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AN IMPLICIT SEMIANALYTIC NUMERICAL METHOD FOR THE SOLUTION OF NONEQUILIBRIUM CHEMISTRY PROBLEMS

By

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R. E. Boughner

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July 1974

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
LANGLEY RESEARCH CENTER, HAMPTON, VIRGINIA 23665

1. Report No.
NASA TM X-71985

2. Government Accession No.

3. Recipient's Catalog No.

4. Title and Subtitle
An Implicit Semianalytical Numerical Method for the Solution of Nonequilibrium Chemistry Problems

5. Report Date
July 1974

6. Performing Organization Code

7. Author(s)
R. A. Graves, Jr., P. A. Gnoffo, R. E. Boughner

8. Performing Organization Report No.

9. Performing Organization Name and Address
Langley Research Center
Hampton, VA 23665

10. Work Unit No.

11. Contract or Grant No.

12. Sponsoring Agency Name and Address
NASA Langley

13. Type of Report and Period Covered
Technical Memorandum

14. Sponsoring Agency Code

15. Supplementary Notes
Previously published as Langley Working Paper LWP-1151, Feb. 1, 1974

16. Abstract

Most nonequilibrium chemistry problems, and many other physical phenomena, are modeled by systems of first order nonlinear ordinary or partial differential equations which for many applications are defined as stiff. These stiff systems are generally difficult to solve using classical techniques because of the rapid error growth and unless a very small time step is used the results can be greatly in error. However, because of the first order differential equation form these systems of equations can be solved by a simple and relatively accurate implicit semianalytic technique which is derived from a quadrature solution of the governing equation. This method is mathematically simpler than most implicit methods and has the exponential nature of the problem embedded in the solution. From the sample problems solved using this technique the method is shown to be both computationally fast and relatively accurate.

17. Key Words (Suggested by Author(s)) (STAR category underlined)
Mathematics
Chemistry
Numerical Analysis

18. Distribution Statement
Unclassified-unlimited

19. Security Classif. (of this report)
Unclassified

20. Security Classif. (of this page)
Unclassified

21. No. of Pages

22. Price*

*Available from {The National Technical Information Service, Springfield, Virginia 22151
STIF/NASA Scientific and Technical Information Facility, P.O. Box 33, College Park, MD 20740

AN IMPLICIT SEMIANALYTIC NUMERICAL METHOD FOR THE SOLUTION OF NONEQUILIBRIUM CHEMISTRY PROBLEMS

By R. A. Graves, Jr., P. A. Gnoffo, and R. E. Boughner

INTRODUCTION

Many physical phenomena are modeled by systems of linear and/or nonlinear ordinary differential equations (see for example references 1 to 5) which are defined as stiff systems when a large spread in negative eigenvalues exists. Such stiff systems commonly arise in nonequilibrium chemistry problems involving kinetic and photochemical reactions. The governing equations for these stiff systems are difficult to solve numerically using classical techniques because the error growth is rapid, and unless the equations are integrated using a very small time step, the results can be meaningless. To alleviate the problems involved with stiff systems, a great deal of effort has been expended in developing numerical solution techniques, both explicit and implicit, for stiff ordinary differential equations. References 6 to 9 review some of the more popular numerical methods and present the results of numerical comparisons between the methods. A generalized conclusion resulting from the studies of references 6 to 8 is that the implicit methods are more desirable because of their increased stability and, in some instances, significantly fewer mathematical operations. In these and other studies, a rather simple (yet fundamental) implicit technique was not investigated because these studies used a generalized equation which did not take advantage of the form of the governing conservation equation for chemical species. The governing conservation equations for systems of chemical reactions can generally be written in the form of first-order ordinary differential equations. These equations can be solved by a simple implicit semianalytic technique which is derived from a quadrature solution of the governing equations. This method is mathematically simpler than most implicit methods and has the exponential nature of the problem embedded in the solution.

The objective of this paper is to present the development of the semianalytic technique (SAT) and to compare its efficiency to that of several of the more popular methods available.

SYMBOLS

a,b	general coefficients, see equation (1)
C_1,C_2	curve fit coefficients, see equation (5)
$\bar{C}_1,\bar{C}_2$	curve fit coefficients, see equation (6)
HS	Hermite-Simpson
R_n	$[Y_n - Y(X_n)]/Y(X_n)$
h	step size
RK4	fourth-order Runge-Kutta
DEQ	Adams' fourth-order P-C
TM	Treanor's method
DIFSYS	modified midpoint rule
TR	Trapezoidal rule
TR-EX	Trapezoidal rule with extrapolation
CAL	Calahan's method
LW1	Liniger-Willoughby - Method 1

LW3	Liniger-Willoughby - Method 3
SAT	semianalytic technique
λ	eigenvalue
Y_n	calculated value
$Y(X_n)$	"exact value"
ξ	transformed coordinate, see equation 3a

MATHEMATICAL DEVELOPMENT

The governing equation for the conservation of chemical species in nonequilibrium chemically reacting systems can generally be written in the form of a first-order ordinary differential equation (see ref. 10):

$$\frac{dY_i}{dt} + a(t)Y_i = b(t) \qquad (1)$$

where a(t) and b(t) generally represent the loss and production rates of species i, respectively. The solution of equation 1 in terms of quadratures is: (This procedure is similar to that used in ref. 11.)

