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Application of Invariant Imbedding to the Estimation of Process Duration*

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This work deals with the application of invariant imbedding to solve a particularly important design problem, namely, the duration of the process. A numerical example is used to illustrate the approach. The advantage of this approach is its straightforward nature and uses only the usual design data. It avoids any iterations and thus no convergence problems need to be considered.

1. INTRODUCTION

An important problem in process industry is the design of equipment. An example is to estimate the size of equipment to produce a desired product given the raw material. This forms a typical boundary value problem with the given raw material and the desired product as boundary conditions. Some sample design problems of the above type are to determine the following: length of a distillation column, length of a tubular reactor, time for the movement of a particle from one position to another, time for the concentration of a drug to reach a certain level in some part of our body, and the time required for a chemical reaction process.

Chandrasekhar [3], Bellman and co-workers [4, 5, 11], Lee [6], Casti and Kalaba [7], Mingle [8], Scott [9], and Shimizu and Aoki [10] have made

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major contributions to the solution of boundary value problems by the invariance principles introduced by Amberzumian [1, 2].

Meyer [12] applied the method of lines to linear one-dimensional parabolic free boundary problems. The author [13] extended the method of lines to multi-dimensional parabolic free surface problems. Meyer [14] also used the method of lines to solve Poisson's equation with nonlinear or free boundary conditions and combined the method of lines and invariant imbedding for elliptic and parabolic free boundary problems [15].

This paper involves the application of invariant imbedding and the method of characteristics to solve free boundary value problems.

2. INVARIANT IMBEDDING AND THE METHOD OF CHARACTERISTICS

Consider a system whose behavior can be represented by the following nonlinear second-order differential equation:

$$\frac{d^2x}{dt^2} = P_1 \frac{dx}{dt} + P_2 x^2 \quad (1)$$

with input data

$$x(0) = C_1 \quad (2)$$

$$x'(0) = C_2$$

$$x(T) = C_3. \quad (3)$$

The problem is to find the length of the above process, T , as a function of the given boundary conditions.

Equations (1)–(3) are transformed into the following first-order differential equations:

$$\frac{dx}{dt} = y = f_1 \quad (4)$$

$$\frac{dy}{dt} = P_1 \cdot y + P_2 \cdot x^2 \quad (5)$$

with input data

$$x(0) = C_1$$

$$y(0) = C_2 \quad (6)$$

$$x(T) = C_3.$$

By using the standard procedure [6], we obtain the following imbedding equation for T as a function of C_1 and C_2 :

$$T(C_1, C_2) = \Delta + T(C_1 + \Delta \cdot f_1, C_2 + \Delta \cdot f_2) \quad (7)$$

where $T(C_1, C_2)$ = length of the process represented by Eqs. (4)–(6) starting at time a and with $x(a) = C_1$ and $y(a) = C_2$.

Expanding Eq. (7) by Taylor series, we have

$$T(C_1, C_2) = \Delta + T(C_1, C_2) + \frac{T}{C_1} \cdot \Delta \cdot f_1 + \frac{T}{C_2} \cdot \Delta \cdot f_2 + 0(\Delta). \quad (8)$$

In the limit as Δ tends to zero, Eq. (8) becomes

$$\frac{\partial T}{\partial C_1} \cdot f_1 + \frac{\partial T}{\partial C_2} \cdot f_2 = -1. \quad (9)$$

There are various computational techniques available for solving Eq. (9). The two frequently used techniques are the various versions of finite-difference methods and the method of characteristics [16–21]. In this work, the method of characteristics is used. The characteristic equation of Eq. (9) is [21]

