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Contents

KINETIC ANALYSIS OF CONSECUTIVE-REACTION MODEL SYSTEMS

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ABSTRACT

Numerical solutions are needed to carry out kinetic calculations of multiple-reaction systems.

Two types of consecutive-reaction models are studied here: consecutive-competitive, and consecutive-reversible (with one reversible step). For the consecutive-competitive reaction model, we determine the effect of an excess of either of two reactants on (a) the time for the system to react to a given conversion, and on (b) the relative yields of intermediate and final products. An excess of either reactant is an important design factor, because it may minimize the required reactor volume and maximize the production rate of the desired product.

Several different kinds of consecutive-reversible cases are studied. These include cases where all the reaction steps are first-order and cases in which there is at least one second-order step. Except for isolated second-order cases, only the all-first-order cases can be solved analytically. The second-order cases are solved numerically using a fourth-order Runge-Kutta method. In cases which contain a second-order step, the proportions of intermediate and final products are dependent upon the initial reactant concentration regardless of which reaction step is second-order.

For plug-flow or batch reactors, we present the calculational results as graphs or tables of either conversion or dimensionless concentrations as a function of dimensionless time for each model considered. For continuous stirred-tank reactors, graphical results are given for the consecutive-competitive model and for certain consecutive-reversible systems. The graphs and tables are useful both for design and for interpretation of experimental data. The required calculations were done on the IBM 650 and 7090 Computers.

I. INTRODUCTION

Kinetic calculations on multiple-reaction systems are difficult to carry out, not only because of the large number of parameters involved but also because analytic solutions for these reaction models often do not exist; additionally, numerical solutions may not be available.

Two types of consecutive-reaction model systems are analyzed in this work; the consecutive-competitive type, and the consecutive-reversible type. The models are as follows:

Type 1. $A + B \rightarrow C$

$A + C \rightarrow D$

Type 2. $aA \rightleftharpoons bB$

$b'B \rightleftharpoons cC$

Type 1, the consecutive-competitive model, is studied to determine the effect of an excess of either reactant on the time required to reach a given conversion, and on the relative yields of intermediate C and final product D. An excess of either of the reactants is an important design factor that aids in minimizing the required reactor volume or maximizing the production of the desired product. In Type 2, which is the general consecutive-reversible model, the cases covered involve three of the four possible reactions, with all three reactions first-order or with combinations of one second-order and two first-order reactions. Numerical solutions are obtained for the second-order consecutive-reversible models and they are compared to the corresponding first-order cases. For the plug-flow reactors and the single-compartment continuous stirred-tank reactors, product yields and time to react to a given conversion are compared. Also, equations are presented that one can use to determine the concentrations of reactants and products in each tank of a series of continuous stirred-tank reactors. Constant volume and temperature, with ideal reactor behavior, are assumed for all the calculations. The results of the calculations are presented as graphs and tables of conversion, in terms of reduced concentrations, as functions of dimensionless time. These results are useful for both design problems and for determination of reaction-mechanism and rate coefficients from experimental data.

The consecutive-competitive reaction has been the subject of numerous studies, but mainly for the case of equivalent amounts of initial reactants. Also, past work has been oriented primarily toward determination of rate coefficients from experimental data. Frost and Schwemer[1] presented an algebraic solution for the yield structure in the case of equivalent amounts of reactants, along with graphs of conversion versus dimensionless time, and tables of time ratios. Burkhard[2] gave more complete tables of time ratios and dimensionless time as a function of conversion. Our work is focused mainly on the problem of design rather than on the determination of rate coefficients. Here, we determine the effect of an excess of either reactant on the time required to react to a given conversion, and on the product yields at a given time. Graphs of conversion versus dimensionless time are presented for three ratios of initial reactant concentrations, and graphs of yield structure are given over a full range.

