Orthogonal Collocation-based Steady-State and Transient Response Simulation of Two-pass Shell and Tube Heat Exchangers

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Abstract
An orthogonal collocation-based approach to the simulation of the steady-state and transient response of a two-pass shell and tube heat exchanger is presented. The analytical solution of the steady-state temperature profiles in the heat exchanger are derived. These are then used for selection of the parameters of the orthogonal solution such that the Euclidean norm of the error between the analytical and orthogonal collocation solution is minimized. The lumped parameter ordinary differential equations (ODEs) obtained from the application of the orthogonal collocation method are used to simulate the dynamic response of the system using the state transition matrix approach. Very good results were obtained consistent with other reported applications of the orthogonal collocation method to other types of heat exchangers in the literature. The orthogonal collocation approach is attractive in the efficient simulation of single or interconnected heat exchanger systems such as heat exchanger networks or heat exchanger-reactor systems.

Keywords: Heat exchangers, orthogonal collocation, steady-state, state transition matrix, and transient response.

1.0 INTRODUCTION

Heat exchangers are equipment that enable the transfer of thermal energy between two or more fluids at different temperatures. As a result, they are widely employed in several types of applications, including but not limited to power generation; process, chemical and food industries; electronics; environmental engineering; waste heat recovery; manufacturing industry; air conditioning; refrigeration; space industry etc. (Kakac and Liu, 2002; Gvozdenac, 2012). In these applications, heat exchangers are frequently subjected to external disturbances and control which make them undergo transients. Consequently, there is often the need to carry out simulations of the transient responses for optimal operation and real-time regulation and control of the heat exchangers (Roetzel et al., 2002). The knowledge of the steady-state and dynamic behaviour of heat exchangers is also required both at the design and operational stages in order to lower future possible failures, and hence maintenance cost. The simulation of the dynamic response behaviour can help forecast potentially extreme operating conditions which may induce adverse thermal stresses in the metal parts of the heat exchanger (Bracco et. al., 2007).

Heat exchangers have been studied extensively, and have frequently been used to typify distributed parameter systems (DPS) analysis (Gutierres and Cooper, 1979). They may be classified into five categories (Kakac and Lui, 2002): (i) Recuperators or regenerators; (ii) Transfer processes: direct contact and indirect contact; (iii) Geometry of construction: tubular, plates and extended surfaces; (iv) Heat Transfer mechanism: single-phase and two-phase, and (v) Flow arrangement: parallel, counter- and cross-flow.

Some of the early studies on heat exchangers are included in the review of Ronsenbrock (1962), and the text books of Harriot (1964), Gould (1969), Friedly (1972). More recent studies include those of Correa and Marchetti (1987), Xia et al. (1991), Williams and Adeniyi (1989, 1991), Sharifi (1995), Roetzel and Xuan (1992, 1999), Roetzel et al.(2002), Bracco et et., 2007), Gvozdenac (2012), Fratczak et al. (2014, 2016) and Ebrahimzadeh et al.(2016a,b) to mention a few. A recent comprehensive review of double-pipe heat exchangers is presented by Omidi et al.(2017). From these works, it is seen that studies of heat exchanger dynamics have largely been based on frequency domain techniques (i.e. transfer functions and frequency responses), and sometimes numerical inversion of the transfer function to obtain time domain responses, see for examples: Gould 1969), Friedly (1972), Roetzel and Xuan (1999), Roetzel et al.(2002) and Luo et al. (2003).

When direct time domain techniques have been used, they have largely been based on lumping of the partial differential equations that model the systems in the spatial domain using classical finite difference techniques. The resulting set of ordinary differential equations (ODEs) are then integrated using a suitable integration routine. The major drawback to using the finite difference method is that it often requires a large number of grid points to accurately approximate the PDE, and hence resulting in a very high-order lumped model that will take longer to simulate, see for examples: Xia et al. (1991), Nevriva etl. (2009). Moreover, such a very high-order lumped model is not suitable for control system design (Friedly, 1972, Srivastava and Joseph, 1984; Williams and Adeniyi, 1989, 1991). Due to these limitations, researchers in the field are increasingly employing the orthogonal collocation method (Finlayson, 1972. 1980; Villadsen and Michelsen, 1978) as a more efficient approach to lump the PDE models with resulting much lower-order set of ODEs. Williams and Adeniyi (1989, 1991) presented the successful application of the orthogonal collocation method to a steam heated exchanger. More recently, Fratczak (2014, 2016) and Ebrahimzadeh (2016a,b) have presented the successful application of the orthogonal collocation method in the simulation of the dynamics of plate-type heat exchangers.

The present paper is concerned with the expansion of the application of the orthogonal collocation method in the study of the steady-state and dynamic response behaviour of other types of heat exchanger systems. The type of system considered in this study is the two-pass shell and tube heat exchanger which is also commonly employed in several thermal exchange applications. As far as the authors know, no dynamic simulation studies utilising the orthogonal collocation method has appeared in the open literature for this type of exchanger system. Yet, this type of heat exchanger systems can also benefit, computationally, from the highly efficient and resulting relatively, low-order model through application of the orthogonal collocation method. Thus a key objective of this work is the development of low-order steady-state and dynamic models that can be used for quick simulations and/or control system analysis/design of the heat exchanger system considered.

2 METHODOLOGY

2.1 Mathematical Model of Two-Pass Shell and Tube Heat Exchanger Systems

The mathematical model of a heat exchanger is developed by writing an energy balance on a microscopic element of the exchanger.

The schematic diagram of a two-pass shell and tube heat exchanger is shown in Figure 1. This type of configuration is also called a 2-pass, double-pipe heat exchanger.

