J. King Saud Univ., Vol. 21, *Eng. Sci.* (2), pp. 87-91, Riyadh (2009/1430H.)

Studies on the Method of the Orthogonal Collocation VIII: A Spline Collocation Method for Distillation Columns Simulation

Moustafa A. Soliman
Chemical Engineering Department, College of Engineering, King Saud University, P.O. Box 800, Riyadh 11421, Saudi Arabia
mostf34@hotmail.com

(Received 21 April 2007; accepted for publication 08 December 2007)

Keywords: Distillation, Simulation, Spline collocation.

Abstract. The author (1992) developed a spline collocation method that was successfully applied to continuous systems described by differential equations. It is based on selecting the spline point such that the second derivative of the independent variable is zero at the spline point. This method is now extended to discrete systems described by different equations and is applied to the simulation of distillation columns.

Introduction

The application of the method of orthogonal collocation to systems with steep profiles requires the division of the domain of interest to elements in which the collocation method is applied individually. Some continuity conditions should be satisfied at the elements partition.

Srivastava and Joseph (1987) applied a global collocation scheme for key component equations, whereas for non-key components, the equations are solved using collocation on two regions for each component. The boundary between the two regions is determined by the smallness or largeness of the absorption factor (L/KV) using an arbitrary criterion. Interpolation is required to transfer information between different collocation schemes.

Choi *et al*. (1991) suggested the use of cubic spline functions for model reduction of distillation columns. They have shown that they are better than quadratic Lagrange polynomials.

Seferlis and Hrymak (1994) based the elements partition on the equi-distribution of the material, and energy balances residuals around the envelopes in the column to track irregularities in mole fraction profiles.

Huss and Westerberg (1994) suggested two variable transformations for the stage number, and mole fractions to straighten irregular mole fraction profiles. An exponential transformation maps zero to an infinite number of trays onto the range 0-1. Jacobi polynomials can be used for the application of the collocation method to the transformed problem. The second transformation uses a hyperbolic tangent function for the mole fractions.

The author (1992) developed a spline collocation method for boundary value problems which is based on determining the spline points by the requirement that the second derivative of the independent variable is zero. In this paper, this approach is extended to distillation columns design.

Model Formulation

In modeling the distillation column, the following assumptions are made:

1. The column separates a binary mixture and has a total condenser.
2. In each of the rectifying and stripping sections, the molar flowrates of the liquid and vapor are constant.
3. Each section has its own constant relative volatility.

Numbering the stages starting from the feed plate as shown in Fig. 1, plate component material balance for the rectifying section can be written as:

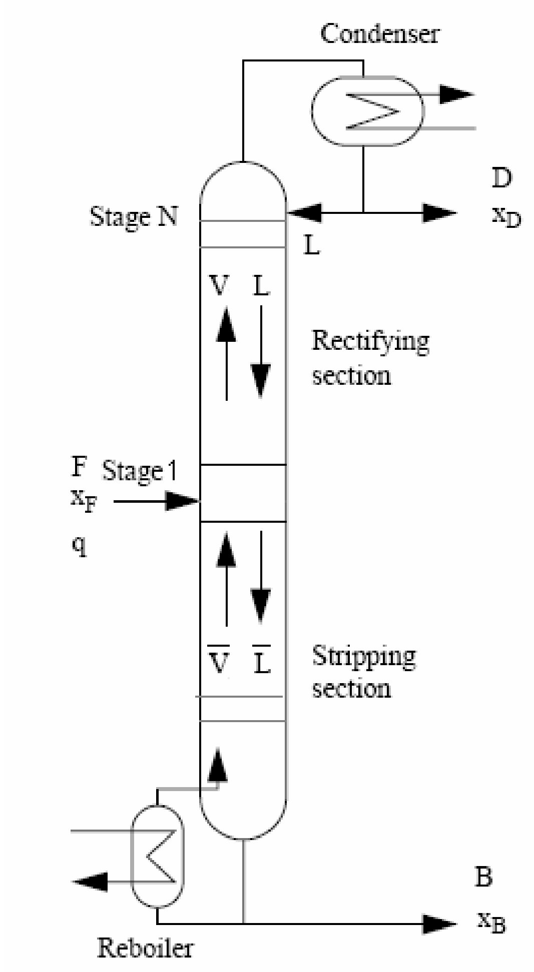


Fig. 1. A two-product distillation column.

