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How Simple Can it be? – A Look at the Models for Batch Distillation

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Abstract

Reduced order models provide an efficient alternative to the rigorous models and are based on simplifying assumptions. In general, the accuracy of a model increases with increasing level of model complexity. However, the improved accuracy is often at the expense of the computational efficiency. The rigor of the models used in practice is therefore governed by a compromise between accuracy and computational efficiency. This paper introduces a novel concept of "Optimal Model Reduction" where the trade-offs between accuracy and efficiency are decided using nonlinear optimization techniques. The effectiveness of this new approach is presented in the context of batch distillation, for which a hierarchy of models exist in the literature.

Keywords: Aggregation, Model reduction, Abstraction, Batch distillation, Compartmental models, Shortcut Model.

1. Introduction

Reduced order, dynamic models of chemical processes are desirable in a number of applications including evaluations of alternative control strategies, development of advanced on-line control schemes, analysis of operability etc. These simplified or reduced order models are abstractions of the rigorous models and their accuracy depends upon the simplifying assumptions employed. The process of model reduction can therefore be viewed as a trade-off between simplicity and accuracy. Undoubtedly, the usefulness of the simplified models depends upon the guarantee they provide in reflecting the behavior of the system in reality. So, the question naturally arises as to the extent to which one can go "simpler" in the modeling without compromising on reality.

This paper addresses this question and presents, for the first time, the concept of an "Optimal Model Reduction." The approach involves selecting an appropriate low order model using optimization techniques. This problem is posed as that of maximizing a degree of simplicity constrained by the error bounds on the specified characteristics of the system. The degree of simplicity is defined in terms of the computational efforts required and the order of the model, while the constraints are expressed in terms of the tolerance on the statistical coefficient of determination (the R^2 value) for the transient profiles. This novel strategy is applied to the domain of hierarchical models for batch distillation presently available in the literature. The non-integer nature of the models allows the optimal model reduction problem to be posed as a nonlinear optimization problem. The results of the study will allow for confidence in the selection of a model, with an appropriate level of rigor (or simplicity), based on the specific needs of the user. The approach used and the results of the study are presented and discussed here.

2. Model Abstraction in Batch Distillation

Development of simplified models for batch distillation and their use in optimization and optimal control seems to be the recent trend in batch distillation studies. BATCH-DIST, a comprehensive package for multicomponent, multifraction batch distillation columns (Diwekar and Madhavan 1991a) provides a hierarchy

Table 1: Model Equations for the Short-cut Method

Overall Material Balance	*Differential Material Balance*
$\frac{dB_1}{dt} = \frac{-V}{R_t+1}, B_0 = F,$	$\frac{dx_B^{(i)}}{dt} = \frac{V}{R_t+1}(x_B^{(i)} - x_D^{(i)}),\ x_{B_0}^{(i)} = x_F^{(i)}, i = 1,2,\ldots,n$
Hengstebeck-Geddes' Equation	*Fenske Equation*
$x_D^{(i)} = \left(\frac{\alpha_i}{\alpha_1}\right)^{C_1} \frac{x_D^{(1)}}{x_B^{(1)}} x_B^{(i)}, i = 2,3,\ldots,n$	$N_{min} \approx C_1$
Summation of Fractions	$x_D^{(1)}$ *estimation*
$\sum_{i=1}^{n} x_D^{(i)} = 1$	$x_D^{(1)} = \frac{1}{\sum_{i=1}^{n}\left(\frac{\alpha_i}{\alpha_1}\right)^{C_1}\frac{x_B^{(i)}}{x_B^{(1)}}}$
Underwood Equations	
$\sum_{i=1}^{n} \frac{\alpha_i x_B^{(i)}}{\alpha_i - \phi} = 0$	$R_{min\ u} + 1 = \sum_{i=1}^{n} \frac{\alpha_i x_D^{(i)}}{\alpha_i - \phi}$
Gilliland Correlation	C_1 *Estimation*
$R_{min\ g} = F(N, N_{min}, R)$	$\frac{R_{min\ g}}{R} - \frac{R_{min\ u}}{R} = 0$

of models for simulation, ranging from the most simplified model to the most rigorous model based on differential material and energy balance equations for each stage. These simplified models offer an efficient alternative for handling the versatility of batch distillation which otherwise poses challenging design and analysis problems. The most simplified model in BATCH-DIST uses the short-cut method (Diwekar and Madhavan, 1991b), which is based on the assumption that batch distillation column can be considered as a continuous distillation column with changing feed at any time instant. This simplified assumption allowed the modification of the short-cut method (Fenske-Underwood-Gilliland (FUG) method) for continuous distillation columns to batch distillation columns.