$$Y_i^{J+1} = Y_i^J e^{-\int_{t^J}^{t^{J+1}} a(t)dt} + \int_{t^J}^{t^{J+1}} b(t) e^{-\int_{t}^{t^{J+1}} a(t')dt'} dt \qquad (2)$$

This equation can be further simplified by introducing the transformation

$$\xi = \int_{t}^{t^{J+1}} a(t')dt'$$

$$d\xi = -a(t)dt$$

hence, equation 2 becomes:

$$Y_i^{J+1} = Y_i^J e^{-\xi_1} + \int_0^{\xi_1} \frac{b(\xi)}{a(\xi)} e^{-\xi} d\xi \tag{3}$$

where

$$\xi_1 = \int_{t^J}^{t^{J+1}} a(t)dt \tag{4}$$

For the least complicated case, the coefficients $a(t)$ and $b(\xi)/a(\xi)$ can be approximated by linear functions.

$$a(t) = C_1 + C_2 (t - t^J) \tag{5}$$

where

$$C_1 = a(t^J)$$

$$C_2 = \frac{a(t^{J+1}) - a(t^J)}{\Delta t}$$

$$\frac{b(\xi)}{a(\xi)} = \overline{C}_1 + \overline{C}_2\xi \tag{6}$$

where

$$\overline{C}_1 = \frac{b(0)}{a(0)}$$

$$\overline{C}_2 = \frac{\frac{b(\xi_1)}{a(\xi_1)} - \frac{b(0)}{a(0)}}{\Delta\xi}$$

It should be noted that due to the transformation from t to ξ that

$$\frac{b(0)}{a(0)} = \frac{b(t^{J+1})}{a(t^{J+1})} \quad \text{and} \quad \frac{b(\xi_1)}{a(\xi_1)} = \frac{b(t^J)}{a(t^J)}$$

Introducing equation 6 into equation 3 results in:

$$Y_i^{J+1} = Y_i^J e^{-\xi_1} + \int_0^{\xi_1} (\overline{C}_1 + \overline{C}_2\xi)e^{-\xi}d\xi \tag{7}$$

This equation can now be integrated by parts to obtain the following semianalytic implicit result:

$$Y_i^{J+1} = Y_i^J e^{-\xi_1} + (\overline{C}_1 + \overline{C}_2)(1 - e^{-\xi_1}) - \overline{C}_2 \xi_1 e^{-\xi_1} \qquad (8)$$

(Note: To have stability and accuracy, it is necessary that $\left| e^{-\xi_1} \right| < 1.$) Equation 8 is semianalytic in nature and includes the inherent exponential behavior of the stiff problem directly in the solution. Equation 8 must be solved implicitly (iteratively) as the constants ξ_1, $\overline{C}_1$, and $\overline{C}_2$ depend on the conditions at the advanced time t^{J+1}.

An error analysis was performed, using the method of chapter 2 of reference 12, to determine the errors incurred in making the linear approximations for the coefficients $a(t)$ and $b(\xi)/a(\xi)$. The lowest order error terms are:

$$E = -\frac{1}{12} \left\{ \Delta\xi^3 \gamma''(\omega) + \Delta t^3 \beta''(\eta)(\overline{C}_1 + Y_i^J) \right\}$$

where $\gamma''(\omega)$ is the second derivative of the ratio $b(\xi)/a(\xi)$ on the interval $0 \leq \omega \leq \xi_1$ and $\beta''(\eta)$ is the second derivative of $a(t)$ on the interval $t^J \leq \eta \leq t^{J+1}$.

Numerical Experiments:

System I (ref. 8)

$$Y_1' = -0.04Y_1 + 10^4 Y_2 Y_3$$

$$Y_2' = 0.04Y_1 - 10^4 Y_2 Y_3 - 3 \times 10^7 Y_2^2$$

$$Y_3' = 3 \times 10^7 Y_2^2$$

$$Y_1(0) = 1 \qquad Y_2(0) = 0 \qquad Y_3(0) = 0$$

This system is nonlinear, and no exact solution for this system exists. The eigenvalues, determined from the Jacobian matrix of the system at $X = 0$

are $\lambda_1 = 0$, $\lambda_2 = 0$ and $\lambda_3 = -0.04$. $|\lambda_{max}|$ changes from 0.04 to 2405 for $0 \leq X \leq 0.02$. The eigenvalues for $0 < X < 40$ are all strictly negative or zero, with $\lambda_1 = 0$, $\lambda_2 \simeq -10^{-1}$ and $\lambda_3 \simeq -10^3$ to -10^4. The sharp increase in the magnitude of λ, makes this a particularly difficult stiff system to work with. In addition this system presents some starting problems for SAT since $a_2(0) = 0$ and hence $b_2(\xi_1)/a_2(\xi_1)$ is meaningless. To circumvent this problem for Y_2, two techniques using constant h were tried: first, the Hermite-Simpson method, reference 13, and secondly, the Runge-Kutta fourth-order method. The RK4 start gave the best results. Table I gives the results for this system on the CDC 6600 as well as the results of Lapidus and Seinfeld, reference 8, for the IBM 7094. (The CDC 6600 is approximately 10 times faster than the IBM 7094.) It should be noted that due to the nature of this system $Y_3(X)$ was calculated by $Y_3(X) = 1 - Y_2(X) - Y_1(X)$.