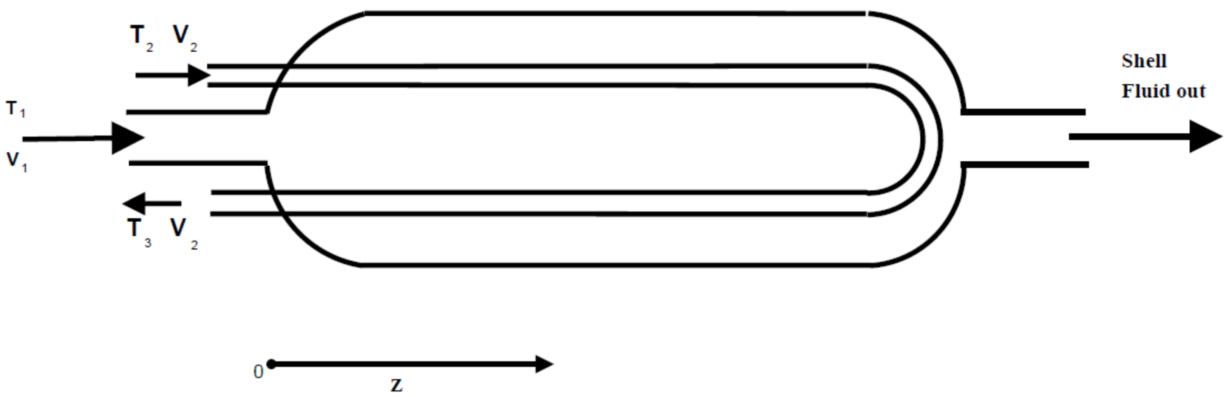


Figure 1: Schematic diagram of a two-pass shell and tube heat exchanger (Friedly, 1972)

To derive the mathematical of model of the system, we make the following assumptions (cf. Friedly, 1972): (i) both fluids are in plug flow, (ii) no temperature variation in the radial direction, (iii) fluid properties such as densities and heat capacities are constant, (iv) there is no heat conduction axially and radially, (v) the outer tube is completely insulated or lagged, with no heat loss to the environment, (vi) heat transfer in the radial direction can be represented by a lumped relation of the form of Newton's Law of Cooling with constant heat transfer coefficient, (vii) uniform cross-sectional area, (viii) potential energy and kinetic energy are negligible and there is no work, (ix) thermal capacities of the walls of exchanger are zero or negligible; then writing an energy balance on a microscopic element of the heat exchanger, one obtains the following model:

$$\rho_1 A_1 C_{p1}\frac{\partial T_1}{\partial t'} = -\rho_1 A_1 v_1 C_{p1}\frac{\partial T_1}{\partial z'} - U_1 S_1 (T_1 - T_2) - U_1 S_1 (T_1 - T_3) \quad (1)$$

$$\rho_2 A_2 C_{p2}\frac{\partial T_2}{\partial t'} = -\rho_2 A_2 v_2 C_{p2}\frac{\partial T_2}{\partial z'} + U_2 S_2 (T_1 - T_2) \quad (2)$$

$$\rho_2 A_2 C_{p2}\frac{\partial T_3}{\partial t'} = \rho_2 A_2 v_2 C_{p2}\frac{\partial T_3}{\partial z'} + U_2 S_2 (T_1 - T_3) \quad (3)$$

Eqs. (1) to (3) model the dynamics of the two-pass, shell and tube heat exchanger system, subject to the following initial and and boundary conditions:

$$At \quad t' = 0, \quad T_1(z',0) = \overline{T}_1(z'), \quad T_2(z',0) = \overline{T}_2(z')$$
$$T_3(z',0) = \overline{T}_3(z')$$

$$At \quad z' = 0, \quad T_1(0,t') = f_1(t'), \qquad T_2(0,t') = f_2(t')$$
$$At \quad z' = L \quad T_3(L,0) = T_2(L,t')$$

If we normalize the independent variables z' and t' by defining

$$z = z'/L, \quad t = v_1 t'/L$$

and use the deviation variables

$$x_1 = T_1 - \overline{T}_1(z), \quad x_2 = T_2 - \overline{T}_2(z), \quad x_3 = T_3 - \overline{T}_3(z)$$
$$x_{1f} = f_1(t) - \overline{f}_1, \quad x_{2f} = f_2(t) - \overline{f}_2$$

where $\overline{T}_1(z)$, $\overline{T}_2(z)$ and $\overline{T}_3$ are the steady-state temperature profiles in the exchanger at $\overline{f}_1$ and $\overline{f}_2$ conditions, then Eqs. (1) to (3) can be simplified to (cf. Friedly, 1972):

$$\frac{\partial x_1}{\partial t} = -\frac{\partial x_1}{\partial z} - a_1(x_1 - x_2) - a_1(x_1 - x_3) \quad (4)$$

$$r\frac{\partial x_2}{\partial t} = -\frac{\partial x_2}{\partial z} + a_2(x_1 - x_2) \quad (5)$$

$$r\frac{\partial x_3}{\partial t} = \frac{\partial x_3}{\partial z} + a_2(x_1 - x_3) \quad (6)$$

Subject to the conditions

- Initial conditions

$$x_1(z,0) = 0 \quad x_2(z,0) = 0 \quad x_3(z,0) = 0 \quad (7)$$

- Boundary conditions

$$x_1(0,t) = x_{1f} \quad x_2(0,t) = x_{2f} \quad x_3(1,t) = x_2(1,t) \quad (8)$$

where

$$a_1 = \frac{U_1 S_1 L}{\rho_1 C_{p1} A_1 v_1} \quad a_2 = \frac{U_2 S_2 L}{\rho_2 C_{p2} A_2 v_2} \quad r = \frac{v_1}{v_2} \quad (9)$$

Eqs. (4) to (6) is a set of first-order, linear, hyperbolic partial differential equations subject to the simple, algebraic initial and boundary conditions given by Eqs. (7) and (8), respectively.

2.2 Steady-state Analytical Solutions Method

Unlike the case of a single-pass, shell and tube heat exchanger where it is very easy to obtain the steady-state analytical solutions, that of the two-pass configuration is a bit tedious to obtain as can be seen in Appendix A. The expressions obtained for the analytical solutions are as follows:

$$\bar{x}_1(z) = c_1 + c_2 e^{\phi_1 z} + c_3 e^{\phi_2 z} \quad (10)$$

$$\bar{x}_2 = c_1 + c_2 e^{\phi_1 z} + c_3 e^{\phi_2 z} + \left(\frac{1}{2a_1} - \frac{1}{a_2}\right)\left(c_2\phi_1 e^{\phi_1 z} + c_3\phi_2 e^{\phi_2 z}\right) - \frac{1}{2a_1 a_2}\left(c_2\phi_1^2 e^{\phi_1 z} + c_3\phi_2^2 e^{\phi_2 z}\right) \quad (11)$$

$$\bar{x}_3 = c_1 + c_2 e^{\phi_1 z} + c_3 e^{\phi_2 z} + \left(\frac{1}{2a_1} + \frac{1}{a_2}\right)\left(c_2\phi_1 e^{\phi_1 z} + c_3\phi_2 e^{\phi_2 z}\right) + \frac{1}{2a_1 a_2}\left(c_2\phi_1^2 e^{\phi_1 z} + c_3\phi_2^2 e^{\phi_2 z}\right) \quad (12)$$

