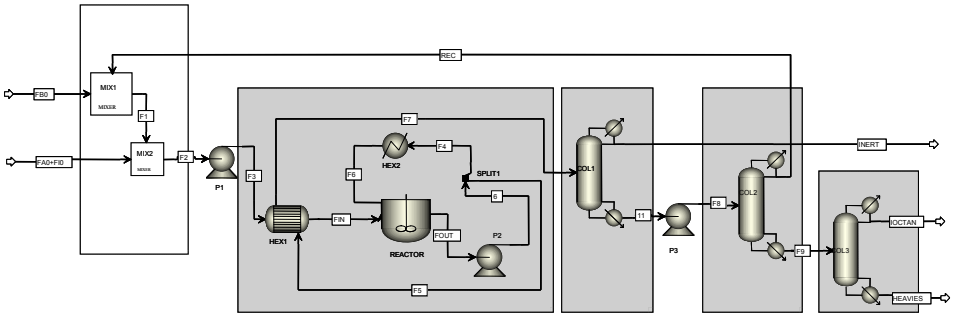

Figure 1. The iso-butane alkylation plant.

The linear model. The original plantwide model is linearized around the nominal operating point. Linearization shows three positive eigenvalues. The heat-integrated reactor and the reaction-separation-recycle structure might be possible reasons, but the origin of the third positive eigenvalue is still unclear.

The balanced model. Obtaining the balanced model fails, as the MATLAB algorithm complains about the unstable system and some ill-conditioned matrices. The use of reduced-order models for designing the plantwide control seems hopeless. Heuristic methodologies become strong candidates.

Exploiting the structure. The plant is split into groups of units (reactor and heat-exchangers around it) or units (distillation columns, mixing vessels) that can be individually analyzed (Figure 1). It turns out that the reaction sub-system is unstable, but it can be easily stabilized by a temperature controller manipulating cooling duty. Unexpectedly, the first and third distillation columns are also unstable. We observe that the dynamic model specifies (realistically) the reflux on a mass basis, in contrast to the steady state simulation which uses moles. Realizing the large relative volatilities and the very different molar weights, multiple or unstable steady states becomes a possibility [5]. Indeed, providing temperature controllers or switching to mole-based specifications stabilize the columns. For each stable or stabilized unit, linear models are obtained, with component flow rates, temperature and pressure of the inlet and outlet streams chosen as inputs and outputs, respectively. Reduction of the linear balanced models is attempted. For the distillation units, a significant reduction is achieved with excellent accuracy (Figure 2a). The model of the reactor has only 15 states, the agreement between the nonlinear and linear models is good, but significant order-reduction at high accuracy is not possible.

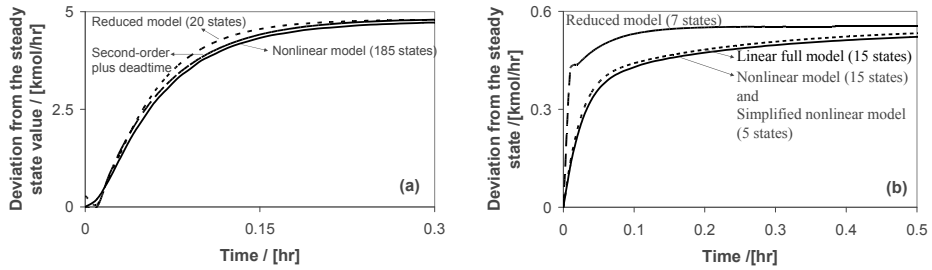

Figure 2. Order-reduction of unit models. The dynamic responses show the *iso*-octane outlet flow rate. a) Distillation column COL1, for 5 kmol/h change of the *iso*-octane inlet flow (b) Reactor, for a 5 kmol/h change of the butene inlet flow.

Preserving the nonlinearity. A second approach is taken to reduce the size of the reactor model. A dynamic model was written, consisting of five component balances, and considering constant temperature and physical properties. The agreement with the AspenDynamics model is excellent (Figure 2b).