The most successful application of the SAT was to use the RK4 one step to obtain $Y_1(0.0005)$, $Y_2(0.0005)$, and $Y_3(0.0005)$ and then use the SAT with a step size of 0.2 to compute the solution from $5 \times 10^{-4} \leq X \leq 40$. As can be seen in figures 1 and 2 the linear approximation for $b(\xi)/a(\xi)$ is very accurate for this system.

System II (ref. 8)

$$Y' = -200\,(Y - F(X)) + F'(X)$$

$$Y(0) = 10$$

$$F(X) = 10 - (10 + X)e^{-X}$$

$$\text{Exact Solution} \quad Y(X) = F(X) + 10e^{-200X}$$

Here, $F(X)$ is a slowly decaying solution component and $10e^{-200X}$ decays rapidly. The large negative eigenvalue of -200 makes $\exp(-200X)$ negligible compared to $\exp(-X)$ in the $F(X)$ component. Results using SAT on the CDC 6600 are compared to results obtained by Lapidus and Seinfeld in Table 2.

At equivalent step sizes, SAT produced R_n less than or equal to the error encountered using other methods, and worked faster than any other method (times for this system are based on computing over a range $0 \leq X \leq 15$)

System III (ref. 8)

$$Y_1' = -0.1Y_1 - 49.9Y_2$$

$$Y_2' = -50Y_2$$

$$Y_3' = 70Y_2 - 120Y_3$$

$$Y_1(0) = 2 \qquad Y_2(0) = 1 \qquad Y_3(0) = 2$$

Exact Solution:

$$Y_1(X) = e^{-0.1X} + e^{-50X}$$

$$Y_2(X) = e^{-50X}$$

$$Y_3(X) = e^{-50X} + e^{-120X}$$

Eigenvalues $\lambda_1 = -120,\ \lambda_2 = -50,\ \lambda_3 = -0.1$

Because the solution components due to λ_1 and λ_2 decay rapidly, a stiff method which was not restricted by the magnitude of these values is desired. The SAT (which yields the exact solution of $Y_2(X)$ for any h since the linear approximation to $a(X)$ and $b/a(\xi)$ gives the true variation of these functions) is compared to results obtained by Lapidus and Seinfeld in Table 3. An $h = 0.01$ produced results which were better than the results obtained by any other method. However as the step size increased, the accuracy dropped off rapidly and at an $h = 0.2$, the solution was very different from the exact solution (except, of course, for $Y_2(X)$ which remained exact).

After examining the problem, it was found that on an interval of $0 \leq \lambda \leq 0.2$, with $h = 0.2$, the linear approximation to $b/a(\xi)$ was very poor. For example, $b/a(X) = -400e^{-50X}$ and $b_3/a_3(X) = (70/120)e^{-50X}$ (see fig. 3). The effect of these terms on $b/a(\xi)$ decays rapidly after $X = 0.2$, and they can be approximated by a linear function, so a method was tried using $h = 0.01$ to arrive at $X = 0.2$ and then proceed from $X = 0.2$ with $h = 0.2$. This method was the fastest and yielded reasonable results.

System IV

$$Y_1' = 0.8Y_2 - 0.01Y_1^2 - 10^7Y_1Y_2Y_3 + 10Y_1Y_3 - 100Y_1Y_2$$

$$Y_2' = -0.8Y_2 - 10Y_1Y_3 + 10^6Y_2Y_4 + 10^4Y_1Y_4$$

$$Y_3' = 0.01Y_1^2 + 10^7Y_1Y_2Y_3 + 2000Y_4^2 - 10^4Y_1Y_4$$

$$Y_4' = -10^6Y_2Y_4 + 100Y_1Y_2 - 20000Y_4^2$$

$$Y_1(0) = 0.9; \quad Y_2(0) = 0.05; \quad Y_3(0) = 0.05; \quad Y_4(0) = 0$$

No exact solution for this nonlinear system was obtained. The eigenvalues for this system, calculated from the Jacobian using values of Y from RK4, are widely separated in magnitudes. All of the eigenvalues are negative or ≈ 0 on a range $6.146 \times 10^{-6} < X < 7.36 \times 10^{-6}$. Typical values on the range are at $X = 7 \times 10^{-6}$, $\lambda_1 = -1.017 \times 10^5$, $\lambda_2 = -4.979 \times 10^4$, $\lambda_3 = -2.7102 \times 10^1$ and $\lambda_4 = -2.515 \times 10^{-9}$. Results for this system appear in Table 4. This system was only stiff for a short time and none of the methods had problems with stability on a range $0 \leq X \leq 2 \times 10^{-5}$. Using RK4 with $h = 1 \times 10^{-8}$ as a standard of comparison, the tables indicate that for any given step size, RK4 was more accurate than any implicit method. SAT gave accuracy comparable to other implicit methods and ran at approximately the same speeds as these methods for equivalent step sizes. In this system, SAT showed no advantage over any other method. However, this system does indicate that SAT gives reasonable results for nonstiff nonlinear systems.