in which

$$\phi_1 = -a_1 + \sqrt{a_1^2 + a_2^2} \quad (13)$$

$$\phi_2 = -a_1 - \sqrt{a_1^2 + a_2^2} \quad (14)$$

$$c_1 = \frac{\bar{x}_{1f}(q_1 q_4 - q_2 q_3) - \bar{x}_{2f}(q_4 - q_3)}{(q_1 q_4 - q_2 q_3) - (q_4 - q_3)} \quad (15)$$

$$c_2 = \frac{q_4(\bar{x}_{2f} - \bar{x}_{1f})}{(q_1 q_4 - q_2 q_3) - (q_4 - q_3)} \quad (16)$$

$$c_3 = \frac{q_3(\bar{x}_{1f} - \bar{x}_{2f})}{(q_1 q_4 - q_2 q_3) - (q_4 - q_3)} \quad (17)$$

with q_1, q_2, q_3 given by the following:

$$q_1 = 1 + \left(\frac{1}{2a_1} - \frac{1}{a_2} \right) \phi_1 - \frac{\phi_1^2}{2a_1 a_2} \tag{18}$$

$$q_2 = 1 + \left(\frac{1}{2a_1} - \frac{1}{a_2} \right) \phi_2 - \frac{\phi_2^2}{2a_1 a_2} \tag{19}$$

$$q_3 = \frac{2}{a_1} \phi_1 e^{\phi_1} + \frac{1}{a_1 a_2} \phi_1^2 e^{\phi_1} \tag{20}$$

$$q_4 = \frac{2}{a_2} \phi_2 e^{\phi_2} + \frac{1}{a_1 a_2} \phi_2^2 e^{\phi_2} \tag{21}$$

The steady-state temperature profiles for streams 1, 2 and 3 are $\bar{x}_1(z), \bar{x}_2(z)$ and $\bar{x}_3(z)$, respectively; while $\bar{x}_{1f}$ and $\bar{x}_{2f}$ are the corresponding steady-state inlet temperatures of the two streams.

2.3 Orthogonal Collocation-Based Solution Method

The mathematical model of the two-pass shell and tube heat exchanger is given by Eqs. (4) to (6) with the initial and boundary conditions, Eqs. (7) and (8). Even though they are linear, it is difficult to obtain analytical solution to these equations. The usual approach would be to apply the Laplace transform method and then carry-out numerical inversion to determine the transient response to specific input types. The drawbacks of this approach and other approaches such as use of finite difference techniques have earlier been highlighted. The approach that is adopted here is to discretize the modeling equations in the spatial variable using the orthogonal collocation method (Finlayson, 1972, 1980; Villadsen and Michelsen, 1978; Young, 2019), and then to solve the resulting system of ODEs using the state transition solution. The orthogonal collocation method belongs to the general class of method of weighted residuals (Finlayson, 1972).

The orthogonal collocation method is an attractive technique for obtaining approximate solution of differential equations by fitting a trial solution at selected points. The method attempts to minimize the residuals that result when the trial solution is substituted into the differential equations modeling the system, and the residuals are set to zero at selected points (known as the collocation points) in the spatial direction of interest. By choosing the collocation points to be zeros of some orthogonal polynomials, the accuracy of the solution is greatly improved (Villadsen and Michelsen, 1978).

To lump the set of PDEs to ODEs using orthogonal collocation method, we assume the following trial solutions:

$$x_1(z,t) = \sum_{k=0}^{n+1} \ell \qquad) \tag{22}$$

$$x_2(z,t) = \sum_{k=0}^{n+1} \ell \qquad) \tag{23}$$

$$x_3(z,t) = \sum_{k=0}^{n+1} \ell \qquad) \tag{24}$$

in which ℓ $\ldots$ are Lagrange polynomials (Villadsen and Michelsen, 1978).

Substituting the trial solutions in Eqs. (4) to (6), setting the residuals to zeros at the collocation points, and including the boundary conditions, we have:

$$\frac{dx_{1_j}(t)}{dt} = -\sum_{k=1}^{n+1} A_{jk} x_{1_k}(t) - A_{j,0} x_{1f} - a_1(x_{1_j} - x_{2_j}) - a_1(x_{1_j} - x_{3_j}), \quad j = 1,2,\ldots \tag{25}$$

$$r\frac{dx_{2_j}(t)}{dt} = -\sum_{k=1}^{n+1} A_{jk} x_{2_k}(t) - A_{j,0} x_{2f} + a_2(x_{1_j} - x_{2_j}), \quad j = 1,2,\ldots \tag{26}$$

$$r\frac{dx_{3_j}(t)}{dt} = \sum_{k=0}^{n} A_{jk} x_{3_k}(t) + A_{j,n+1} x_{2,n+1} + a_2(x_{1_j} - x_{3_j}), \quad j = 0,1,\ldots \tag{27}$$

in which we have used the boundary conditions:

$$x_{1_0} = x_{1f}, \; x_{2_0} = x_{2f} \text{ and } x_{3_{n+1}} = x_{2_{n+1}}$$

In eqs. (25) - (27), A_{jk} is the first collocation matrix given by:

$$A_{jk} = \frac{d\ell}{dz}\Big|_{z=z_j} \tag{28}$$

and the collocation points $z_j, j = 0,1,\ldots$ are the roots of the orthogonal Jacobi Polynomial (Villadsen and Michelsen, 1978):

$$\int_0^1 z^{\beta}(1-z)^{\alpha} z^j P_n^{(\alpha,\beta)}(z)dz = 0, \quad \alpha,\beta > -1, \; j = 0,1,\ldots \tag{29}$$

The resulting set of ODEs can be easily rearranged into the standard, linear state-space form:

$$\dot{} \qquad \mathrm{b}_1 u \tag{30}$$

$$\mathbf{y} = \mathbf{cx} \tag{31}$$

where the matrices A_1, B_1, and the state and input vectors are given by the following:

$$\mathbf{A}_1 = \begin{bmatrix} -(2a_1\mathbf{I} + \mathbf{A}) & a_1\mathbf{T}_1 & a_1\mathbf{T}_2 \\ (a_2/r)\mathbf{I} & -(a_1\mathbf{I} + \mathbf{A})/r & \mathbf{0} \\ (a_2/r)\mathbf{T}_3 & (\mathbf{T}_4)/r & (\end{bmatrix} \in \Re^{(3n+3)\times(3n+3)} \tag{32}$$

$$\mathbf{B}_1 = \begin{bmatrix} -A_{1,0} & -A_{2,0} \cdots & \cdots & \cdots \\ 0 & 0 \cdots & \cdots & \cdots \end{bmatrix} \quad {}^{+1)\times 2} \tag{33}$$