For consecutive-reversible models, only the first-order cases can be solved analytically (except for isolated second-order cases). Lowry and John[3] present a general equation for these first-order cases where either or both steps are reversible. An approximation method for cases with a second-order reaction step was proposed by Hill;[4] this method seems inherently inaccurate and difficult to use. McDaniel and Smoot[5] developed an approximate solution for one of the first-order cases but have not extended it to the corresponding second-order case. Higgins[6] has demonstrated the use of both digital and analog computers for solving typical enzyme reactions, which are generally consecutive but non-competitive. The Michaelis-Menten mechanism[7] was solved for a limited range of rate-coefficient ratios and initial reactant proportions, using the analog computer. The Michaelis-Menten mechanism is as follows:

and

$$A + B \rightleftharpoons C \ ,$$
$$C \rightarrow D \ .$$

In our work, second-order cases are solved numerically on the IBM 7090 Computer using the Runge-Kutta method.[8] To estimate the truncation error for the solutions of the second-order cases, a first-order case is solved both numerically and analytically and the two results are compared. Also, a first-order and a second-order case are compared in terms of the dimensionless time to react to a given conversion and yield structure. Graphs of dimensionless time versus dimensionless concentrations are presented for three kinds of consecutive-reversible models, and tables are presented for five other models. In addition, graphs are given for determining the three rate coefficients in one of the second-order/first-order cases by a time-ratio method.

The analysis of the consecutive-competitive reaction model is given in Sec. II which covers the derivation of equations, method of calculation, and a discussion and interpretation of results. Section III presents the analysis of the consecutive-reversible models. The first two models considered are all-first-order cases; each of the next six cases include a second-order reaction step. Analytical solutions are given for the all-first-order cases. An outline of the derivation of the fourth-order Runge-Kutta equations, which are used to solve the second-order cases, is given in the Appendix. Examples are given which illustrate the use of the graphs for solving various types of problems.

II. CONSECUTIVE-COMPETITIVE REACTION MODEL

We now consider the following reaction:

$$A + B \xrightarrow{k_1} C,$$

and

$$A + C \xrightarrow{k_2} D\ .$$

This complex reaction is consecutive with respect to B and C, and parallel with respect to A. Reactant B and intermediate C compete for coreactant A; both reaction steps are second-order. A common example of this reaction model is the saponification of a symmetrical diester such as ethyl succinate. The reactant A represents the hydroxide ion, B represents the diester, and C the monoester. Another example is the hydrolysis of an acetal in which the hemiacetal is formed as an intermediate; in this case the first step is much slower than the second step and the reaction appears to be a simple second-order reaction.

This reaction model has been the subject of many previous studies which cover only the case where the initial concentration of A is twice that of B. These proportions are the equivalent amounts for complete reaction, in which all of A and B disappear to yield only D. In the present work, this model is examined to determine the effect of an excess of either reactant.

A. Plug-Flow or Batch Reactors

1. Equations

The rate equations are

$$dA/dt = -k_1AB - k_2AC, \qquad (1)$$

$$dB/dt = -k_1AB, \qquad (2)$$

$$dC/dt = k_1AB - k_2AC, \qquad (3)$$

and

$$dD/dt = k_2AC\ . \qquad (4)$$

By material balance we obtain

$$C = 2(B_o - B) - (A_o - A), \qquad (5)$$

and

$$D = B_o - B - C, \qquad (6)$$

where A, B, C, and D, are now the concentrations of the respective components; k_1 and k_2 are the rate coefficients; and subscript o designates initial reactant concentrations. The algebra is simplified by introducing dimensionless variables α, β, and τ, and parameters κ and ω, where $\alpha = A/A_o$, $\beta = B/B_o$, $\tau = B_o k_1 t$, $\kappa = k_2/k_1$, and $\omega = A_o/B_o$. Substituting Eq. (5) into Eq. (1) and expressing the resulting equation in terms of the dimensionless variables and parameters, we obtain

$$\frac{d\alpha}{d\tau} = - \alpha\beta - \kappa\alpha\ (2 - 2\beta + \omega\alpha - \omega)\ . \tag{7}$$