The focus of the present article is on the constant reflux mode of operation of batch distillation columns, for which Table 1 presents the governing equations as used in the short-cut method. At any time instant t, the change in the still composition of all components ($x_B^{(i)}, i = 1,2,\ldots,n$) can be calculated by the differential material balance equations (Table 1). The distillate composition ($x_D^{(i)}, i = 1,2,\ldots,n$) is then related to the new still composition in terms of a constant C_1, using the Hengstebeck-Geddes' equation. The constant C_1 in the Hengstebeck-Geddes' equation is equivalent to the minimum number of plates N_{min} in the Fenske equation. At this stage C_1 and $x_D^{(1)}$ are the unknowns. Summation of distillate compositions could be used to obtain $x_D^{(1)}$ and the FUG equations to obtain C_1.

The short-cut method demonstrated for the first time the power of aggregation in the context of batch distillation. This method represents an abstraction and is very useful in identifying global properties like feasible region of operation. However, the short-cut method cannot be directly applied to columns where holdup effects are significant.

While the assumption of negligible holdup is reasonable for certain applications, holdup effects do play an important role in several other batch distillation columns. Holdup affects the performance of a batch distillation column in two basic ways namely, the dynamic "flywheel" effect, and the steady state "capacitance effect". The flywheel effect can be characterized by the parameter $\tau = \frac{holdup}{reflux \times distillate\ rate}$. For large τ, the initial composition profile predicted by the zero holdup models departs significantly from the results of a rigorous model. The capacitance effect is observed at the end of the total reflux condition, when the given charge distributes itself throughout the column. Associated with the capacitance effect is the concept of equilibration time. However, the short-cut method assumes instant equilibration at the total reflux condition.

For a wider applicability, a modified short-cut model using the lumped parameter approach applied to the short-cut method was presented recently (Diwekar, 1992). The model is based on the compartmental approach proposed by Benallou et.al. (1986). In this approach a staged column is considered as a compartmental system in which a number of stages are lumped to form an equivalent stage. The short-cut