$$\mathbf{x} = \begin{bmatrix} x_{1_1} & x_{1_2} \cdots & \cdots & \cdots \end{bmatrix}^T$$

$$\mathbf{u} = \begin{bmatrix} x_{1f} & x_{2f} \end{bmatrix}$$

$$\mathbf{A} = \left[a_{ij} \right], \ i, j = 1, 2, \ldots$$

$$\tilde{} \quad \left[\quad \right] \quad i, j = 0, 1, \ldots$$

are given by the first collocation matrix, while matrices $\mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3, \mathbf{T}_4$ are given by the following:

$$\mathbf{T}_1 = \begin{bmatrix} \mathbf{I}_1 & 0 \\ 0 & 2 \end{bmatrix} \in \Re^{(n+1)\times(n+1)} \tag{34}$$

$$\mathbf{T}_2 = \begin{bmatrix} 0 & \mathbf{I}_1 \\ 0 & 0 \end{bmatrix} \in \Re^{(n+1)\times(n+1)} \tag{35}$$

$$\mathbf{T}_3 = \begin{bmatrix} 0 & 0 \\ \mathbf{I}_1 & 0 \end{bmatrix} \in \Re^{(n+1)\times(n+1)} \tag{36}$$

$$\mathbf{T}_4 = \begin{bmatrix} 0 & 0 & \cdots & & 4_{0,n+1} \\ 0 & 0 & \cdots & & 4_{1,n+1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & & 4_{n,n+1} \end{bmatrix} \quad \Re^{(n+1)\times(n+1)} \tag{37}$$

in which $\mathbf{I} \in \Re^{(n+1)\times(n+1)}$, $\mathbf{I}_1 \in \Re^{n\times n}$ are identity matrices with indicated dimensions.

2.3.1 Orthogonal-based Steady-State and Transient Solution Methods

The steady-state behaviour of the linear system given by Eq. (30) can be obtained by setting the left hand side (the time derivative) to zero, and solving the set of linear algebraic equations using the Gaussian Elimination routine of Villadsen and Michelsen (1978) i.e.

$$\mathbf{A}_1\mathbf{x}_s + \mathbf{B}_1\mathbf{u}_s = 0 \tag{38}$$

If the matrix inverse A_1^{-1} exists, then one can solve for x_s as

$$\mathbf{x}_s = -\mathbf{A}_1^{-1}\mathbf{B}_1\mathbf{u}_s \tag{39}$$

where x_s gives the steady-state solutions at the collocation points.

The dynamic response behaviour of the linear system given by Eq. (30) can be obtained by carrying out discrete-time simulation using the state-transition method. This is known to be computationally more efficient than carrying out numerical integration (Martens, 1969; Moler and Van Loan, 1978).

The process is summarized as follows: the continuous-time system given by Eq. (30) is converted to the discrete-time equivalent given by:

$$\mathbf{x}(k+1) = \mathbf{F}\mathbf{x}(k) + \mathbf{G}\mathbf{u}(k) \tag{40}$$

$$\mathbf{y}(k+1) = \mathbf{C}\mathbf{x}(k+1) \tag{41}$$

where $\mathbf{F}$ and $\mathbf{G}$ were computed using the basic Taylor series expansion method (cf. Director and Rohrer, 1972):

$$\mathbf{F} = e^{\mathbf{A}_1\tau} = \sum_{k=0}^{\infty} \frac{1}{k!}(\mathbf{A}_1\tau)^k \tag{42}$$

$$\mathbf{G} = \int_0^{\tau} e^{\mathrm{A}_1 t}\, \mathbf{b}_1\, dt = \tau \left[\sum_{k=0}^{\infty} \frac{1}{(k+1)!} (\mathbf{A}_1 \tau)^k \right] \mathbf{b}_1 \tag{43}$$

Williams and Adeniyi (2001) describe reliable FORTRAN 77 routines developed to carry out the exponential matrix and its integral reliably and accurately.

3 RESULTS AND DISCUSSION

All the computations and simulations were carried using FORTRAN 77 due to the ready availability of the collocation routines and others in this programming language.

3.1 Steady-State Solutions

The steady-state collocation solution of the two-pass shell and tube heat exchanger was computed following the procedure described above.

In doing this however, one must specify the collocation parameters: α, β and number of collocation points (including the exit $z = 1$), $N = n + 1$. A FORTRAN 77 program was written to determine the best values of the collocation parameters which minimize the Euclidean norm between the collocation and the analytical solutions at the collocation points using the nominal heat exchanger parameters specified. The parameters α and β were varied between -0.5 to 5.0 in steps of 0.5, while N was varied between 2 and 7. The summary of results are given in Table 1.

Table 1: Effect of number of collocation points (N) and best values of α and β which minimize the Euclidian norm between the steady-state collocation and analytical solutions at the collocation points

RESULTS OF DETERMINATION OF BEST VALUES FOR THE
COLLOCATION PARAMETERS: ALPHA, BETA AND N FOR THE TWO-PASS
SHELL AND TUBE HEAT EXCHANGER

NOMINAL HEAT EXCHANGER PARAMETERS ARE

PA1= 4.000

PA2 = 1.000

R = 1.000

FOR XFS(1) = 1.0 XFS(2) = 0.0

N	ALFA1M	BETA1M	E1MIN	ALFA2M	BETA2M	E2MIN	ALFA3M	BETA3M	E3MIN
2	-0.5	5.0	0.4862E-03	-0.5	5.0	0.1408E-03	2.5	3.5	0.1009E-01
3	-0.5	5.0	0.6202E-03	-0.5	5.0	0.1169E-03	0.0	0.5	0.7923E-03
4	-0.5	5.0	0.8843E-03	0.0	0.0	0.5712E-04	0.0	0.5	0.7848E-04
5	0.5	0.0	0.2463E-03	0.0	0.0	0.7725E-05	0.0	0.5	0.7728E-05
6	0.5	0.0	0.2523E-04	0.0	0.0	0.7522E-06	0.0	0.5	0.6330E-06
7	0.5	0.0	0.1849E-05	0.5	0.0	0.5485E-07	0.0	0.5	0.4426E-07