$$\frac{dC_1}{f_1} = \frac{dC_2}{f_2} = -\frac{dT}{1}. \quad (10)$$

From the first two terms of Eq. (10), we have

$$\frac{dC_2}{dC_1} = \frac{f_2}{f_1}. \quad (11)$$

Solving Eq. (11) either analytically or numerically, we can obtain

$$C_2 = f(C_1). \quad (12)$$

From the second and third terms of Eq. (10), we have

$$\frac{dC_1}{f_1} = -\frac{dT}{1}. \quad (13)$$

Integrating Eq. (13), we obtain

$$T(C_1, C_4) = -\int_0^{C_1} \frac{dC_1}{f_1} + \psi. \quad (14)$$

From the definition of $T(C_1, C_2)$, we see that

$$T(x(T), y(T)) = 0.$$

Thus, Eq. (14) becomes

$$-\int_0^{x(T)} \frac{dC_1}{f_1} + \psi = 0. \quad (15)$$

From Eq. (3) and Eq. (15), we obtain

$$\psi = \int_0^{C_3} \frac{dC_1}{f_1}. \quad (16)$$

Substituting Eq. (16) in Eq. (14), we have

$$T(C_1, C_2) = + \int_{C_1}^{C_3} \frac{dC_1}{f_1}. \quad (17)$$

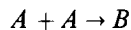
The computational procedure is summarized below:

(i) With the given values of $x(0)$, $x'(0)$, and Eqs. (11) and (12), obtain the C_2 values at various C_1 values.

(ii) Using C_1 , C_2 , and C_3 in Eq. (17), calculate the value of T .

3. CHEMICAL REACTOR MODEL

Consider the chemical reaction [6]



which is taking place in a homogeneous tubular flow chemical reactor with axial mixing. Assuming that the change of volume in the reactor is negligible, the following equation can be established easily by the use of material balance on reactant A [6]:

$$\frac{1}{N_{pe}} \cdot \frac{d^2x}{dt^2} - \frac{dx}{dt} - R \cdot x^2 = 0$$

or

$$\frac{d^2x}{dt^2} = N_{pe} \cdot \frac{dx}{dt} + N_{pe} \cdot R \cdot x^2 \quad (18)$$

with input data

$$\begin{aligned} x(0) &= C_1 \\ x'(0) &= C_2 \\ x(T) &= C_3 \end{aligned} \quad (19)$$

where

N_{pe} = the dimensionless Peclet group Lv/D

R = the reaction rate group kL/v

x = concentration of reactant A

t = dimensionless reactor length, $0 < t < 1$

L = total reactor length

v = flow velocity of the reaction mixture (constant)

D = mean mass axial dispersion coefficient (constant)

k = specific chemical reaction rate (constant).

The notations and assumptions of this model are the same as those in Ref. [6]. The problem is to determine the length of the chemical reaction process, T , by using invariant imbedding and the method of characteristics.

Equations (18) and (19) can be rewritten as

$$\frac{dx}{dt} = y \quad (20)$$

$$\frac{dy}{dt} = N_{pe} \cdot y + N_{pe} \cdot R \cdot x^2 \quad (21)$$

with input data

$$\begin{aligned} x(0) &= C_1 \\ y(0) &= C_2 \\ x(T) &= C_3. \end{aligned} \quad (22)$$

Using Eq. (9) for the above system, we obtain the invariant imbedding equation for $T(C_1, C_2)$ as

$$\frac{\partial T}{\partial C_1} \cdot C_2 + \frac{\partial T}{\partial C_2} \cdot (N_{pe} \cdot C_2 + N_{pe} \cdot R \cdot C_1^2) = -1. \quad (23)$$

As per Eq. (10), the characteristic equation for Eq. (23) becomes

$$\frac{dC_1}{C_2} = \frac{dC_2}{N_{pe} \cdot C_2 + N_{pe} \cdot R \cdot C_1^2} = -\frac{dT}{1}. \quad (24)$$

Applying Eqs. (11), (12), and (13) to Eq. (24), we obtain

$$\frac{dC_2}{dC_1} = \frac{N_{pe} C_2 + N_{pe} R C_1^2}{C_2} \quad (25)$$

$$C_2(C_1 = x(0)) = y(0) \quad (26)$$

and

$$\frac{dC_1}{C_2} = -\frac{dT}{1} \quad (27)$$

respectively.

Thus, according to Eq. (17), we have

$$T(C_1, C_2) = \int_{C_1}^{C_3} \frac{dC_1}{C_2}.$$

The numerical values used in the calculation are

$$x(0) = C_1 = 0.83129$$

$$y(0) = x'(0) = C_2 = -1.0122$$

$$x(T) = C_3 = 0.38727$$

$$N_{pe} = 6$$

$$R = 2.$$

This problem is solved using the above computational procedure. The results are listed in Table I. At $c_3 = 0.38727$, the value of T should be 1.0. Considering the various computational errors, the value of 1.026 obtained is very close to the correct one.