CONCLUDING REMARKS

As developed herein the crucial approximation is the linearization of the coefficients within the integral in the quadrature form which allows the semianalytic form to be obtained. In some cases this approximation is very good but in some applications, the linear approximation can be in error for what appear to be not unreasonable time steps. As demonstrated, this problem was overcome by having a variable time step which is small in the region where the Linear Approximation is in error.

Additionally, quadratic and exponential curve fits were tried. However these approximations produced results which were approximately equivalent to those obtained with the linear approximation. Because the linear approximation was the simplest to program and because of the consistently good results it yielded, it was chosen as the most desirable approximation evaluated.

An important feature of the semianalytic technique is that it will allow the computation of nonequilibrium chemical systems to and including the equilibrium state. For systems where the rates are large (typical of approaching equilibrium) the SAT equilibrium condition is the exact solution for equilibrium.

As demonstrated in the example problems, the semianalytic technique is both rapid and accurate and should be applicable to those stiff problems which can be modeled by an equation like that used in this development.

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TABLE I.- COMPARISON OF RESULTS FOR SYSTEM I

Method	h	R_{1_N}		R_{2N}		R_{3_N}		Time, sec	
		X = 0.4	X = 10	X = 0.4	X = 10	X = 0.4	X = 10	IBM 7094	CDC 6600
RK4	0.001	0	0	0	0	0	0	-	-
DEQ	0.001	-	-	-	-	-	-	-	-
TM	0.01	-	-	-	-	-	-	-	-
DIFSYS	0.001	-	-	-	-	-	-	-	-
TR	0.2	$1.35x10^{-3}$	$1.05x10^{-3}$	$2.12x10^{-1}$	$2.4x10^{-1}$	$9x10^{-2}$	$1.5x10^{-2}$	9.3	-
TR-EX	0.2	$1.72x10^{-5}$	$3.6x10^{-4}$	$3.5x10^{-2}$	$4.3x10^{-4}$	$6.8x10^{-4}$	$1.2x10^{-3}$	34	-
CAL	0.005/0.02	$2.4x10^{-3}$	$1.01x10^{-1}$	$2.5x10^{0}$	$6.0x10^{-1}$	$1.62x10^{-1}$	$5.4x10^{-1}$	10	-
LW1	0.2	$1.6x10^{-4}$	$4.9x10^{-4}$	$2.4x10^{-4}$	$1.3x10^{-4}$	$3.2x10^{-3}$	$4.4x10^{-4}$	20	-
LW3	0.2	$5.9x10^{-4}$	$7.1x10^{-5}$	$2.9x10^{-3}$	$1.1x10^{-3}$	$4x10^{-2}$	$1.9x10^{-3}$	23.3	
RK4	0.0005	0	0	0	0	0	0	-	20.7
HS	0.001	$2.5x10^{-5}$	$6.88x10^{-3}$	$1.26x10^{-4}$	$2.86x10^{-2}$	$1.66x10^{-3}$	$3.65x10^{-2}$	-	168
SAT (HS Start)	0.001	$4.07x10^{-5}$	$2.54x10^{-4}$	$1.25x10^{-3}$	$1.97x10^{-4}$	$1.87x10^{-2}$	$6.52x10^{-4}$	-	37
SAT (HS Start)	0.001/0.1	$3.79x10^{-5}$	$2.42x10^{-4}$	$1.25x10^{-3}$	$1.95x10^{-4}$	$1.88x10^{-2}$	$6.33x10^{-4}$	-	4
SAT (RK4 Start)	0.0005/0.2	$2.26x10^{-6}$	$1.31x10^{-5}$	$1.62x10^{-7}$	$1.74x10^{-5}$	$1.97x10^{-5}$	$4.44x10^{-5}$	-	1.43
SAT (RK4 Start)	0.0005 to X = 0.1 then 0.3	$1.97x10^{-5}$	$3.96x10^{-5}$	$9.04x10^{-5}$	$1.62x10^{-4}$	$1.31x10^{-3}$	$2.1x10^{-4}$	-	.9

TABLE 2.- COMPARISON OF RESULTS FOR SYSTEM II

Method	h	X = 0.4	X = 10	IBM 7094 Time, sec	CDC 6600 Time, sec
RK4	0.01	1.0×10^{-5}	2.0×10^{-9}	11	-
DEQ	0.005	3.0×10^{-9}	2.0×10^{-9}	18	-
TM	0.2	6.7×10^{-8}	1.0×10^{-9}	16.5	-
DIFSYS	0.1	(a)	(a)	(a)	-
TR	0.2	1.85×10^{-2}	4.3×10^{-5}	2	-
TR-EX	0.2	1.4×10^{-4}	1.0×10^{-8}	36	-
CAL	0.01/0.2	1.7×10^{-2}	4.0×10^{-8}	1	-
LW1	0.2	1.1×10^{-3}	5.0×10^{-8}	3	-
LW3	0.2	1.8×10^{-3}	9.0×10^{-8}	4	-
SAT	0.2	9.35×10^{-4}	4.1×10^{-8}	-	0.09