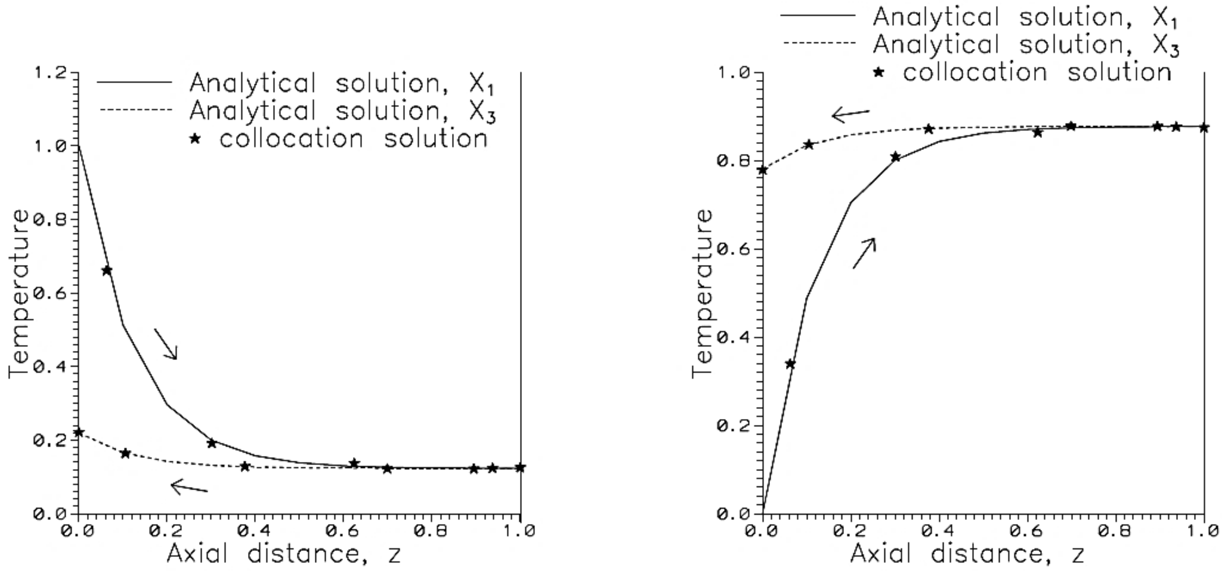
FOR XFS(1) = 0.0 XFS(2) = 1.0

N	ALFA1M	BETA1M	E1MIN	ALFA2M	BETA2M	E2MIN	ALFA3M	BETA3M	E3MIN
2	-0.5	5.0	0.4862E-03	-0.5	5.0	0.1408E-03	2.5	3.5	0.1009E-01
3	-0.5	5.0	0.6202E-03	-0.5	5.0	0.1169E-03	0.0	0.5	0.7923E-03
4	-0.5	5.0	0.8843E-03	0.0	0.0	0.5712E-04	0.0	0.5	0.7848E-04
5	0.5	0.0	0.2463E-03	0.0	0.0	0.7725E-05	0.0	0.5	0.7728E-05
6	0.5	0.0	0.2523E-04	0.0	0.0	0.7522E-06	0.0	0.5	0.6330E-06
7	0.5	0.0	0.1849E-05	0.5	0.0	0.5485E-07	0.0	0.5	0.4426E-07

where ALFA1M, BETA1M; ALFA2M, BETA2M; and ALFA3M, BETA3M are the α and β that give the minimum Euclidian norms: E1MIN, E2MIN, and E3MIN at each N for streams 1, 2, and 3, respectively.

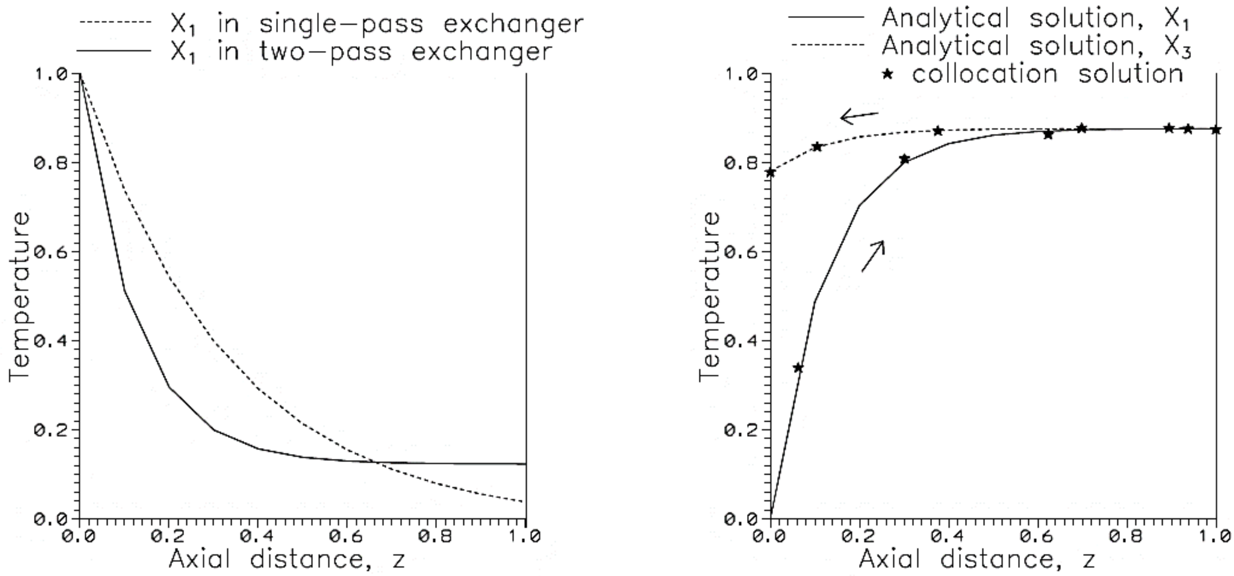
It is seen from the results in this table that, as expected, the accuracy of the collocation solution improves as the number of collocation points, N is increased. However, it is seen that the best values of α and β vary somewhat with N and the fluid streams. We observe that for stream 1, the best values of (α, β) = (-0.5,5.0) for $N \leq 4$, but (α, β) = (0.5,0.0) for $5 \leq N \leq 7$. On the other hand, for stream 3, the best values of (α, β) = (2.5,3.5) for $N = 2$, but (α, β) = (0.0,0.5) for $3 \leq N \leq 7$; whereas in the case of stream 2, the best values of (α, β) = (-0.5,5.0) for $N = 2,3$ while (α, β) = (0.0,0.0) for $N = 4,5,6$, and (α, β) = (0.5, 0.0) for $N = 7$.
No explanations can be adduced for the observed variations in the values of N, α, β which result in the minimization of the defined Euclidean norm for the different streams. However, it suffices to note that Cho and Joseph (1983) have pointed out that the optimal choice of N, α, β is dependent on the particular problem. Since no general systematic guideline is available for the choice of the orthogonal collocation parameters, they are best determined through exploratory simulation experiments such as presented here.

