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Computational performance of aggregated distillation models

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ABSTRACT

Compartmental and aggregated modeling is used to derive low-order (reduced) dynamic models from detailed models of staged processes. In this study, the aggregated modeling method of [Lévine, J., & Rouchon, P. (1991). Quality control of binary distillation columns via nonlinear aggregated models. Automatica, 27, 463] is revised with the objective of deriving computationally efficient models for real-time control and optimization applications. A simple implementation of the original method not requiring the specification of compartments is presented. The resulting DAE models are converted into ODE models by pre-solving and substituting the algebraic equations resulting from the reduction procedure, which is the key step to increase simulation speed. To study this, the performances of several full and reduced distillation models, with and without base-layer controllers, are compared using different numerical integrators. It is found that while the reduced DAE models are computationally not advantageous, the reduced ODE models decrease the simulation time by a factor of 5–10.

1. Introduction

With the establishment of dynamic real-time optimization and model predictive control as state-of-the-art methods to efficiently operate industrial processes, reduced models with low computational complexity are in the focus of current research (Allgöwer & Zheng, 2000; Marquardt, 2001; van den Berg, 2005). In particular, reduced nonlinear physically based models are of high interest for the prediction of the system behavior over a wide range of operating conditions. Many model reduction techniques have been developed for nonlinear systems (Marquardt, 2001; van den Berg, 2005), most of which produce models of lower order. This, however, does not guarantee that the reduced models show a computationally better performance than the original models they were derived from (van den Berg, 2005). This is because a reduced model is most likely less accurate than the original full model, and because the numerical complexity of the full model is often retained in the equations of the reduced model.

For nonlinear model reduction of distillation columns, several model reduction and simplification methods have been developed in the past (Benallou, Seborg, & Mellichamp, 1986; Cho & Joseph, 1983; Khowinij, Bian, Henson, Belanger, & Megan, 2004; Khowinij, Henson, Belanger, & Megan, 2005; Kienle, 2000; Kumar & Daoutidis, 2003; Lévine & Rouchon, 1991; Marquardt, 1990; Skogestad, 1997). Among these are the method of compartmental modeling (Benallou et al., 1986) and later the improved variant of aggregated modeling by Lévine and Rouchon (1991). The latter method is used for deriving the reduced models investigated in this study. It is based on partitioning a distillation column into "compartments" consisting of "steady-state" trays and dynamic "aggregation" trays, and using a singular perturbation argument (Kokotovic, Khalil, & O'Reilly, 1986) to derive a reduced-order model. Among its advantages is the perfect steady-state agreement with the original model, a simple derivation, and good control of the reduced model complexity.

Originally, these methods were intended for nonlinear controller design, for which a low-order model is necessary. More recently, they have been used to reduce the simulation time in real-time applications (Bian, Khowinij, Henson, Belanger, & Megan, 2005; Khowinij et al., 2004, 2005). However, it is shown in this study that while only transforming the original system into a reduced system in differential-algebraic equation (DAE) form does not improve the simulation speed of the reduced model, a subsequent elimination of the algebraic equations is necessary to obtain a reduced model in ordinary differential equation (ODE) form, which shows a significantly improved computational performance compared to the original model. On a more fundamental level, it is shown that the notion of compartments is not necessary in the derivation of the reduction method. This greatly simplifies the derivation and makes

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the extension of the method to more complex systems straightforward.

The paper is organized as follows: In Section 2, the full model for a binary distillation column, and the derivation of reduced models from this using aggregated modeling is described. Important implementation details and properties of the models are given. In Section 3, the framework for testing the computational performance of the models is explained, discussing the input signal, the model parameters and the numerical solvers used for simulating the models. The results of the simulations are given in Section 4. Section 5 discusses the results of the simulations, and details and possible extensions of the reduction method. A summary and conclusions are given in Section 6.

2. Models

2.1. System and modeling assumptions

The system investigated is a binary distillation column with 72 trays plus reboiler and condenser. Two variants of this system are studied:

1. An "uncontrolled" column with level controllers for condenser and reboiler, but with no temperature or composition control. The reflux L and the boil-up V remain as degrees of freedom ("LV-configuration").
2. A "controlled" column with an additional composition controller in the lower column part that manipulates the boil-up rate V.

The controlled column is shown schematically in Fig. 1. In the following, the uncontrolled system is used to explain the system equations and the reduction procedure. Later, in Section 2.4, the inclusion of the composition controller is explained.

All assumptions made in this simplified distillation model are discussed in detail by Skogestad (1997). The major modeling assumptions are: Ideal trays, which means that liquid and vapor are in equilibrium at each tray; ideal mixture, which means that the vapor composition y can be expressed as a function of the liquid composition x assuming the constant relative volatility

$$y = k(x) = \frac{\alpha x}{1+(\alpha-1)x}, \tag{1}$$

where α is the relative volatility; constant molar flows, which means that the energy balance is simplified; constant molar holdup on each tray and negligible mass in the vapor phase.

