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A New Technique of Model Order Reduction Based on Weighted Residuals in Discrete Domain

L. D. Ribeiro, A. R. Sechi, E. C. Biscaia Jr

Chemical Engineering Program - PEQ/COPPE - Universidade Federal do Rio de Janeiro, Av. Horácio Macedo, 2030 - CT - G116 CP.68502 - Ilha do Fundão - 21941-972 - Rio de Janeiro, RJ – Brazil {ldorigo, evaristo, arge}@peq.coppe.ufrj.br

Abstract

In this work we present a new technique of model order reduction applied to staged processes. The proposed method reduces the dimension of the original system based on null values of moment-weighted sums of heat and mass balances residuals on real stages. To compute these sums of weighted residuals a discrete form of Gauss-Lobatto quadrature is developed, allowing a high degree of accuracy on these calculations. Balances related to upstream and downstream devices (such as condenser, reboiler, and feed tray of a distillation column) are considered as boundary conditions of the corresponding difference-differential equations system. The chosen number of moments is the dimension of the reduced model being much lower than the dimension of the complete model and do not depend on the size of the original model. Scaling of the discrete independent variable related with the stages was crucial for the computational implementation of the proposed method, avoiding accumulation of round-off errors presented even in low-degree polynomial approximations in the original discrete variable. Dynamical simulations of distillation columns were carried out to check the performance of proposed reduction technique and, the differential-algebraic nature of the equations was exploited. The obtained results show the superiority of the new procedure in comparison with traditional orthogonal collocation method. Global heat and mass balances are fulfilled in this new method. Moreover, in traditional orthogonal collocation method the points where the residuals are canceled are fixed, and in the new method moving collocation points are obtained, characterizing a desirable adaptive nature of this technique. Lower computational costs were obtained in dynamic simulations with reduced models, maintaining predictive capacity of the complete model, revealing that this new technique can be used in real-time applications.

Keywords: Model order reduction, discrete domain, weighted residuals, orthogonal collocation, distillation column.

1. Introduction

Rigorous dynamic mathematical models of staged separation systems with mass and energy balances lead to a large set of differential-algebraic equations, making them impractical for real-time applications. The challenge to reduce the computational cost of such systems motivated the development of different model order reduction techniques, such as compartmental models (España and Landau, 1978; Benallou et al., 1986; Musch and Steiner, 1993) and its variants aggregated modeling (Lévine and Rouchon, 1991; Linhart and Skogestad, 2009) and time-scale separation (Kumar and Daoutidis, 2003) based on singular perturbation analysis, nonlinear wave propagation (Marquardt, 1986;

Kienle, 2000), model linearization (Georgakis and Stoever, 1982), and orthogonal collocation.

Wong and Luus (1980) were the first to apply orthogonal collocation for order reduction of staged separation systems, by transforming the difference-differential equations into partial differential equations with subsequent application of the orthogonal collocation method in a continuous domain. Cho and Joseph (1983) showed that is possible to apply the orthogonal collocation method directly in the discrete domain by adequate selection of polynomials, and further Stewart et al. (1985) showed the Hahn's polynomials are the best choice for better results as well as more reliable reduced models. Following this approach, Pinto and Biscaia (1987) presented four different order reduction strategies dealing with the discontinuities that happen between the sections of staged separation systems, whereas Seferlis and Hrymak (1994) treated all discontinuous stages as discrete stages and applied order reduction for each section between these discrete stages using orthogonal collocation on finite elements technique with different polynomials for the vapor and liquid phases.

In this work we present a new technique of model order reduction of staged separation systems based on null values of moment-weighted sums of heat and mass balances residuals on real stages. To compute these sums of weighted residuals a discrete form of Gauss-Lobatto quadrature is developed, allowing a high degree of accuracy on these calculations. Balances related to upstream and downstream devices (such as condenser, reboiler, and feed tray of a distillation column) are considered as boundary conditions of the corresponding difference-differential equations system, dealing nicely with the discontinuities that may occur at these points using only one polynomial for each section. Scaling of the discrete independent variable related with the stages is also introduced in this work, which was a drawback for applying discrete orthogonal collocation methods, avoiding accumulation of round-off errors presented even in low-degree polynomial approximations in the original discrete variable.