Equation (2) in dimensionless form is

$$\frac{d\beta}{d\tau} = - \omega\alpha\beta\ . \tag{8}$$

Dividing Eq. (7) by Eq. (8), τ is eliminated and we have

$$\frac{d\alpha}{d\beta} - \frac{\kappa}{\beta}\ (\alpha) = \frac{\beta + \kappa\ (2-2\beta-\omega)}{\omega\beta}\ . \tag{9}$$

Equation (9) integrates to

$$\alpha = \left[\frac{1}{\omega(1-\kappa)}\right]\beta^{\kappa} + \left[\frac{1-2\kappa}{\omega(1-\kappa)}\right]\beta + (1-\frac{2}{\omega})\ , \tag{10}$$

or

$$(1-\alpha)\omega = 2 - \left[\frac{1}{1-\kappa}\right]\ \beta^{\kappa} - \left[\frac{1-2\kappa}{1-\kappa}\right]\beta\ .$$

The material-balance equations in dimensionless form are

$$\frac{C}{(1-\beta)B_o} = 2 - \frac{(1-\alpha)\omega}{1-\beta}, \tag{11}$$

and

$$\frac{D}{(1-\beta)B_o} = \frac{(1-\alpha)\omega}{1-\beta} - 1\ . \tag{12}$$

For the special case of $\kappa = 1.0$, Eq. (9) integrates to give

$$\alpha = - \frac{\beta}{\omega}\ \ell n\beta + \frac{2\beta}{\omega} + 1 - \frac{2}{\omega}\ , \tag{13}$$

or

$$(1-\alpha)\omega = 2 + \beta\,\ell n\beta - 2\beta\ .$$

Thus Eqs. (10), (11), (12), and (13), give the yield structure for the plug-flow or batch reactor.

Equation (8) is used to determine the elapsed time of the reaction. Substituting for α in Eq. (8) from Eq. (10), we obtain

$$\frac{d\beta}{d\tau} = \left[\frac{1}{\kappa - 1}\right] \beta^{\kappa+1} + \left[\frac{1-2\kappa}{\kappa-1}\right] \beta^2 + (2-\omega)\beta \, . \tag{14}$$

Equation (14) can be integrated only when $\kappa = 0,\ 0.5,$ or ∞, provided also that $\omega = 2.0$. The following equations for τ and α are then obtained:

$$\kappa = 0, \quad \tau = \ln\left[\frac{\beta+1}{2\beta}\right], \quad \alpha = \frac{\beta+1}{2} \; ; \tag{15}$$

$$\kappa = 0.5, \quad \tau = \frac{1-\alpha}{\alpha}, \quad \alpha^2 = \beta \; ; \tag{16}$$

and

$$\kappa = \infty, \quad \tau = \frac{1-\beta}{2\beta}, \quad \alpha = \beta \, . \tag{17}$$

For other values of κ and ω, Eq. (14) must be integrated numerically. A program for the IBM 650 Computer was written to compute values of α for given values of β with Eq. (10) or (13), and to integrate numerically the equation

$$\tau = \frac{1}{\omega} \int_{\beta}^{1.0} \frac{d\beta}{(\alpha)(\beta)} = \frac{1}{\omega} \sum_{\beta}^{1.0} \frac{\Delta\beta}{(\bar{\alpha})(\bar{\beta})} \, , \tag{18}$$

where $\Delta\beta$ is the increment, $\bar{\beta}$ is the average value of β in the increment, and $\bar{\alpha}$ is the value of α calculated from $\bar{\beta}$.