Plantwide control structures. At this point, different plantwide control structures can be considered and evaluated. Here, we only discuss two of them (Figure 3). In control structure CS1, the fresh feeds of both reactants are fixed. In CS2, the butene fresh feed is fixed, but *iso*-butane is brought in the process on inventory control. CS1 has the advantage of setting directly the production rate and product distribution. However, it has the disadvantage of extremely high sensitivity to disturbances, as it will be shown later. The reduced-order models of the units can be coupled. As CS1 and CS2 differ only in the way reactants are brought in the process, this means that the reduced-order models of the reaction section and separation units can be easily reused.

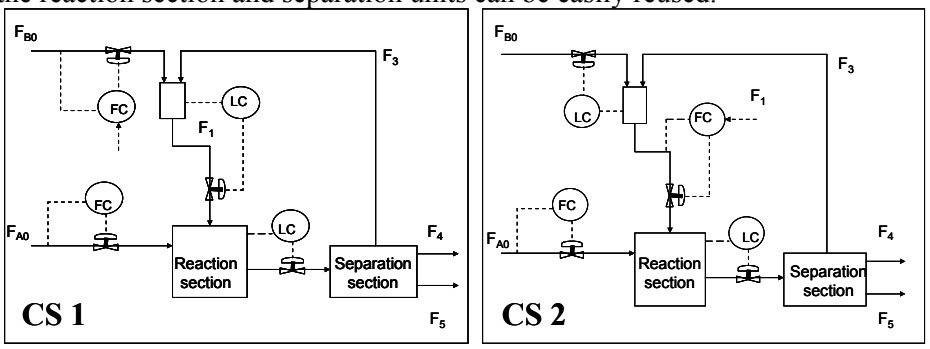

Figure 3. Control structures for the alkylation plant.

Evaluating the reduced-order models and the control structures. At this point, three different models are available: the original AspenDynamics nonlinear model (M1) which will be taken as reference, the reduced-order linear model (M2) and the reduced-order nonlinear model (M3). When control structures CS1 and CS2 are applied, all models predict a stable plant. However,

when the butene feed is decreased by 10%, the control structure CS1 is not able to control the plant: the amount of butene fed in the process is not enough to consume the *iso*-octane. Reactant accumulation occurs, reflected by the slow but continuous increase of the recycle flow. This behaviour is correctly predicted by the nonlinear models M1 and M3, but not by the linear model M2. In contrast, CS2 performs very well. For the same disturbance, a new steady state is reached in relatively short time (Figure 4). The excellent accuracy of the nonlinear reduced-order model is obvious. The reduction in computation time, from about 3 minutes to less than 30 seconds, should also be remarked.

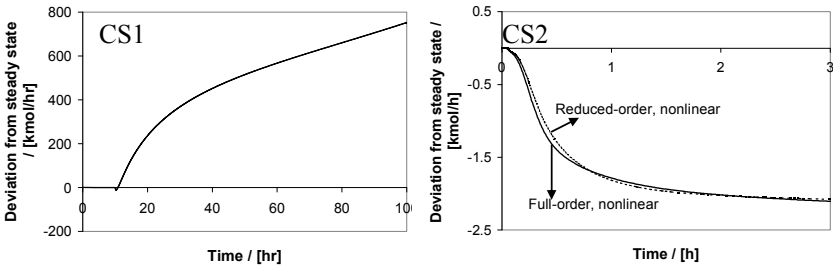

Figure 4. Dynamic simulation results, for 10% decrease of the fresh butene flow rate. CS1: recycle flow rate; CS2: production rate

4. Conclusions

This paper proposes and demonstrates the advantage of considering the inherent structure that exists in a chemical plant for developing reduced-order models to be used during design of plantwide control. The recommended procedure is to apply model reduction to individual units of the plant, and then to couple together these reduced-order models. The procedure is flexible. The solution time is significantly reduced. The nonlinearity of the original model can be preserved, which is a highly desirable feature. The maintenance and adaptation to future plant changes is facilitated by the modularity of the reduced model.

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