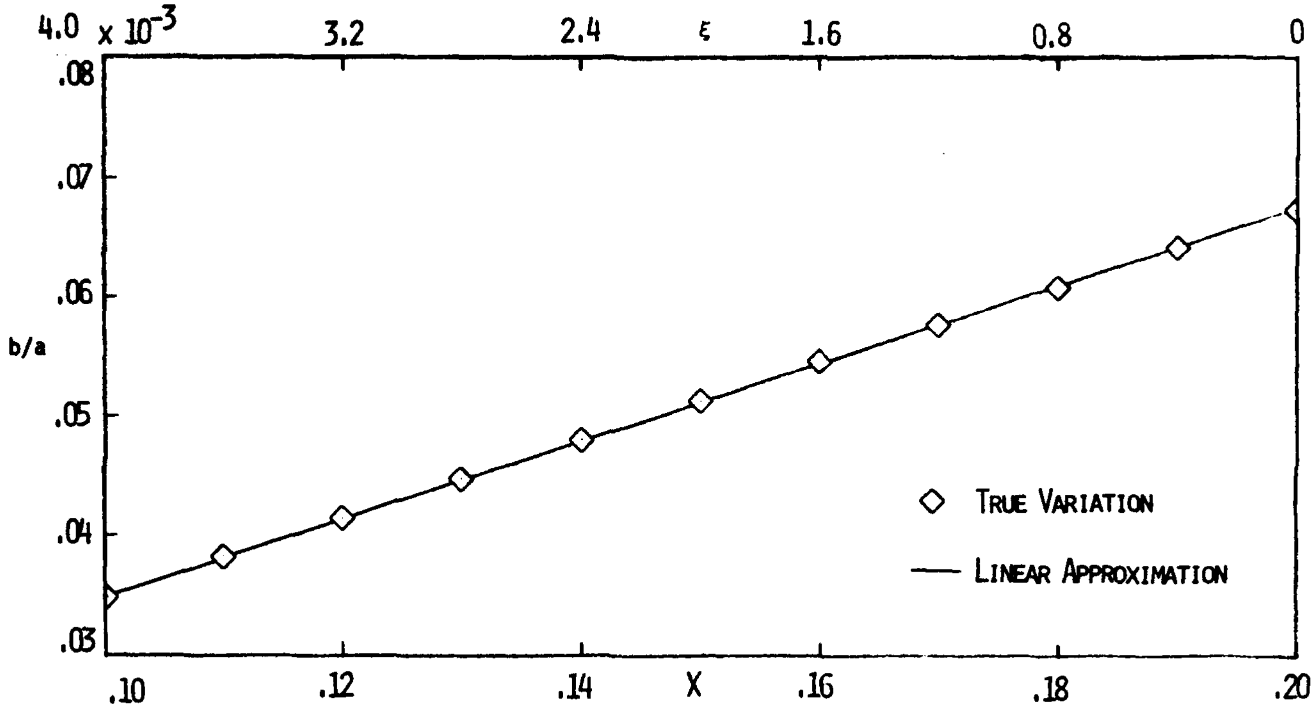
(a) Unstable

TABLE 3.- COMPARISON OF RESULTS FOR SYSTEM III

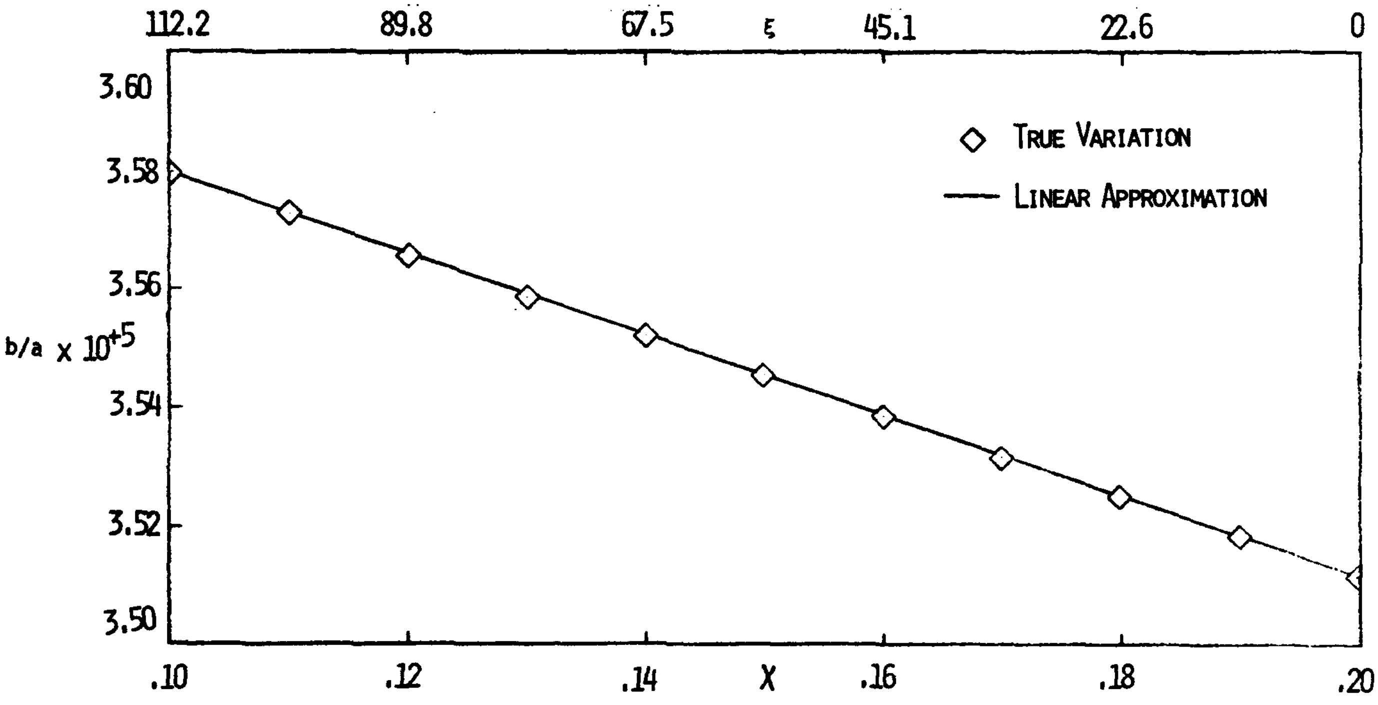
Method	h	R_{1_N}		R_{2_N}	R_{3_N}	Time, sec	Time, sec
		X = 0.4	X = 10	X = 0.4	X = 0.4	IBM 7094	CDC 6600
RK4	0.01	2.0×10^{-7}	5.4×10^{-7}	3.0×10^{-1}	3.0×10^{-1}	20	-
DEQ	0.01	2.0×10^{-4}	8.1×10^{-7}	9.5×10^{-1}	7.4×10^{5}	23	-
TM	0.2	4.0×10^{-4}	1.35×10^{-4}	1.1×10^{5}	1.2×10^{5}	1	-
DIFSYS	0.1	5.0×10^{-4}	2.16×10^{-4}	9.4×10^{-1}	8.3×10^{2}	22	-
TR	0.2	1.0×10^{-3}	2.7×10^{-4}	6.5×10^{7}	1.3×10^{5}	1.3	-
TR-EX	0.2	4.0×10^{-5}	8.1×10^{-4}	5.7×10^{1}	8.0×10^{1}	30	-
CAL	0.01/0.2	2.0×10^{-3}	2.7×10^{-6}	2.5×10^{5}	1.6×10^{5}	1	-
LW1	0.2	4.0×10^{-3}	1.1×10^{-2}	5.0×10^{5}	5.0×10^{5}	3	-
SAT 0.01 to X = 0.2 0.2 after X = 0.2		2.13×10^{-2}	2.08×10^{-2}	0	5.3×10^{2}	-	0.27