It should be emphasized that the main advantage of this approach is its straightforward nature. No iterations are involved and thus no convergence problems need to be considered. This forms a big advantage when modern computers are used.

TABLE I
Length of Chemical Reaction Process, T

C_1	C_2	t
$x(0) = 0.83129$	$x'(0) = -1.0122$	0
0.786888	-0.916744	0.046114
0.742486	-0.825192	0.097187
0.698084	-0.737563	0.154127
0.653682	-0.653815	0.218097
0.609280	-0.573752	0.290623
0.564878	-0.496781	0.373812
0.520476	-0.421124	0.470852
0.476074	-0.345160	0.580353
0.431672	-0.226559	0.743211
$x(T) = 0.38727 = C_3$	-0.006369	1.026337 = T

In actual applications, the number of conditions given is frequently greater than the number of unknowns to be determined. In this overspecified situation, the method of least-squares can be used. The other computational procedures remain essentially the same.

REFERENCES

1. V. A. AMBARZUMIAN, Diffuse reflection of light by a foggy medium, *C. R. Acad. Sci. U.R.S.S.* **38** (1943), 229–232.
2. V. A. AMBARTSUMIAN (AMBARZUMIAN), "Theoretical Astrophysics," Pergamon, Elmsford, N. Y., 1958.
3. S. CHANDRASEKHAR, "Radiative Transfer," Dover, New York, 1960.
4. R. E. BELLMAN, R. E. KALABA, AND M. PRESTRUD, "Invariant Imbedding and Radiative Transfer in Slabs of Finite Thickness," Amer. Elsevier, New York, 1963.
5. R. E. BELLMAN, R. E. KALABA, AND M. PRESTRUD, "Invariant Imbedding and Time Dependent Transport Processes," Amer. Elsevier, New York, 1964.
6. E. S. LEE, "Quasilinearization and Invariant Imbedding," Academic Press, New York, 1968.
7. J. CASTI, AND R. KALABA, "Imbedding Methods in Applied Mathematics," Addison-Wesley, Reading, Mass., 1973.
8. J. O. MINGLE, "The Invariant Imbedding Theory of Nuclear Transport," Amer. Elsevier, New York, 1973.
9. M. R. SCOTT, "Invariant Imbedding and Its Application to Ordinary Differential Equations—An Introduction," Addison-Wesley, Reading, Mass., 1973.
10. R. SHIMIZU AND R. AOKI, "Application of Invariant Imbedding to Reactor Physics," Academic Press, New York, 1973.
11. R. E. BELLMAN AND G. M. WING, "Introduction to Invariant Imbedding," Wiley, New York, 1975.
12. G. H. MEYER, One-dimensional parabolic free boundary problems, *SIAM Rev.* **19** (1977), 17–34.
13. G. H. MEYER, An alternating direction method for multidimensional parabolic free surface problems, *Internat. J. Numer. Methods Engrg.* **11** (4) (1977), 741–752.
14. G. H. MEYER, The method of lines for Poisson's equation with nonlinear or free boundary conditions, *Numer. Math.* **29** (3) (1978), 329–344.
15. G. H. MEYER, The method of lines and invariant imbedding for elliptic and parabolic free boundary problems, *SIAM J. Numer. Anal.* **18** (1) (1981), 150–164.
16. R. COURANT AND K. O. FRIEDRICHS, "Supersonic Flow and Shock Waves," Wiley-Interscience, New York, 1948.
17. G. E. FORSYTHE AND W. R. WASOW, "Finite-Difference Methods for Partial Differential Equations," Wiley, New York, 1960.
18. R. ARIS, "The Optimal Design of Chemical Reactors," Academic Press, New York, 1961.
19. R. COURANT AND D. HILBERT, "Methods of Mathematical Physics," Vol. II, Wiley-Interscience, New York, 1962.
20. W. F. AMES, "Nonlinear Partial Differential Equation in Engineering," Academic Press, New York, 1965.
21. M. B. ABBOTT, "An Introduction to the Method of Characteristics," Amer. Elsevier, New York, 1966.