2. Order Reduction Technique

In order to introduce the proposed model order reduction technique, let us consider a generic section of a staged separation system described by the following difference-differential equations:

$$\frac{dx_i}{dt} = f(x_{i-1}) + g(x_i) + h(x_{i+1}) \quad , \; j = 1, 2, \ldots, N \tag{1}$$

with the boundary conditions $x_0(t) = p(t)$ e $x_{N+1}(t) = q(t)$. Applying a polynomial approximation of degree $n + 1$ in the state variables $x_i(t)$, using the following scaled independent variable representing the stages of the system:

$$s_i = \frac{i-1}{N} \tag{2}$$

and considering the internal points $0 < s^{(1)} < s^{(2)} < \ldots < s^{(n)} < 1$ and the extreme points $s^{(0)} = -\frac{1}{N}$ and $s^{(n+1)} = \frac{N+1}{N}$ as interpolation points, the polynomial can be written as:

$$x(s,t) \cong x^{(n+1)}(s,t) = \sum_{j=0}^{n+1} \ell_j(s)\, x(s^{(j)},t) = \sum_{j=0}^{n+1} \ell_j(s)\, x_j(t) \tag{3}$$

where $\ell_j(s)$ are the Lagrange interpolating polynomials and for the sake of notation $x_j(t) \equiv x(s^{(j)},t)$. For each interpolating points, i = 0, 1, 2, …, n + 1, the following residual function are defined:

$$\Re^{(n+1)}(s^{(i)},t) = \frac{dx_i(t)}{dt} - f\left[x^{(n+1)}(s^{(i)}-1,t)\right] - g\left[x_i(t)\right] - h\left[x^{(n+1)}(s^{(i)}+1,t)\right] \tag{4}$$

where the first-order negative and positive differences are evaluated as:

$$f\left[x^{(n+1)}(s^{(i)}-1,t)\right] = \sum_{j=0}^{n+1} \ell_j(s^{(i)}-1)\, f\left[x_j(t)\right] = \sum_{j=0}^{n+1} A_{i,j}^{-}\, f\left[x_j(t)\right] \tag{5}$$

$$h\left[x^{(n+1)}(s^{(i)}+1,t)\right] = \sum_{j=0}^{n+1} \ell_j(s^{(i)}+1)\, h\left[x_j(t)\right] = \sum_{j=0}^{n+1} A_{i,j}^{+}\, h\left[x_j(t)\right] \tag{6}$$

In the traditional method of discrete orthogonal collocation, $x_i(t)$ are find such that the residuals at the internal points, i = 1, 2, …, n, are canceled (collocation points):

$$\Re^{(n+1)}(s^{(i)},t) = 0 = \frac{dx_i(t)}{dt} - \sum_{j=0}^{n+1} A_{i,j}^{-}\, f\left[x_j(t)\right] - g\left[x_i(t)\right] - \sum_{j=0}^{n+1} A_{i,j}^{+}\, h\left[x_j(t)\right] \tag{7}$$

and the boundary conditions $x_0(t) = p(t)$ e $x_{n+1}(t) = q(t)$ complete the system of n + 2 equations. In order to skip the discontinuities that may occur in the boundaries, a similar approach of Seferlis and Hrymak (1994) can be applied in the traditional method by adding two extra collocation points at the extreme stages of the section of the separation system, and for these points the residuals are defined as:

$$\Re^{(n+1)}(s^{(0)},t) = 0 = \frac{dx_0(t)}{dt} - f\left[x_{-1}(t)\right] - g\left[x_0(t)\right] - \sum_{j=0}^{n+1} A_{0,j}^{+}\, h\left[x_j(t)\right] \tag{8}$$

$$\Re^{(n+1)}(s^{(n+1)},t) = 0 = \frac{dx_{n+1}(t)}{dt} - \sum_{j=0}^{n+1} A_{n+1,j}^{-}\, f\left[x_j(t)\right] - g\left[x_{n+1}(t)\right] - h\left[x_{n+2}(t)\right] \tag{9}$$

where the boundary conditions are $x_{-1}(t) = p(t)$ e $x_{n+2}(t) = q(t)$. However, this modified approach has the disadvantage of increasing the size of the system, or reducing the degree of the orthogonal polynomial by two if keeping the same size of the traditional method.