2. Calculations

The integration was performed for 13 values of κ and three values of ω, with a β range of 1.0 to 0.001. A total of 139 β increments were used, in the following sequence:

β Range			β Increment
1.0	to	0.3	0.02
0.3	to	0.1	0.01
0.1	to	0.03	0.005
0.03	to	0.01	0.001
0.01	to	0.005	0.0003
0.005	to	0.001	0.0001

For the case of $\kappa = 0.5$ and $\omega = 2.0$, the analytical solution given by Eq. (16) and the numerical computer solution compare as shown below:

β	τ by Eq. (16)	τ by Computer	Error ,%
0.50	0.41416	0.41416	-
0.28	0.88967	0.88965	0.002
0.02	6.07100	6.06195	0.15

3. Discussion of Results

Figure 1 is a graph of conversion of B as a function of the amount of A reacted divided by B_o, or $(1-\alpha)\omega$, with parameters of κ. The slopes of the curves, at any conversion of B, correspond to the rate of disappearance of B with respect to that of A (i. e., dB/dA). At $\kappa = 0$, only the first step of the reaction occurs; thus $1-\beta$ plotted against $(1-\alpha)\omega$ is linear with a slope of unity. At values of κ greater than 0, the rate of disappearance of B is less than that of A, which results in slopes less than unity. At low values of κ (with the first reaction step being fast relative to the second step), the initial slope is close to unity, but decreases as the conversion of B increases; this decrease occurs because the concentration of the intermediate builds up rapidly. As κ approaches infinity, the slope approaches a constant value of 0.5 because the concentration of C remains low during the course of the reaction; thus the complex reaction appears to be a simple second-order reaction.

Figure 1 shows that exactly equivalent amounts of A and B are reacted at complete conversion of B when ω is equal to or greater than 2 (equivalent amounts of reactants or excess A). With ω less than 2 (excess B) and complete conversion of A, $(1-\alpha)\,\omega$ becomes equal to ω, the ratio of A reacted to B reacted is less than 2 (but still greater than ω). Hence less than the amount of excess B is left unreacted, and some intermediate C is present.

Figure 2 is a graph of $1-\beta$ versus κ, with $(1-\alpha)\,\omega$ values as parameters. This graph, which is a cross plot of Fig. 1 at selected values of $(1-\alpha)\omega$, is useful for determining the value of κ from experimental data.

Figure 3 presents a graph of the ratio of D produced to B reacted, $D/(1-\beta)B_o$, and C produced to B reacted, $C/(1-\beta)B_o$, as a function of $1-\beta$ with parameters of κ. At high values of κ, the ratio of D produced to B reacted increases sharply with increasing conversion of B; the reverse occurs for low values of κ. At $\kappa = 2$, $(1-\beta)$ versus $D/(1-\beta)B_o$ is linear with a slope of unity; one can easily see this linearity by substituting 2 for κ in Eq. (10), substituting the resulting value of $(1-\alpha)\,\omega$ into Eq. (12) and simplifying to obtain

$$1 - \beta = \frac{D}{(1-\beta)B_o} .$$

Figure 4 shows τ as a function of $1-\beta$ with families of ω and parameters of κ. As shown in Fig. 4, τ changes very little with κ for the case of excess A. This occurs because the time for any given conversion of B becomes less dependent on the amount of A consumed by reaction with the intermediate C. Since B is a reactant for just the first step, excess B spreads the curves for various values of κ to a greater extent than for the case of excess A or equivalent amounts of reactants. In this case κ has a great effect upon the concentration of A, and therefore τ is much more dependent upon κ. At $\tau = \infty$, with $\omega = 1.0$, the terminal points of the τ curves correspond to ratios of A