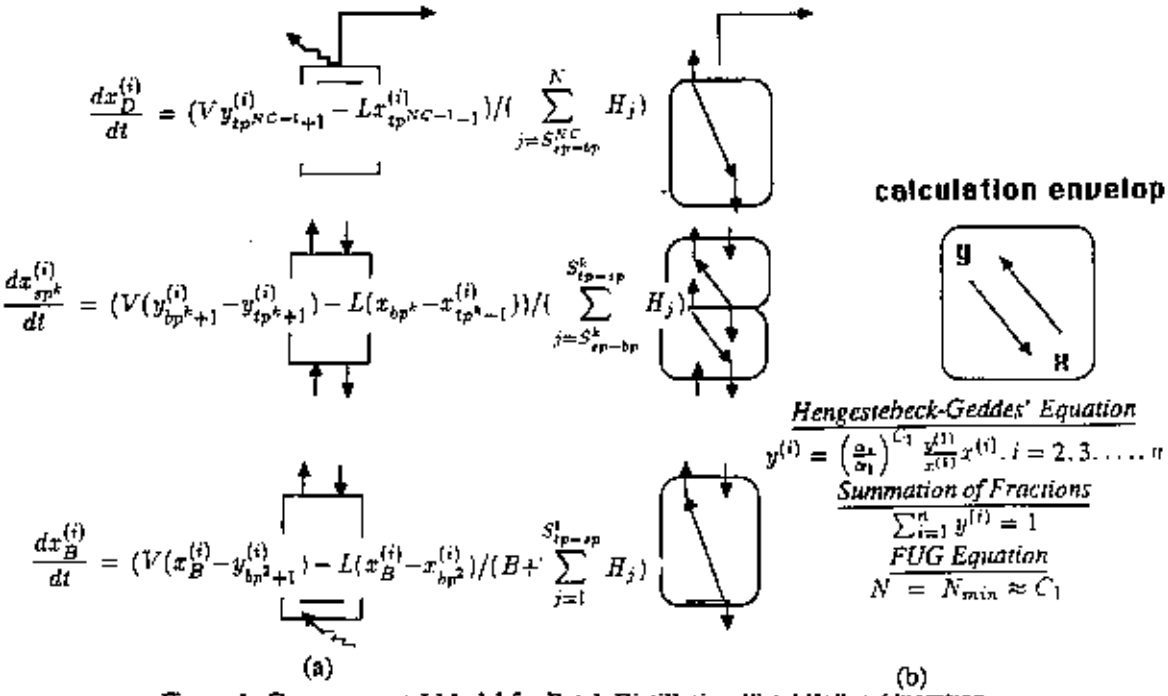


Figure 1: Compartmental Model for Batch Distillation, Total Reflux Operation

model (Table 1) is extended to obtain the composition profiles of the lumped compartment. This technique appears to capture both the capacitance and flywheel effect of holdup and also provides reasonably accurate estimates of the equilibration times (Diwekar, 1992).

Figure 1 shows the batch distillation column consisting of a number of compartments. The figure also shows the overall dynamics of the column in terms of compartmental input, output vapor streams composition y_{bp^k+1} and y_{tp^k} (where tp^k is the top plate of the compartment k and bp^k is the bottom plate), input and output liquid compositions x_{tp^k-1} and x_{bp^k}, and the composition of the sensitive stage x_{sp^k}. It should be noted that the equations in Fig.1 are based on the constant molal assumption, wherein the liquid and vapor flowrates are assumed to be constant throughout the column. The differential equation describing the composition of the sensitive stage is based on the total holdup in the compartment. The compositions, y_{tp^k} and x_{tp^k-1}, leaving each compartment can be found algebraically by applying the short-cut method to the material balance envelopes shown in Fig. 1b. Benallou et al. (1986) used a short cut model based on the absorption, separation factors to calculate the steady state material balance envelop, while Horton et al. (1991) resorted to plate to plate calculation methods. In the present work, the short-cut method based on the FUG method will be representing the steady state compartmental material balances. This is because the short-cut method is proved to be reasonably accurate and very fast. Besides computational efficiency this method has been very effective in identifying feasible region of operation crucial for design, optimization, and control studies. Furthermore, the number of theoretical stages in the short-cut method is not being an integer variable is a very useful concept in the optimization studies presented in this paper. This also allows for exploring the possibility of the sensitive stage being a non-integer which enhances the practical applicability of the results.

For application of the short-cut method to obtaining material balances around the envelopes, the envelopes are further decomposed (fig.1b). Since the objective of the paper is to demonstrate the idea of optimal model reduction, the discussion is focused on the simpler case of total reflux condition. At total reflux, the short-cut method equations for the envelope material balance calculations reduce to the Hengstebeck-Geddes' equation (equivalently the Fenske's equation). At minimum reflux the number of plates equals the minimum number plates, or equivalently, the constant C_1 in the Hengstebeck-Geddes' equation. Therefore, given the number of plates above the sensitive stage S_{sp-tp}, and below the sensitive stage S_{bp-sp}, the material balance can be calculated using the Hengstebeck-Geddes' equation as shown in Fig. 1b.