In the proposed method, $x_i(t)$ are find such that sum of the moment-weighted residuals are canceled for the first n moments:

$$\Re_k^{(n+1)}(t) = \sum_{j=1}^{N} \left(\frac{j-1}{N}\right)^{k-1} \Re^{(n+1)}\left(\frac{j-1}{N},t\right) = 0 \quad , \; k = 1, 2, \ldots, n \tag{10}$$

These sums of weighted residuals are evaluated using a discrete form of Gauss-Lobatto quadrature:

$$\Re_k^{(n+1)}(t) = \sum_{i=0}^{n+1} \omega_i \left(s^{(i)}\right)^{k-1} \Re^{(n+1)}\left(s^{(i)},t\right) = \sum_{i=0}^{n+1} M_{k,i}\, \Re^{(n+1)}\left(s^{(i)},t\right) = 0\ ,\ k = 1, \ldots, n \quad (11)$$

where $M_{k,i} = \omega_i \left(s^{(i)}\right)^{k-1}$ and ω_i are the quadrature weights. This quadrature is exact for polynomial functions up to degree 2 n + 1, which is always the case for the linear case because $\Re^{(n+1)}(s,t)$ is a polynomial of degree n + 1.

As the n equations in (11) are linear, they can be rewritten in the following form:

$$\Re^{(n+1)}\left(s^{(i)},t\right) + V_{i,0}\, \Re^{(n+1)}\left(s^{(0)},t\right) + V_{i,1}\, \Re^{(n+1)}\left(s^{(n+1)},t\right) = 0\ ,\ i = 1, \ldots, n \quad (12)$$

where $\mathbf{V}_0 = \mathbf{M}^{-1}\mathbf{b}_0$ and $\mathbf{V}_1 = \mathbf{M}^{-1}\mathbf{b}_1$ with $b_{i,0} = M_{i,0}$, $b_{i,1} = M_{i,1}$ and $\mathbf{M}$ is the square matrix by removing the first and the last columns. By substituting Eq. (4) in Eq. (12), the following expression can be derived:

$$\frac{dX_i(t)}{dt} = \sum_{j=0}^{n+1} B_{i,j}^{-}\, f\left[x_j(t)\right] + G\left[x_i(t)\right] + \sum_{j=0}^{n+1} B_{i,j}^{+}\, h\left[x_j(t)\right]\ ,\ i = 1, \ldots, n \quad (13)$$

where $X_i(t) = x_i(t) + V_{i,0}\, x_0(t) + V_{i,1}\, x_{n+1}(t)$, $B_{i,j}^{-} = A_{i,j}^{-} + V_{i,0}\, A_{0,j}^{-} + V_{i,1}\, A_{n+1,j}^{-}$, $B_{i,j}^{+} = A_{i,j}^{+} + V_{i,0}\, A_{0,j}^{+} + V_{i,1}\, A_{n+1,j}^{+}$ and $G\left[x_i(t)\right] = g\left[x_i(t)\right] + V_{i,0}\, g\left[x_0(t)\right] + V_{i,1}\, g\left[x_{n+1}(t)\right]$.

The boundary conditions $x_0(t) = p(t)$ e $x_{n+1}(t) = q(t)$ complete the system of n + 2 equations. Note that the traditional orthogonal collocation is reproduced by setting $V_{i0} = 0$ and $V_{i1} = 0$. In both cases, $s^{(1)}$, $s^{(2)}$, …, $s^{(n)}$ are the roots of the Hahn's polynomial of degree n.

Using the proposed scaled discrete independent variable, the roots of the Hahn's polynomial are obtained with high accuracy for any degree, whereas high accumulation of round-off errors are observed in the original discrete variable, even for low-degree polynomials.

It must be emphasized that global heat and mass balances are fulfilled in the proposed method, which are given by the zero-order moment. Moreover, in traditional orthogonal collocation method the points where the residuals are canceled are fixed ($s^{(1)}$, $s^{(2)}$, …, $s^{(n)}$), and in the proposed method moving collocation points are obtained, characterizing a desirable adaptive nature of this technique.

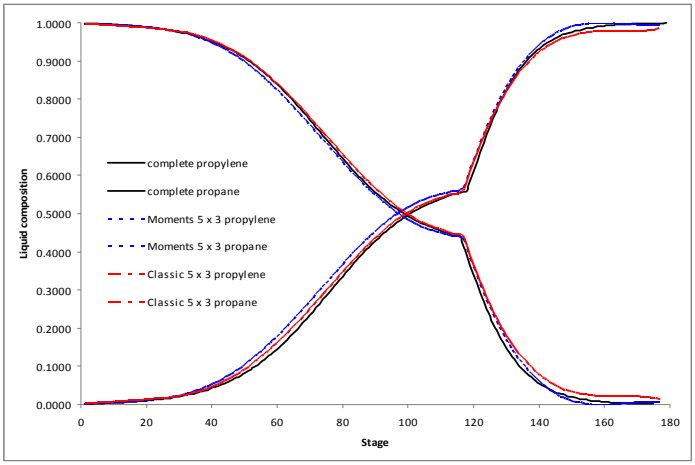
3. Illustrative Example

In order to illustrate the application of the proposed method, a distillation column to separate propane and propylene was used, as described in Seferlis and Hrymak (1994) and with the specifications given in Table 1.