It is clear from the plots in Figure 2 and the results in Table 1 that using 5 collocation points gives steady-state collocation solutions with very good accuracy.



(a) $\bar{x}_{1f} = 1.0, \bar{x}_{2f} = 0.0$; (b) $\bar{x}_{1f} = 0.0, \bar{x}_{2f} = 1.0$;

Figure 2: Comparison of steady-state 5-point collocation and analytical solutions for two-pass heat exchanger system.



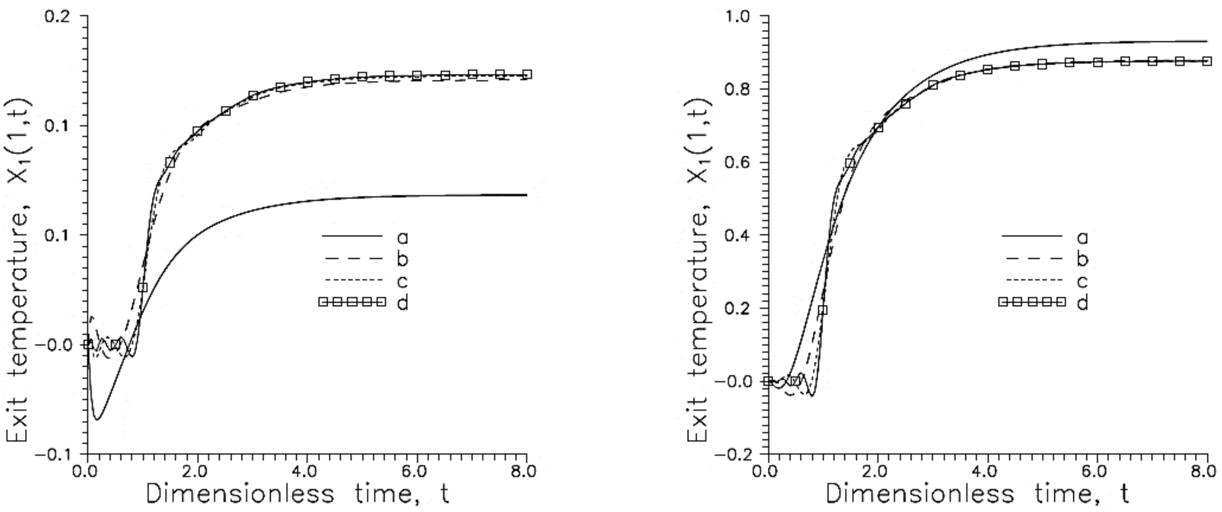
(a) $\bar{x}_{1f} = 1.0, \bar{x}_{2f} = 0.0$; (b) $\bar{x}_{1f} = 0.0, \bar{x}_{2f} = 1.0$;

Figure 3: Comparison of steady-state analytical solutions of x_1 for single- and two-pass shell and tube heat exchanger systems.

Figure 3 shows the comparison of the analytical steady-state temperature profiles of $x_1(z)$ in the single- and two-pass heat exchangers for the same nominal values $a_1 = 4$, $a_2 = 1$, and $r = 1$. It can be seen from this figure that the profile of $x_1(z)$ in the two-pass exchanger changes more rapidly with z than in the single-pass exchanger. The practical implication of this, as expected, is that to effect a given temperature change in x_1 (either for heating or cooling), requires one to use a single-pass exchanger that is longer than the two-pass exchanger. However, this advantage of the two-pass exchanger disappears for about $z > 0.65$. From Figure 3, we also notice that the single-pass exchanger leads to a steady-state exit temperature for x_1 which is lower or greater than that for the two-pass exchanger for cooling or heating of x_1, respectively.

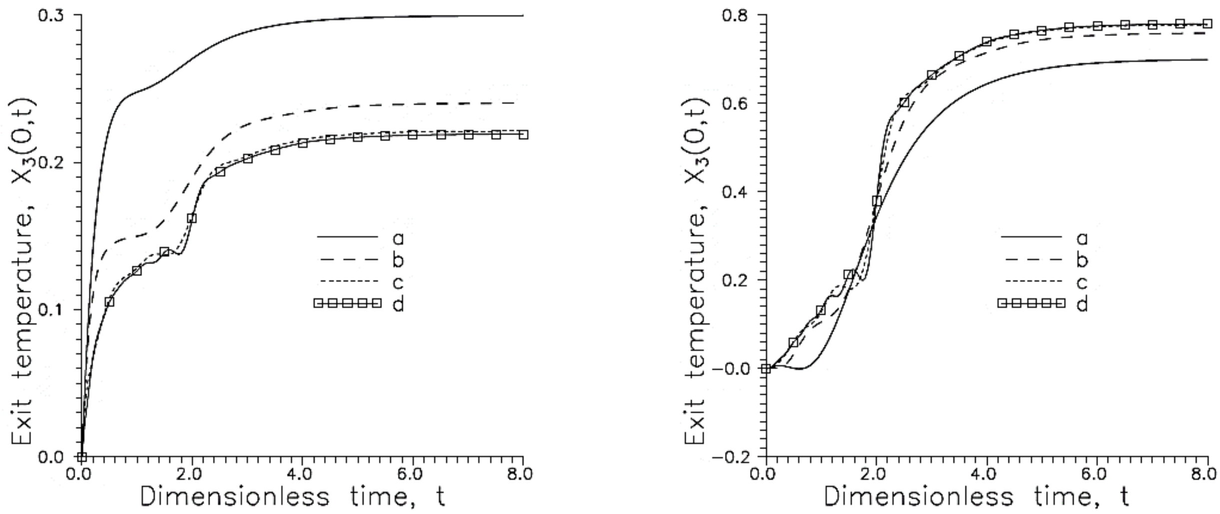
3.2 Orthogonal-Based Transient Response Simulations

For the same nominal heat exchanger parameters specified above, Figure 4 shows the simulated transient response of $x_1(1,t)$ to a unit step change in the disturbance inputs x_{1f} and x_{2f}, while Figure 5 shows the simulated transient response of $x_3(0,t)$ (i.e. exit temperature of stream 3) to the same inputs. The simulated responses were obtained from the lumped models of the two-pass exchanger using orthogonal collocation with 2, 3, 5, and 8 collocation points, and (α, β) = (0.0,0.5).



(a) For unit step change in x_{1f} (b) For unit step change in x_{2f}

Figure 4: Response of the exit temperature of stream 1, $x_1(1,t)$ for two-pass heat exchanger system. Legend: a, b, c and d for 2, 3, 5 and 8 collocation points, respectively.