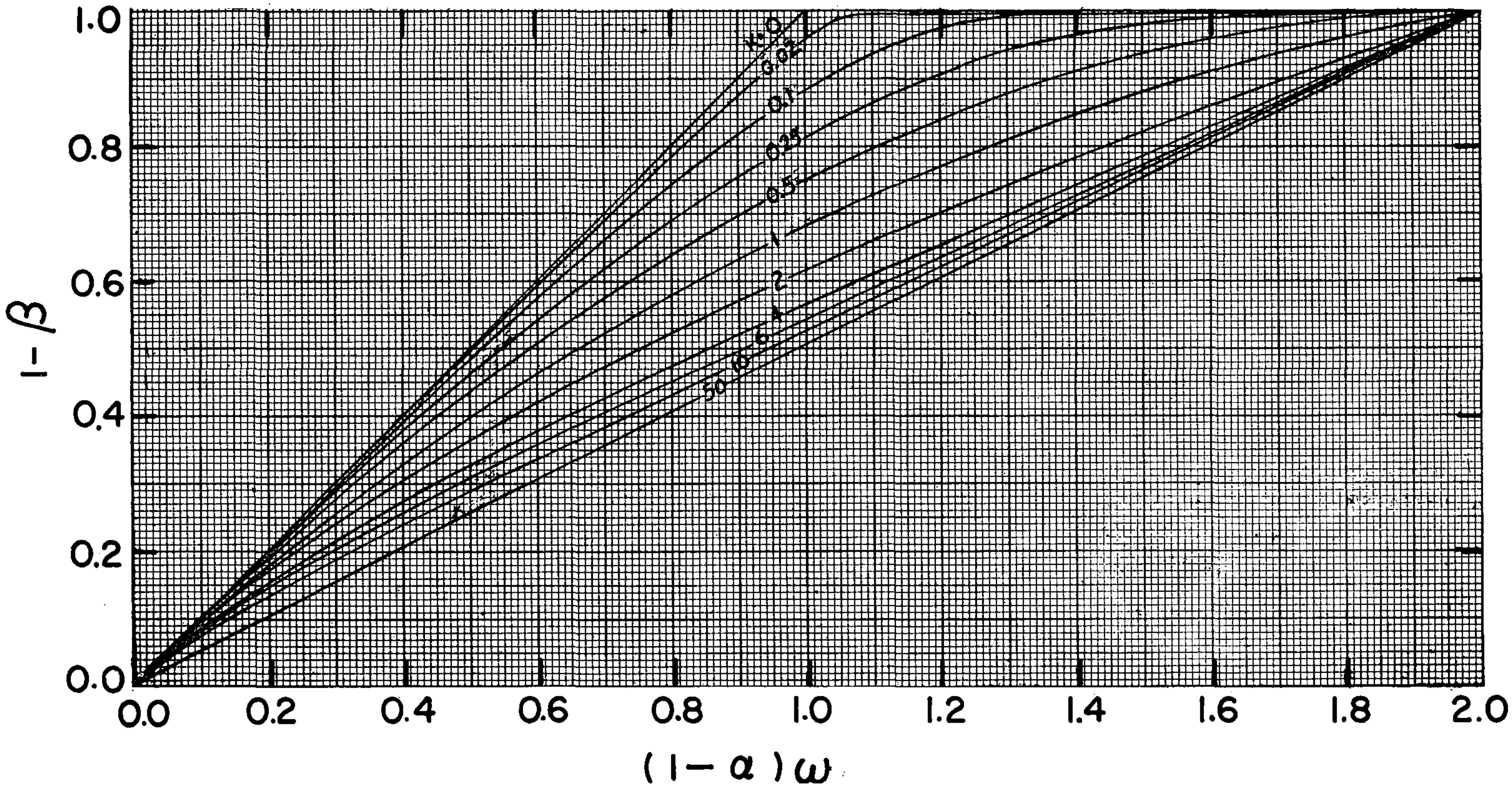

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Fig. 1. Fraction B reacted versus moles A reacted/moles B in feed, for consecutive-competitive second-order reactions: batch or tubular-flow reactor; $\kappa = k_2/k_1$.