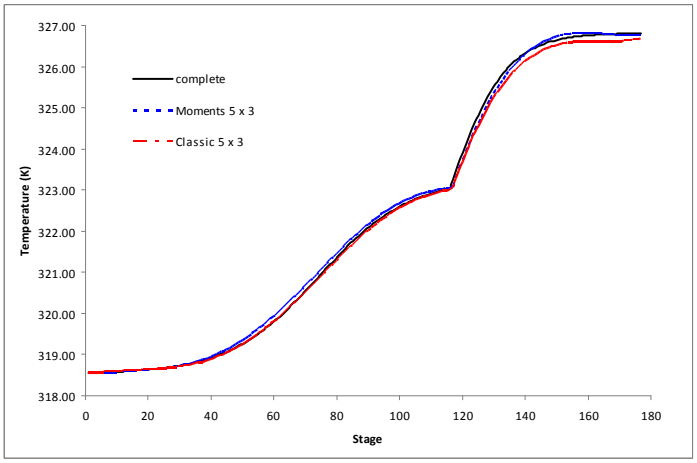
Table 1. Distillation column specifications

number of trays	175
feed tray	116
feed composition (propylene, propane)	[0.8973, 0.1027]
feed flow rate (kmol/d)	1073.4
feed temperature	46.11
operating pressure (kPa)	1860.60
reflux ratio	19.7
distillate flow rate (kmol/d)	965

The Peng-Robinson equation of state was used for evaluation of the thermodynamic properties. In the reduced models, for the rectifying section 5 internal points were used, and for the stripping section only 3 points, i.e., a reduction of 95%. The procedure was implemented in the EMSO simulator. In Figure 1, the liquid molar fraction and temperature steady-state profiles for the complete model and for the reduced models using the proposed method and the traditional orthogonal collocation method are presented, where the superiority of the new approach in comparison with traditional method can be observed for the downstream variables, mainly at the bottom of the column. These results are better visualized in the tables presented in Figure 1, where the absolute square errors relative to the complete model are given for (1) sum of these errors over all stages, (2) maximum error, (3) condenser error, (4) reboiler error, and (5) feed tray.



Errors	Moments	Classic
sum	2.92937	3.46050
max	0.02358	0.03273
top	0.00055	0.00155
bottom	0.00487	0.01379
feed	0.00590	0.01721



Errors	Moments	Classic
sum	12.172	14.787
max	0.202	0.283
top	0.004	0.012
bottom	0.043	0.122
feed	0.025	0.028

Figure 1. Steady-state profiles for complete model, proposed method, and orthogonal collocation.

In order to illustrate the dynamic behavior a step function was applied in the reflux ratio at 0.4 h changing from 19.7 to 22, starting the simulation at the steady-state condition. In Figure 2, the step response of the propylene composition and the temperature in the distillate are presented, showing the predictive capacity of the reduced model even for the transient behavior.

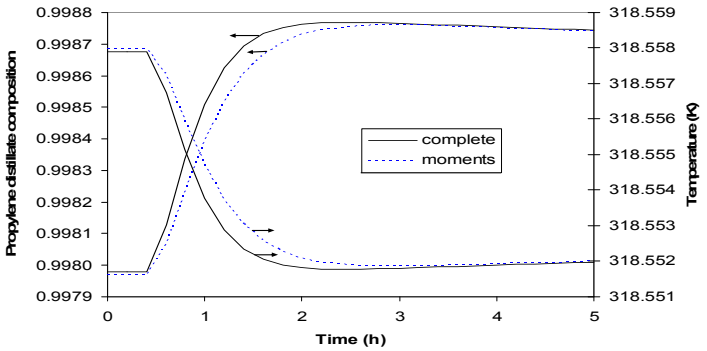


Figure 2. Distillate temperature and composition step response for complete and reduced models.

4. Conclusion

The proposed technique of model order reduction of staged separation systems based on the sum of moment-weighted residuals showed to be superior to the traditional orthogonal collocation method on discrete domain. The scaling of the discrete independent variable was crucial for the accuracy of the roots of Hahn's polynomials. Dynamical simulations results of distillation columns showed the technique can be applied for control purposes and other real-time applications.

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