$$V(y_i - y_{i-1}) = L(x_{i+1} - x_i) \tag{1}$$

where

$$y_i = K_i x_i = \frac{\alpha_r x_i}{1+(\alpha_r - 1)x_i} \tag{2}$$

A total condenser would mean that the vapor leaving the top tray has a mole fraction y_N that is equal to the liquid mole fraction entering this plate x_D, i. e.,

$$x_D = y_N = \frac{\alpha_r x_N}{1+(\alpha_r - 1)x_N} \tag{3}$$

Overall component material balance on the rectifying section gives:

$$V\overline{y_1} = Lx_1 + Dx_D \tag{4}$$

where

$$V = L + D \tag{5}$$

At the feed plate,

$$\overline{L} = L + qF \tag{6}$$

the stripping section plate component material balance is given by:

$$\overline{V}(\overline{y}_i - \overline{y}_{i+1}) = \overline{L}(\overline{x}_{i-1} - \overline{x}_i) \tag{7}$$

where

$$\overline{V} = \overline{L} - B \tag{8}$$

and

$$\overline{y}_i = \frac{\alpha_s \overline{x}_i}{1+(\alpha_s - 1)\overline{x}_i} \tag{9}$$

The column overall component balance is given by:

$$x_f F = Dx_D + Bx_B \tag{10}$$

Numerical Method Development

If the equilibrium curve is linear and its slope is equal to the operating line, we could write the component material balance on the plates as:

$$x_{i+1} - 2x_i + x_{i-1} = 0 \tag{11}$$

Subject to given conditions for the top and bottom compositions, the solution will be linear with the number of plates as:

$$x_i = x_1 + (x_D - x_1)r_i \tag{12}$$

where

$$r_i = (i-1)/N \tag{13}$$

Now, we model the deviation from this ideal situation by:

$$x_i = x_1 + (x_D - x_1)r_i U_i \tag{14}$$

and let U_i satisfies the equation:

$$(r_{i+1}U_{i+1} - 2r_i U_i + r_{i-1}U_{i-1}) = \phi\, r_i U_i / N^2 \quad (15)$$

The right hand side is obtained by substituting Eq. (14) into Eq. (11). The left hand side is introduced to model the deviation. If we let N goes to infinity, Eq. (15) becomes:

$$\frac{d^2(rU)}{dr^2} = \phi\, rU \quad (16)$$

With the boundary conditions:

$$U(1) = 1, U'(0) = 0 \quad (17)$$

The application of the one point collocation to Eq. (16) requires the selection of the collocation point (r_c) such that:

$$r_c^2 = 0.3 \quad (18)$$

to get accurate value for U at r = 0, and U will be a function of the even power of r.

Thus we could write the following equation for U_i,

$$U_i = \frac{(1-r_i^2)U_c + (r_i^2 - r_c^2)}{(1-r_c^2)} \quad (19)$$

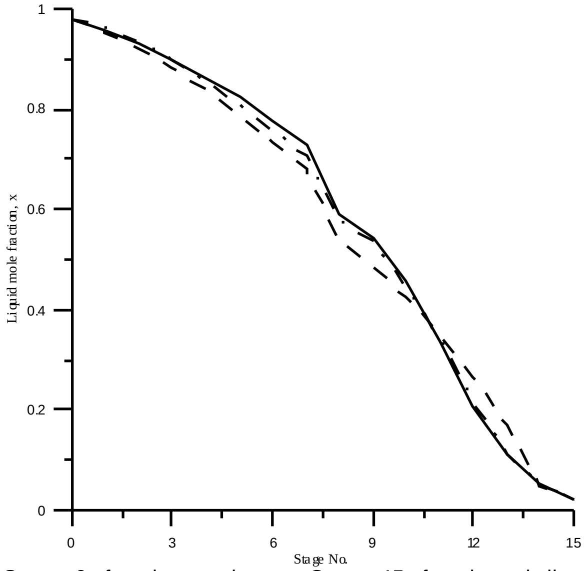
In effect this would mean that we have approximated the composition profile by a cubic polynomial whose second derivative is zero at the plate above the feed point and the plate below the feed point. If one cubic polynomial is not enough to approximate the profile, we consider cubic splines such that at the spline point (subscript s) we have the following condition,

$$x_{s-1} - 2x_s + x_{s+1} = 0 \quad (20)$$

For a continuous system, this condition is equivalent to the requirement that at the spline point the profile has an inflection point; a condition that was successfully used in the development of a spline collocation method (Soliman, 1992). In addition, we require that the spline farther from the feed point starts with inflection point, and the component material balance is satisfied at the spline point of this spline.