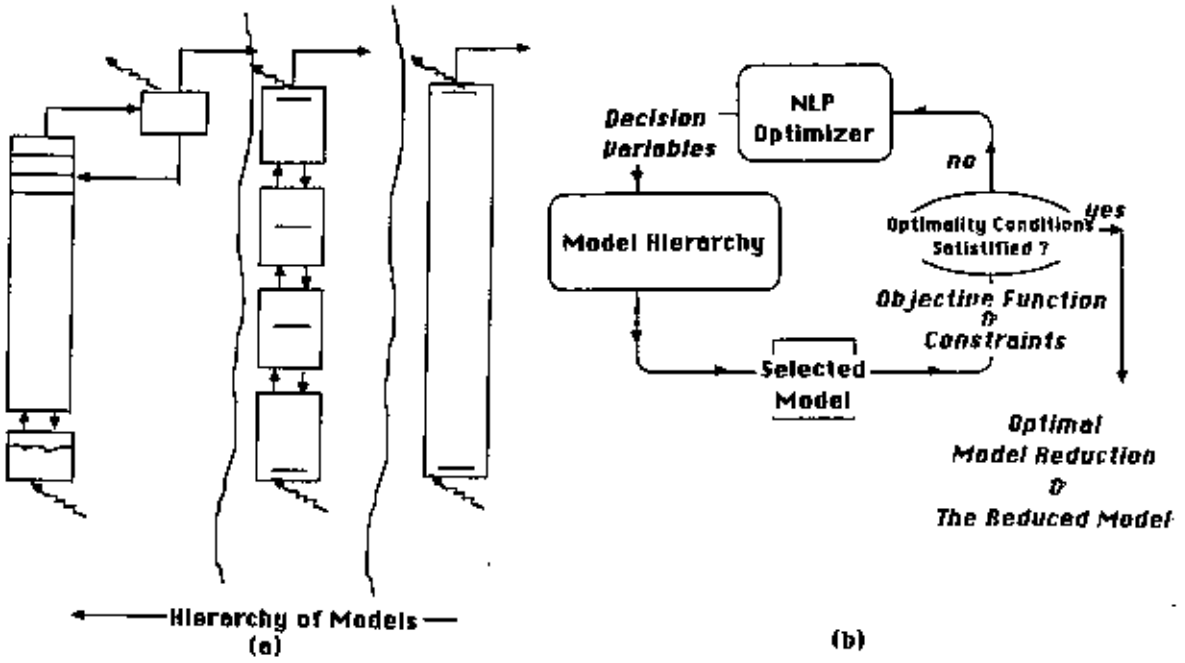


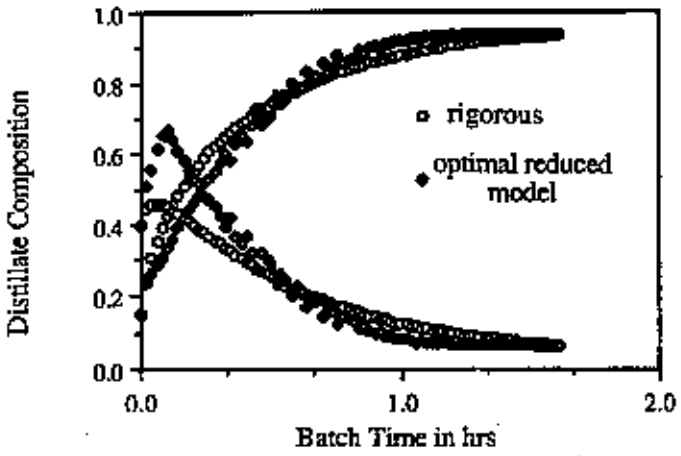
Figure 2: Hierarchy of Models and the Concept of Optimal Model Reduction

3. Hierarchy of Models and Optimal Model Reduction

The compartmental modeling approach for capturing the holdup effects in batch distillation represents a next level of abstraction. However, if observed carefully, the concept of compartmental modeling itself provides a hierarchy of models of increasing complexity with the short-cut method, which can be considered as a single compartmental model, being at the lowest level of hierarchy (Fig. 2a) and the rigorous model, where the number of compartments equals the number of plates N, being at the highest level of hierarchy. Compartmental models have been very popularly used in continuous distillation dynamics and the experiences of the researchers in this area has shown that the decision about the number of compartments and the selection of the sensitive stages are crucial to this approach. Horton et al.(1992) have reported that improper selection of the number of compartments or the sensitive stages associated with each compartment can result in inverse response where none is present in the rigorous full order model. Therefore, the goal of the optimization endeavor is to determine the number of compartments and the associated locations of sensitive stage for each compartment.