The assumption of constant molar flows may not be good if the model is to be used for control purposes (Skogestad, 1997), but the focus here is on longer time scales.

The column has one feed flow F at tray number n_F. z_F denotes the concentration of the first (light) component in the feed. A liquid flow L (or $L+F$ for trays below the feed tray) and a vapor flow V enter and leave each tray. The condenser and reboiler levels are assumed to be controlled using the distillate flow D and bottom flow B, respectively. For simplicity, perfect level control is assumed, such that $D=V-L$ and $B=L+F-V$. Note that the assumption of perfect level control is not important with the LV-configuration. The concentrations in these flows determine the purity of the distillation products and are therefore the most important output variables in the process. The feed flow rate F and the feed concentration z_F can be seen as disturbance variables, and the flows L and V are manipulated variables for control.

2.2. Full uncontrolled model

The full model consists of one component material balance for each tray and the condenser and reboiler. For ease of notation, the condenser and reboiler are written as tray 1 and N:

$$H_1\dot{x}_1 = Vy_2 - Vx_1, \tag{2}$$

$$H_i\dot{x}_i = Lx_{i-1} + Vy_{i+1} - Lx_i - Vy_i, \quad i=2,\ldots,n_F-1 \tag{3}$$

$$H_{n_F}\dot{x}_{n_F} = Lx_{i-1} + Vy_{i+1} - (L+F)x_i - Vy_i + Fz_F, \tag{4}$$

$$H_i\dot{x}_i = (L+F)x_{i-1} + Vy_{i+1} - (L+F)x_i - Vy_i,$$
$$i = n_F+1,\ldots,N-1 \tag{5}$$

$$H_N\dot{x}_N = (L+F)x_{N-1} - (L+F-V)x_N - Vy_N, \tag{6}$$

where H_i is the total liquid molar holdup, x_i and $y_i = k(x_i)$ are the concentrations of the first component in the liquid and vapor phase, respectively, of tray i, N is the number of trays including the condenser and reboiler, n_F is the index of the feed tray, and V, L, F, z_F are as described above.

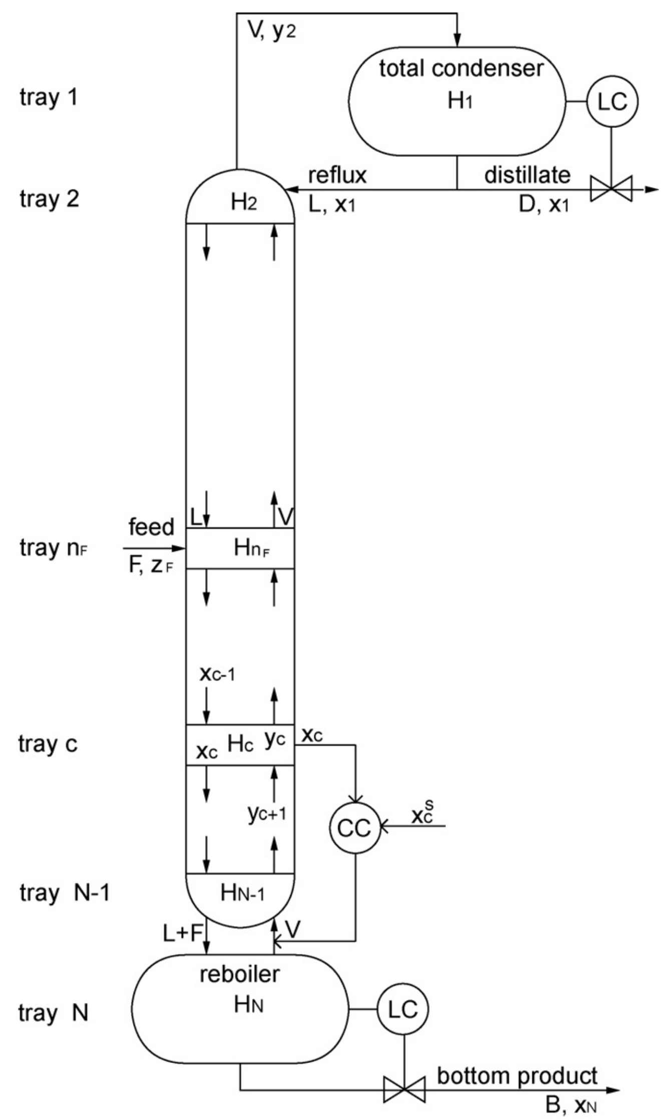

Fig. 1. Schematic diagram of a binary distillation column with a composition controller in the lower column section.