Table 1. Design and operating conditions for the distillation column

Number of plates in the rectifying section	7
Number of plates in the stripping section	7
Total condenser + reboiler	
Feed flowrate	216.0 mol/hr
Feed condition (q)	1
Feed mole fraction (x_f)	0.5
Top product flowrate	108.0 mol/hr
Reflux ratio	2
Relative volatilities	$\alpha_r = 2.0, \alpha_s = 3.0$



Stage 0 for the condenser, Stage 15 for the reboiler, ___ rigorous, __ __ cubic collocation, __ _ __ _ cubic spline collocation

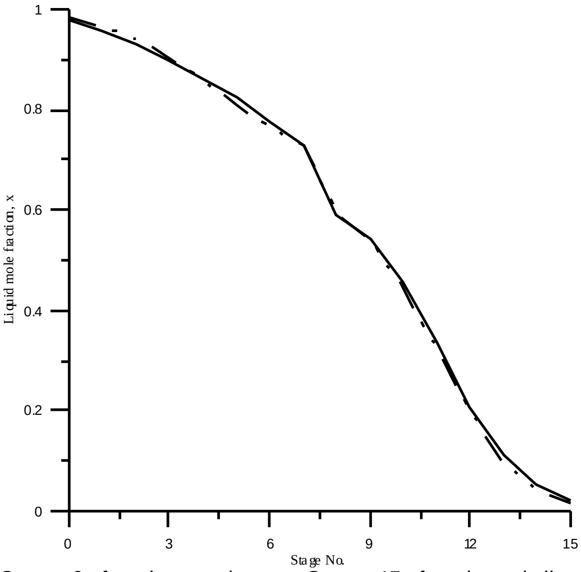
Fig. 2. Composition profile in the distillation column.

Numerical Example

Table 1 shows the design and operating conditions of the distillation column to be simulated.

Results of the numerical testing are shown in Figs. 2 and 3. In Fig. 2, the application of a single cubic polynomial in each of the column sections show some deviation in the composition profile in the stripping section compared to the rigorous solution due to the sigmoidal nature of the profile. When we used two cubic splines in the stripping section, the profile greatly improved. In Fig. 3, the application of Huss and Westerberg (1996) transformation:

$$x = \frac{(1+\tanh(y))}{2} \quad (20)$$



Stage 0 for the condenser, Stage 15 for the reboiler, ___ rigorous, ___ _ _ ___ _ _ Huss and Westerberg transformation

Fig. 3. Composition profile in the distillation column.

and

$$y = \frac{\ln\left(\frac{x}{1-x}\right)}{2} \qquad (21)$$

resulted in almost exact results. y is fitted by a quadratic polynomial, and the collocation point $r_c = 0.5$.

Conclusion

A spline collocation method is developed and successfully applied to the simulation of a distillation column. The keys for the success of this method are the proper selection of the interpolating function (Eqs. (14) and (19)), the proper selection of the collocation point (Eq. (18)), and the proper selection of the criterion at the spline point (Eq. (20)). It can be considered as an alternative if Huss and Westerberg transformation does not work.

References

Choi, S.Y.; Kim, H.S.; Lee, K.S.; Yoo, K.P. and Lee, W.H. "Reduced-order Distillation Model Using Collocation Method with Cubic Splines." *Korean J. of Chem. Eng.*, Vol. 8, No. (1), (1991), 44-52.

Huss, R. and Westerberg, A.W. "Collocation Methods for Distillation Design I- Model Description and Testing." *Ind. Eng. Chem. Res.*, Vol. 35, No. (5), (1996), 1603-1610.

Huss, R. and Westerberg, A.W. "Collocation Methods for Distillation Design II- Applications for Distillation." *Ind. Eng. Chem. Res.*, Vol. 35, No. (5), (1996), 1611-1623.

Seferlis, P. and Hrymak, A.N. "Adaptive Collocation Finite Elements Models for the Optimization of Multi-stage Distillation Units." *Chem. Eng. Sci.*,Vol. 49, (1994), 1369-1382.

Sirvastava, R.K. and Joseph, B. "Reduced Order Models for Staged Separation Columns VI- Columns with Steep and Flat Profiles." *Comput. Chem. Eng.*, Vol. 49, (1997), 1369-1382.

Soliman, M.A. "A Spline Collocation Method for the Solution of Diffusion-convection Problems with Chemical Reactions." *Chem. Eng. Sci.*, Vol. 47, (1992), 4209-4212.

دراسات على طريقة التنظيم ا تعامد ٨:
طريقة تنظيم مقسمة اكاة أعمدة التقط

مصطفى علي سليمان

قسم الهندسة الكيميائية ، كلية الهندسة ، جامعة الملك سعود ،

ص ب ٨٠٠ الرياض ١١٤٢١ ، المملكة العربية السعودية

mostf34@hotmail.com

(قدم للنشر في ٢١/٠٤/٢٠٠٧م؛ وقبل للنشر في ٠٨/١٢/٢٠٠٧م)

ملخص البحث. طور المؤلف طريقة تنظيم مقسمة وطبقت بنجاح على أنظمة مستمرة توصف بمعادلات تفاضلية وتعتمد على اختيار نقطة التقسيم بحيث تكون المشتقة الثانية للمتغير المستقل عند نقطة التقسيم صفرًا، وقد تم تطويرها في هذا البحث لتشمل أنظمة غير مستمرة توصف بمعادلات فرق، ومن ثمَّ طُبقت الطريقة على أعمدة تقطير.