TABLE 4.- COMPARISON OF RESULTS FOR SYSTEM IV

Method	h	Time, sec	R_{1_N}		R_{2_N}		R_{3_N}		R_{4_N}	
		CDC 6600	$X=1x10^{-6}$	$X=2x10^{-5}$	$X=1x10^{-6}$	$X=1x10^{-6}$	$X=1x10^{-6}$	$X=2x10^{-5}$	$X=1x10^{-6}$	$X=2x10^{-5}$
RK4	10^{-8}	2.94	0	0	0	0	0	0	0	0
RK4	10^{-6}	0.0384	$9.17x10^{-6}$	$3.11x10^{-3}$	0	0	$9.24x10^{-3}$	$4.21x10^{-6}$	$1.38x10^{-5}$	$1.26x10^{-4}$
TRAP	$2x10^{-8}$	6.11	0	0	0	$8x10^{-6}$	$2.56x10^{-6}$	0	$2.31x10^{-6}$	0
TRAP	10^{-6}	0.177	$4.67x10^{-4}$	$7.1x10^{-2}$	0	$1.0x10^{-5}$	$5.24x10^{-3}$	$9.59x10^{-5}$	$9.73x10^{-4}$	$8.9x10^{-5}$
SAT	$5x10^{-8}$	4.3	$1.94x10^{-5}$	$5.47x10^{-3}$	$5.90x10^{-4}$	$5.82x10^{-4}$	$2.04x10^{-4}$	$9.48x10^{-6}$	$4.48x10^{-4}$	$5.71x10^{-4}$
SAT	10^{-6}	0.159	$4.65x10^{-4}$	$9.62x10^{-3}$	$1.6x10^{-5}$	$6.0x10^{-6}$	$5.75x10^{-4}$	$8.98x10^{-4}$	$1.30x10^{-3}$	$1.32x10^{-3}$