(a) For unit step change in x_{1f} (b) For unit step change in x_{2f}

Figure 5: Step response of the exit temperature of stream 3, $x_3(0,t)$ for two-pass heat exchanger system. Legend: a, b, c and d for 2, 3, 5 and 8 collocation points, respectively..

These figures show that in general, using 5 collocation points lead to transient response simulation results that compare very well with those obtained using 8 collocation points; this, for all practical purposes, being taken as the converged solution. However, it is to be noted that using just 3 collocation points still gives results that compare well with the converged solution. Furthermore, we observe that the simulation results for the two-pass exchanger in Figure 4 display some small oscillations during the initial period of the transient. These are manifestations of the attempt by the global orthogonal polynomials to approximate the inherent time delay when sharp changes are made at the inlet of systems described by hyperbolic-type partial differential equations.For these cases, the order of the orthogonal collocation lumped model may become high because a large number of collocation points must be chosen so that enough are placed within the region of sharp gradients or abrupt changes to provide an accurate representation of the solution. An alternative is to use the finite difference procedure in which accurate representation of the solution is then possible simply by increasing the number of grid points. However, as well known, this technique can become computationally prohibitive due to the high dimensionality of the resulting system. Note that contrary to the small oscillations in the initial dynamic response observed in Figure 4, much better dynamic response profiles are shown in Figure 5. These plots show that the orthogonal collocation method does not suffer any challenges in computing the dynamic response of $x(0,t)$ to the specified step changes in x_{1f} and x_{2f}.

Remarks

A compromise between the high dimensionality of the finite difference technique and the inability of the orthogonal collocation technique to accurately define profiles with sharp gradients or abrupt changes led to the development of the technique called orthogonal collocation on finite elements (Carey and Finlayson, 1975; Finlayson, 1980) or what Villadsen and Michelsen (1978) called global spline collocation. In this technique, one uses trial functions that are defined over only part of the region and then piece together adjacent functions to provide an approximation over the entire domain. Using this technique, smaller regions can be used near the location of steep gradients or abrupt changes. The orthogonal collocation on finite element technique may be able to provide a better representation of the dynamic solution of the heat exchanger system during the initial transient period. However, a decision would need to be made about accepting the result of the global orthogonal collocation with much lower order against a solution using orthogonal collocation on finite element which will be of much higher order. Since a key objective of this work is the development of low-order steady-state and dynamic models that can be used for quick simulations and/or control system analysis/design, the orthogonal collocation on finite element approach is not investigated in this study.

4 CONCLUSION

This paper has presented the application of the orthogonal collocation method to the steady-state and transient response simulation of a two-pass shell and tube heat exchanger. Very good results were obtained with five (5) collocation points against a converged solution requiring eight (8) collocation points. The results are consistent with studies for other types of heat exchangers reported in the literature. Since the literature shows that as many as twenty (20) to fifty (50) grid points may be required using the finite difference method, the orthogonal collocation approach is attractive in the efficient simulation of single or interconnected heat exchanger systems such as heat exchanger networks or heat exchanger-reactor systems. Since a fifteenth (15)-order lumped parameter system results, this may not be suitable for direct use in control system design without an additional step of model order reduction to bring the order of the system to a more manageable size. This shall be the focus of future work.

Nomenclature

A_1	= Cross-sectional area for flow for stream 1.
A_2	= Cross-sectional area for flow for stream 2.
a_1	= Dimensionless parameter for flow for stream 1.
a_2	= Dimensionless parameter for flow for stream 2
$r = v_1 / v_2$	= Dimensionless ratio of the velocities of fluid stream 1 and fluid

	stream 2.
C_{p1}	= Specific heat capacity of stream 1 fluid (Shell side).
C_{p2}	= Specific heat capacity of stream 2 fluid (Tube side).
L	= Length of heat exchanger in the axial direction.
S_1	= Stream 1 (shell side) heat transfer area per unit length of heat exchanger.
S_2	= Stream 2 (tube side) heat transfer area per unit length of heat exchanger.
t'	= Time, in consistent dimensional unit
t	= Time, dimensionless
$T_1(z',t')$	= Fluid temperature of stream 1 in exchanger.
$\bar{T}_1(z')$	= Initial steady-state fluid temperature of stream 1 in exchanger.
$T_2(z',t')$	= Fluid temperature of stream 2 in exchanger.
$\bar{T}_2(z')$	= Initial steady-state fluid temperature of stream 2 in exchanger.
$T_3(z',t')$	= Fluid temperature of stream 3 in exchanger.
$\bar{T}_3(z')$	= Initial steady-state fluid temperature of stream 3 in exchanger.
U_1	= Shell side (Stream 1) heat transfer coefficient.
U_2	= Tube side (Stream 2) heat transfer coefficient.
v_1	= Shell side (Stream 1) fluid velocity in the exchanger.
v_2	= Tube side (Stream 2) fluid velocity in the exchanger.
ρ_1	= Shell side (Stream 1) fluid density.
ρ_2	= Tube side (Stream 2) fluid density.

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APPENDIX A DERIVATION OF STEADY-STATE ANALYTICAL SOLUTION

Setting the left hand sides of Eqs. (3) to (5) to zero leads to the following ODEs:

$$\frac{d\bar{x}_1}{dz} = -a_1(\bar{x}_1 - \bar{x}_2) - a_1(\bar{x}_1 - \bar{x}_3) \tag{A.1}$$

$$\frac{d\bar{x}_2}{dz} = a_2(\bar{x}_1 - \bar{x}_2) \tag{A.2}$$

$$\frac{d\bar{x}_3}{dz} = a_2(\bar{x}_1 - \bar{x}_3) \tag{A.3}$$

subject to the boundary conditions given by Eq. (8) i.e.

$$\bar{x}_1(0) = \bar{x}_{1f}$$
$$\bar{x}_2(0) = \bar{x}_{2f}$$
$$\bar{x}_3(1) = \bar{x}_2(1)$$

in which $\bar{x}_1, \bar{x}_2, \bar{x}_3$ are the steady-state temperature profiles corresponding to the steady-state inlet temperatures $\bar{x}_{1f}$ and $\bar{x}_{2f}$. This set of ODEs can be converted to a single, third-order ODE which may then be readily solved as shown in what follows.