As mentioned earlier, the prime advantage of reduced order models is their computational efficiency. Accordingly, the objective function for the problem of "Optimal model reduction" is the CPU time required for solving each model level. Although the decisions such as the number of compartments and the locations of the sensitive stages appear to be discrete, use of short-cut method for the steady-state calculations presents the opportunity to represent these decisions as continuous variables (Fig. 2b). The limit on the maximum number of compartments (NC) may be chosen as the number of stages above the sensitive stage (S^i_{lp-sp}) and below the sensitive stage (S^i_{sp-bp}) for each compartment i as the continuous decision variables. The summation of these two variables associated with the compartment i being zero indicates that the respective compartment i does not exist thereby reducing the order of the model. To retain the distillate and still compositions as state variables, the sensitive stages for the first and the last compartments are considered to be the condenser and reboiler stages. So, for each compartment (other than top and bottom) there are two decision variables resulting in $2(NC-1)$ decision variables for all the compartments. The optimization problem may then be written as:

$$\underset{S^1_{sp-bp},\, S^i_{lp-sp},\, S^i_{sp-bp},\, i=2,\ldots,NC-1,\, S^{NC}_{lp-sp}}{\text{Minimize}} \quad CPU\ time$$



Problem Specification

$N = 20$; $V = 100$; $F = 100$;
$T = 2.0$; $\sum_{i=1}^{N} H_i = 11\%$
$A_{spe} = 0.1$; $NC = 3$
$x_F^{(i)} = 0.15, 0.40, 0.45$
$\alpha_i = 1.25, 1.00, 0.75$

Figure 3: Performance of the Optimally Reduced Model

The problem of minimizing the CPU time is constrained by the error bounds on the specified characteristics of the system. The error bounds are defined in terms of the statistical coefficient of determination (the R^2 value) for the transient profile given by:

$$R_z^2 = \frac{\sum z_{red} - \overline{z}_{rig}}{\sum z_{rig} - \overline{z}_{rig}} = \frac{\int_0^T z_{red}\, dt - \frac{\int_0^T z_{rig} dt}{T}}{\int_0^T z_{rig}\, dt - \frac{\int_0^T z_{rig} dt}{T}}$$

where z represents the composition of the key component (which can be either the still composition x_B or distillate composition x_D). For a good fit, R^2 should be closer to unity. So the accuracy requirement (A_{spe}) can be expressed in terms of the following inequality constraint.

$$1 - A_{spe} \leq R^2 \leq 1 + A_{spe}$$

For the total reflux operating condition predictability of equilibration time introduces additional constraint given by;

$$\tau e_{rig} - \tau e_{red} = 0$$

The optimization problem described above is solved using a nonlinear programming algorithm as illustrated in Fig. 2b. The optimizer invokes the model with the values of $2(NC - 1)$ decision variables. These decision variables represent a particular level of the model in the given hierarchy with a specific structure about the sensitive stage. The model equations are used to simulate the transient profiles and the CPU time required is calculated. This simulation feeds back the values of the objective function and constraints to the optimizer. This information, together with the partial derivatives of the objective function and the constraints with respect to decision variables, is utilized by the optimizer to update the values of the decision variables. The partial derivatives are calculated by the optimizer, by perturbation. The iterative sequence shown in Fig. 2b is carried out until the optimality conditions are satisfied. At convergence, the values of decision variables constitute the optimal model reduction level.