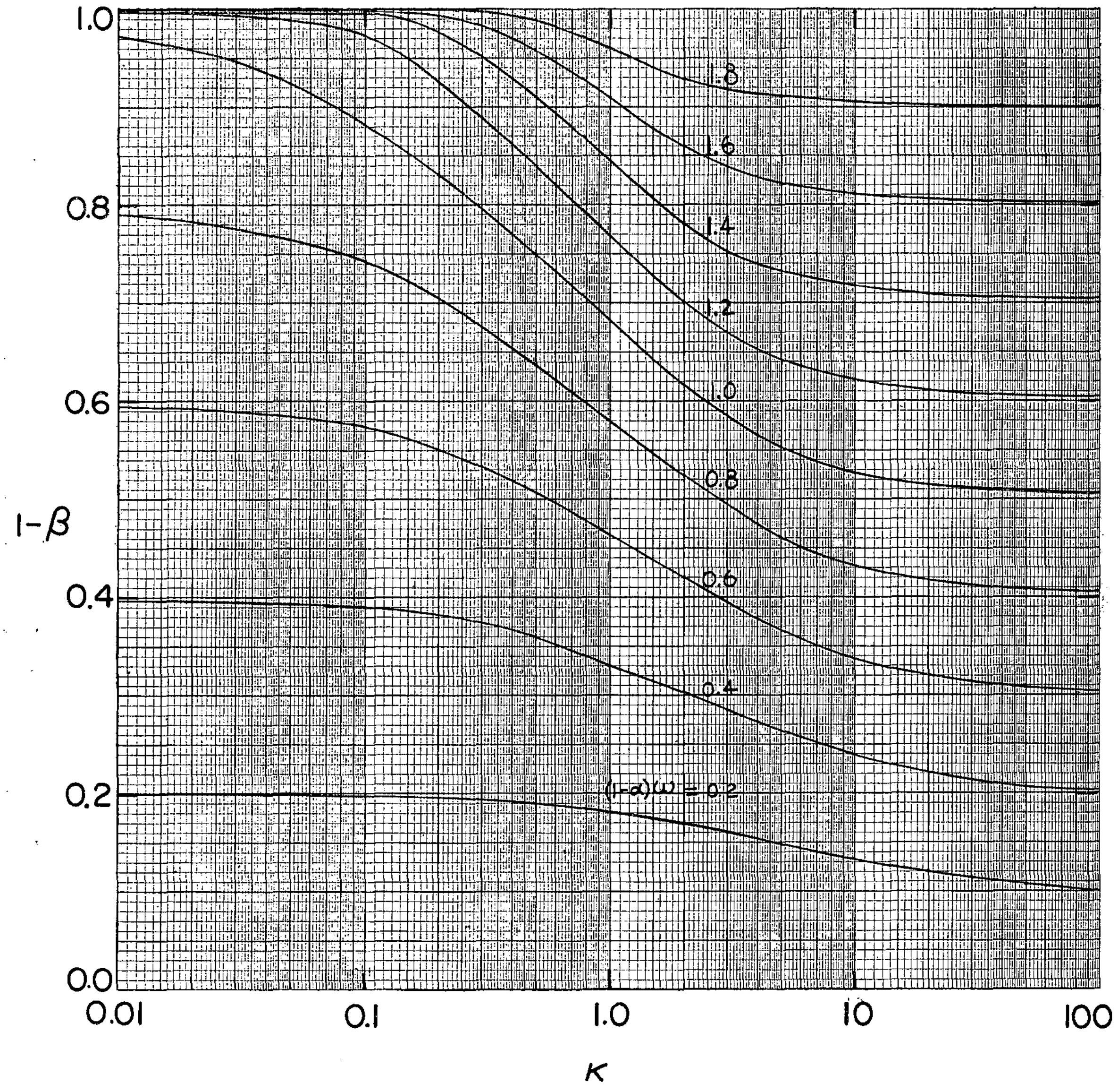

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Fig. 2. Fraction B reacted versus rate-coefficient ratio κ, for consecutive-competitive second-order reactions; contours of constant (moles A reacted/moles B in feed); batch or tubular-flow reactor.