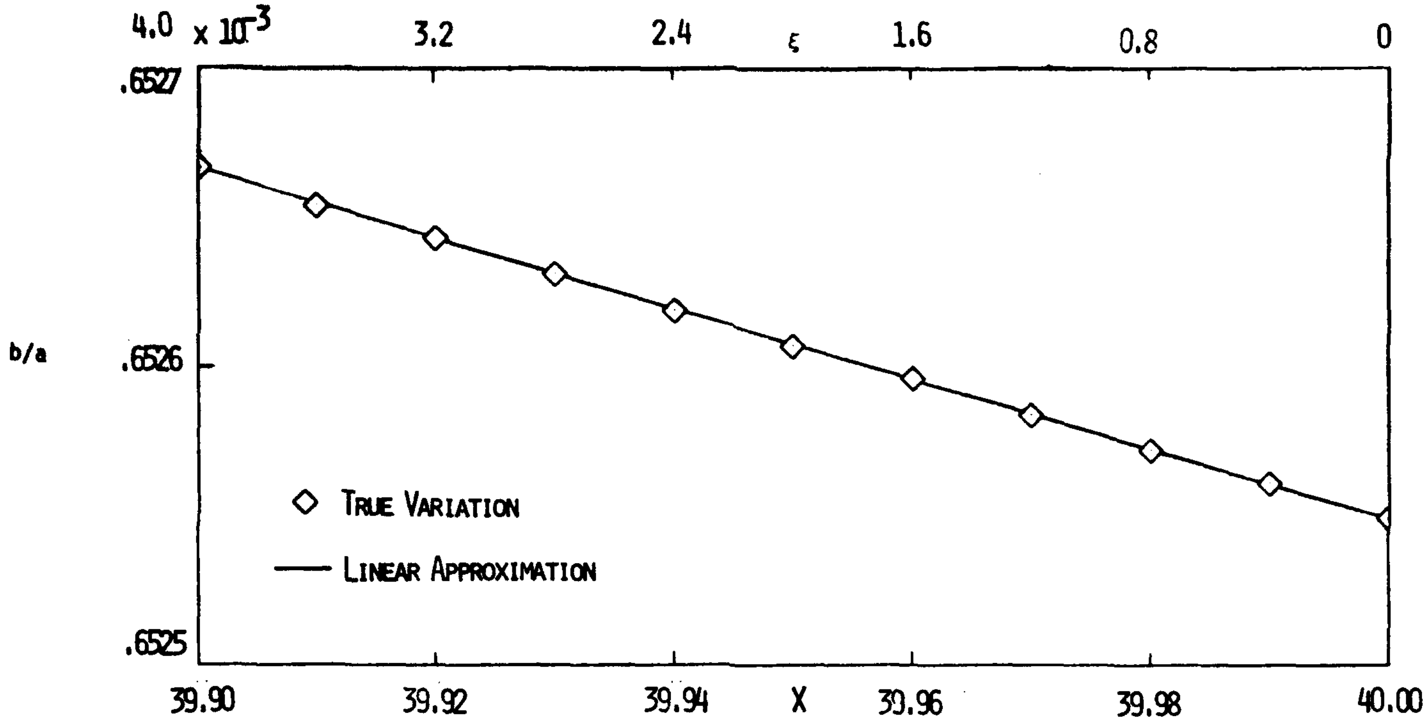


a) REACTION 1

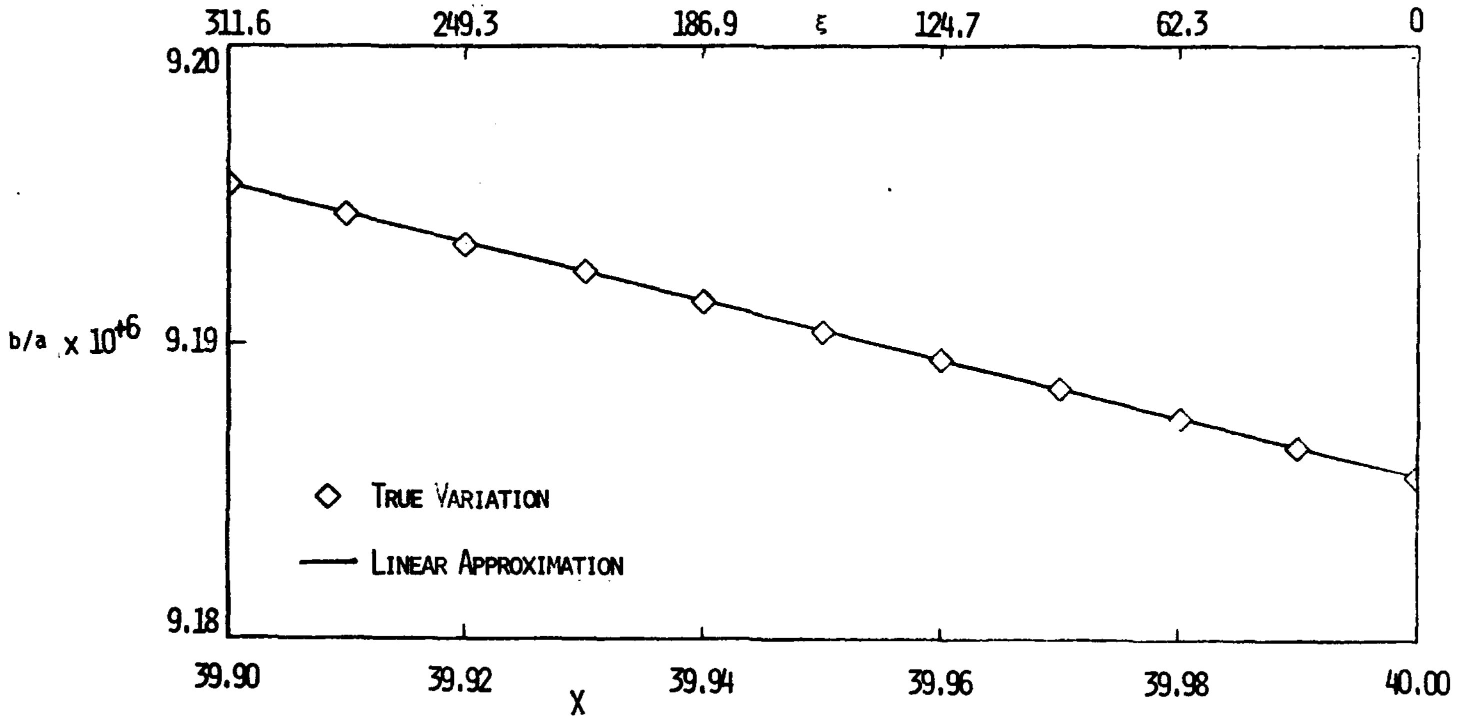


b) REACTION 2

FIGURE 1. VARIATION OF (a/b) FOR SYSTEM I IN THE INTERVAL $.1 \leq X \leq .2$.