4. Results and Discussions

In order to illustrate the concept of "Optimal Model Reduction" for the total reflux operating condition of batch distillation, a 20-plate column with 11% holdup was considered. A number of cases with mixtures

ranging from binary to quaternary systems were used to test the idea of optimal model reduction. In these studies we have chosen the maximum number of compartments NC to be three based on our earlier experience (Diwekar, 1992). The maximum number of compartments may be increased in the later studies, if necessary. The optimization runs were initiated using four decision variables (corresponding to $NC = 3$), ($S^1_{sp-bp}, S^2_{lp-sp}, S^2_{sp-bp}, S^3_{lp-sp}$), and the optimization procedure described earlier, was numerically executed. For the 20-plate column in this study and for $NC = 3$, If all possible combinations are considered (considering the variables to be discrete), the number of column alternatives to be evaluated will be of the order of over 1700, while with this strategy, the best reduced order model could be arrived at in merely a few iterations (mostly 2-3 iterations). The performance of the optimally reduced model and rigorous model was compared. Unlike other optimization problems in process design and synthesis, here the CPU time was directly considered in the form of objective function and since the derivatives are calculated by perturbation, the reproducibility of the CPU time caused some concern especially for lower order models. However, for almost all the cases the optimizer was able to select appropriate model level as well as structural parameters such as location of sensitive stages and size of the compartment. It was also noted that while the R^2 provides a good statistical measure for most of the cases, it is the introduction of the constraint on predictability of the model with respect to equilibration time guaranteed the success of good performance of the reduced model.

Figure 3 presents one of the test cases for a ternary system, for the sake of brevity results of the other systems are not presented here. The accuracy specifications were imposed on the two key components ($0.9 \leq R^2_{x_D1)} \leq 1.1$ and $0.9 \leq R^2_{x_D2)} \leq 1.1$). For this example, the optimizer selected a two compartment model ($S^1_{sp-bp} = 0.5, S^2_{lp-sp} = 1, S^2_{sp-bp} = 19.5, S^3_{lp-sp} = 0.0$). From Fig.3, it can be seen that the performance of the optimally reduced model is in good agreement with the rigorous model and this model was observed to be atleast 15 times faster than the rigorous model.

The test examples and the detailed example presented in Fig. 3, demonstrated the usefulness of the concept of "Optimal Model Reduction". Since aggregation is pervasive in all branches of science, the generalizability of this concept will have wide ranging implications and a more enhanced study will be carried out in the future.

5. Conclusions

A new approach to selecting optimum level of model reduction is proposed. The strategy is illustrated using different levels of compartmental models of batch distillation. The use of short-cut method to represent the compartmental steady-state material balances allowed the transformation of the discrete decision variables such as the number of compartments and the locations of sensitive stages of each compartment as continuous variables. Nonlinear programming optimization is carried out to obtain the trade-offs between accuracy and efficiency. The successful validation of this strategy for the total reflux operation of batch distillation has shown its potential applicability for other operating conditions of batch distillation and also for continuous distillation. The approach will be expanded further to include discrete decisions by using mixed integer nonlinear programming optimization, thereby making it applicable in general for all a wide range of reduced order models.

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Nomenclature

A_{spc}	accuracy specification
bp^k	bottom plate of the compartment k
B_t	amount remaining in the still at time t, [mol]
C_1	constant in the Hengstebeck-Geddes' equation
F	total feed [mol]
H_j	holdup at plate j [mol]
n	number of components
N	number of plates
NC	maximum number of compartments
N_{min}	minimum number of plates
R_{min}	minimum reflux ratio
$R_{min\ g}$	minimum reflux ratio (Gilliland correlation)
$R_{min\ u}$	minimum reflux ratio (Underwood equations)
R_t	reflux ratio at time t
R_z^2	coefficient of determination for z profiles
sp^k	sensitive stage of the compartment k
S^i_{tp-sp}	no. of stages above the sensitive stage in compartment i
S^i_{sp-bp}	no. of stages below the sensitive stage in compartment i
T	batch time [hrs]
tp^k	top plate of the compartment k
V	vapor boil-up rate [moles/hr]
$x_B^{(i)}$	still composition for component i
$x_D^{(i)}$	distillate composition for component i
$x_F^{(i)}$	feed composition for component i
x_p	liquid composition leaving stage p
y_p	vapor composition leaving stage p
z_{red}	key composition (abstract model)
z_{rig}	key composition (rigorous model)
$\overline{z}_{rig}$	avg. key composition (rigorous model)

Greek Symbols

α_i	relative volatility of component i
ϕ_i	Underwood constant
τe_{rig}	equilibration time prediction (rigorous model)
τe_{red}	equilibration time prediction (abstract model)