Differentiating Eq. (A.1) w.r.t. z and rearranging, we obtain

$$\frac{d^2\bar{x}_1}{dz^2} = -2a_1\frac{d\bar{x}_1}{dz} + a_1\left(\frac{d\bar{x}_2}{dz} + \frac{d\bar{x}_3}{dz}\right) \tag{A.4}$$

Adding Eqs. (A.2) and (A.3) and substituting the result into Eq. (A.4), we have

$$\frac{d^2\bar{x}_1}{dz^2} = -2a_1\frac{d\bar{x}_1}{dz} + a_1a_2(\bar{x}_3 - \bar{x}_2) \tag{A.5}$$

Differentiating Eq. (A.5) w.r.t. z, we obtain

$$\frac{d^3\bar{x}_1}{dz^3} = -2a_1\frac{d^2\bar{x}_1}{dz^2} + a_1a_2\left(\frac{d\bar{x}_3}{dz} - \frac{d\bar{x}_2}{dz}\right) \tag{A.6}$$

Subtracting Eq. (A.2) from Eq. (A.3), substituting the result into Eq. (A.6), and rearranging, we have

$$\frac{d^3\bar{x}_1}{dz^3} = -2a_1\frac{d^2\bar{x}_1}{dz^2} - 2a_1a_2^2\bar{x}_1 + a_1a_2^2(\bar{x}_3 + \bar{x}_2) \quad (A.7)$$

From Eq. (A.1), however, we have that

$$a_1(\bar{x}_3 + \bar{x}_2) = \frac{d\bar{x}_1}{dz} + 2a_1\bar{x}_1 \quad (A.8)$$

Using Eq. (A.8) to substitute for $a_1(\bar{x}_2 + \bar{x}_3)$ in Eq. (A.7) and simplifying, leads to the third-order ODE in $\bar{x}_1$ alone

$$\frac{d^3\bar{x}_1}{dz^3} + 2a_1\frac{d^2\bar{x}_1}{dz^2} - a_2^2\frac{d\bar{x}_1}{dz} = 0 \quad (A.9)$$

From standard techniques, the general solution of Eq. (A.9) is

$$\bar{x}_1(z) = c_1 + c_2e^{\phi_1 z} + c_3e^{\phi_2 z} \quad (A.10)$$

where

$$\phi_1 = -a_1 + \sqrt{a_1^2 + a_2^2},\ \phi_2 = -a_1 - \sqrt{a_1^2 + a_2^2}$$

and c_1, c_2 and c_3 are constants to be determined.

Having obtained $\bar{x}_1$, the expessions for the analytical solutions of $\bar{x}_2$ and $\bar{x}_3$ may be obtained from the following considerations.

From Eqs. (A.5) and (A.8), we have

$$-\bar{x}_2 + \bar{x}_3 = \frac{1}{a_1a_2}\left[\frac{d^2\bar{x}_1}{dz^2} + 2a_1\frac{d\bar{x}_1}{dz}\right]$$

$$-\bar{x}_2 + \bar{x}_3 = \frac{1}{a_1}\left[2a_1\bar{x}_1 + 2a_1\frac{d\bar{x}_1}{dz}\right]$$

respectively. Solving for $\bar{x}_2$ and $\bar{x}_3$ from these two equations, we have

$$\bar{x}_2 = \frac{1}{2a_1}\left[2a_1\bar{x}_1 + \frac{\bar{x}_1}{dz}\right] - \frac{1}{2a_1a_2}\left[\frac{d^2\bar{x}_1}{dz^2} + 2a_1\frac{d\bar{x}_1}{dz}\right] \quad (A.11)$$

$$\bar{x}_3 = \frac{1}{2a_1}\left[2a_1\bar{x}_1 + \frac{\bar{x}_1}{dz}\right] + \frac{1}{2a_1a_2}\left[\frac{d^2\bar{x}_1}{dz^2} + 2a_1\frac{d\bar{x}_1}{dz}\right] \quad (A.12)$$

Subsituting Eq. (A.10) into Eqs. (A.11) and (A.12) and simplifying, leads, respectively to the following analytical solutions for $\bar{x}_2$ and $\bar{x}_3$:

$$\bar{x}_2 = c_1 + c_2e^{\phi_1 z} + c_3e^{\phi_2 z} + \left(\frac{1}{2a_1} - \frac{1}{a_2}\right)\left(c_2\phi_1e^{\phi_1 z} + c_3\phi_2e^{\phi_2 z}\right)$$
$$-\frac{1}{2a_1a_2}\left(c_2\phi_1^2e^{\phi_1 z} + c_3\phi_2^2e^{\phi_2 z}\right) \quad (A.13)$$

$$\bar{x}_3 = c_1 + c_2e^{\phi_1 z} + c_3e^{\phi_2 z} + \left(\frac{1}{2a_1} + \frac{1}{a_2}\right)\left(c_2\phi_1e^{\phi_1 z} + c_3\phi_2e^{\phi_2 z}\right)$$
$$+\frac{1}{2a_1a_2}\left(c_2\phi_1^2e^{\phi_1 z} + c_3\phi_2^2e^{\phi_2 z}\right) \quad (A.14)$$

Applying the 3 boundary conditions given earlier and simplifying leads to the following 3 simultaneous linear equations which may be readily solved for c_1, c_2, and c_3:

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & q_1 & q_2 \\ 0 & q_3 & q_4 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} \bar{x}_{1f} \\ \bar{x}_{2f} \\ 0 \end{bmatrix} \tag{A.15}$$

in which

$$q_1 = 1 + \left(\frac{1}{2a_1} - \frac{1}{a_2} \right) \phi_1 - \frac{\phi_1^2}{2a_1 a_2}$$

$$q_2 = 1 + \left(\frac{1}{2a_1} - \frac{1}{a_2} \right) \phi_2 - \frac{\phi_2^2}{2a_1 a_2}$$

$$q_3 = \frac{2}{a_1} \phi_1 e^{\phi_1} + \frac{1}{a_1 a_2} \phi_1^2 e^{\phi_1}$$

$$q_4 = \frac{2}{a_2} \phi_2 e^{\phi_2} + \frac{1}{a_1 a_2} \phi_2^2 e^{\phi_2}$$

Solving for c_1, c_2, and c_3 using Cramer's rule, we obtain

$$c_1 = \frac{\bar{x}_{1f}(q_1 q_4 - q_2 q_3) - \bar{x}_{2f}(q_4 - q_3)}{(q_1 q_4 - q_2 q_3) - (q_4 - q_3)} \tag{A.16}$$

$$c_2 = \frac{q_4(\bar{x}_{2f} - \bar{x}_{1f})}{(q_1 q_4 - q_2 q_3) - (q_4 - q_3)} \tag{A.17}$$

and

$$c_3 = \frac{q_3(\bar{x}_{1f} - \bar{x}_{2f})}{(q_1 q_4 - q_2 q_3) - (q_4 - q_3)} \tag{A.18}$$