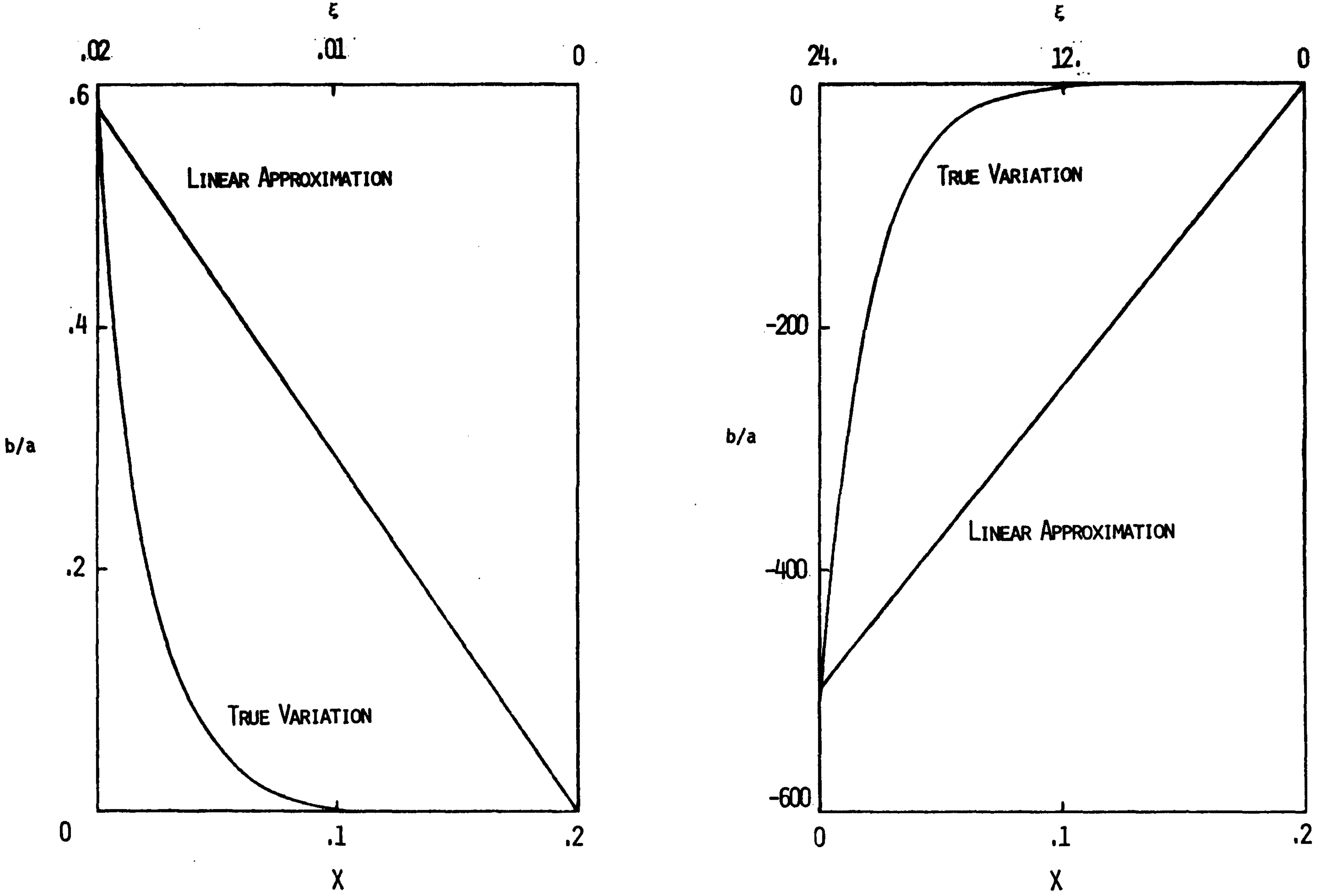


a) Reaction 1



b) Reaction 2

Figure 2. Variation of (b/a) for System I in the interval $39.9 \leq X \leq 40.0$.



a) Reaction 1

b) Reaction 3

Figure 3. Variation of (b/a) for System III.