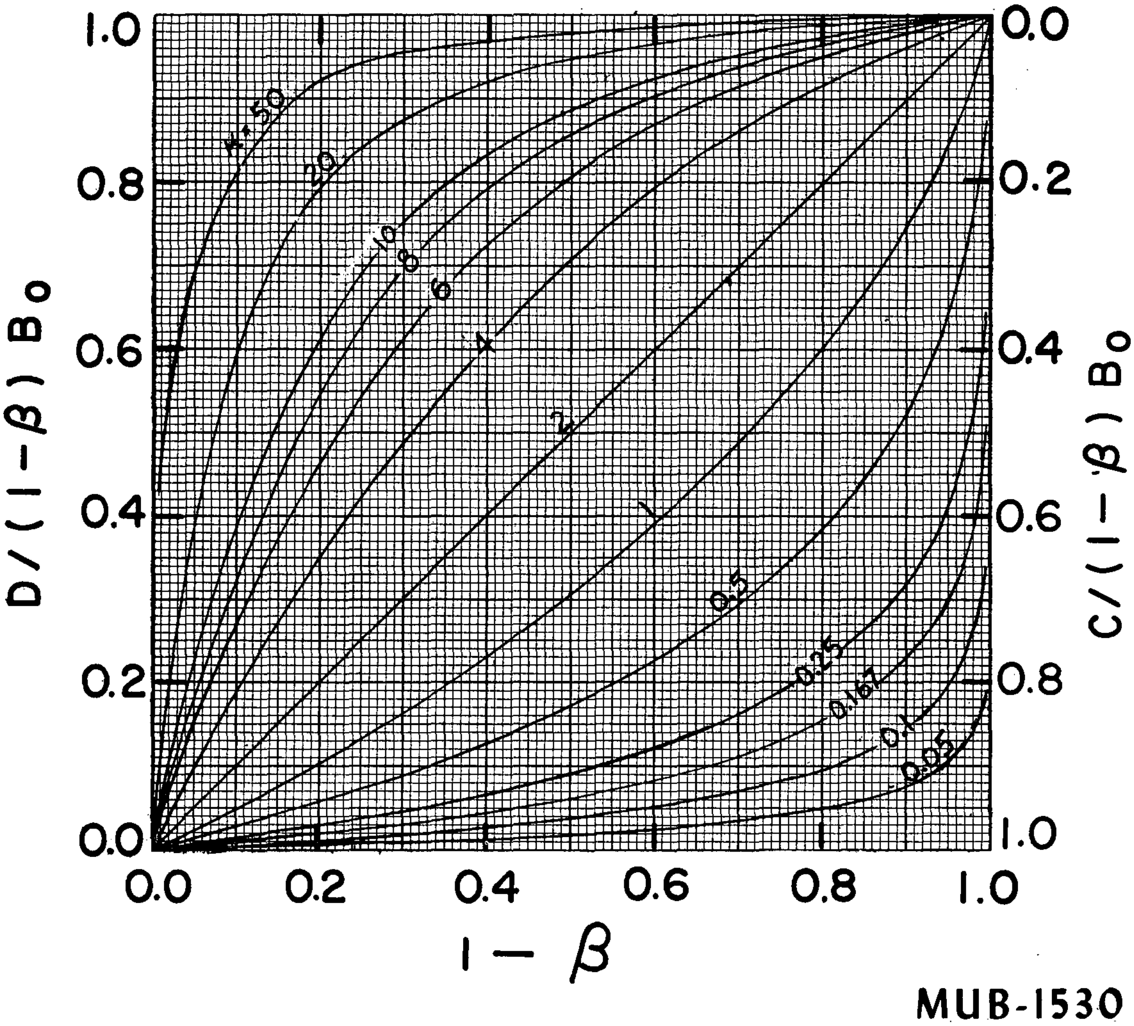

Fig. 3. Yield of products C and D versus fraction B reacted, for consecutive-competitive second-order reactions; batch or tubular-flow reactor; $\kappa = k_2/k_1$.

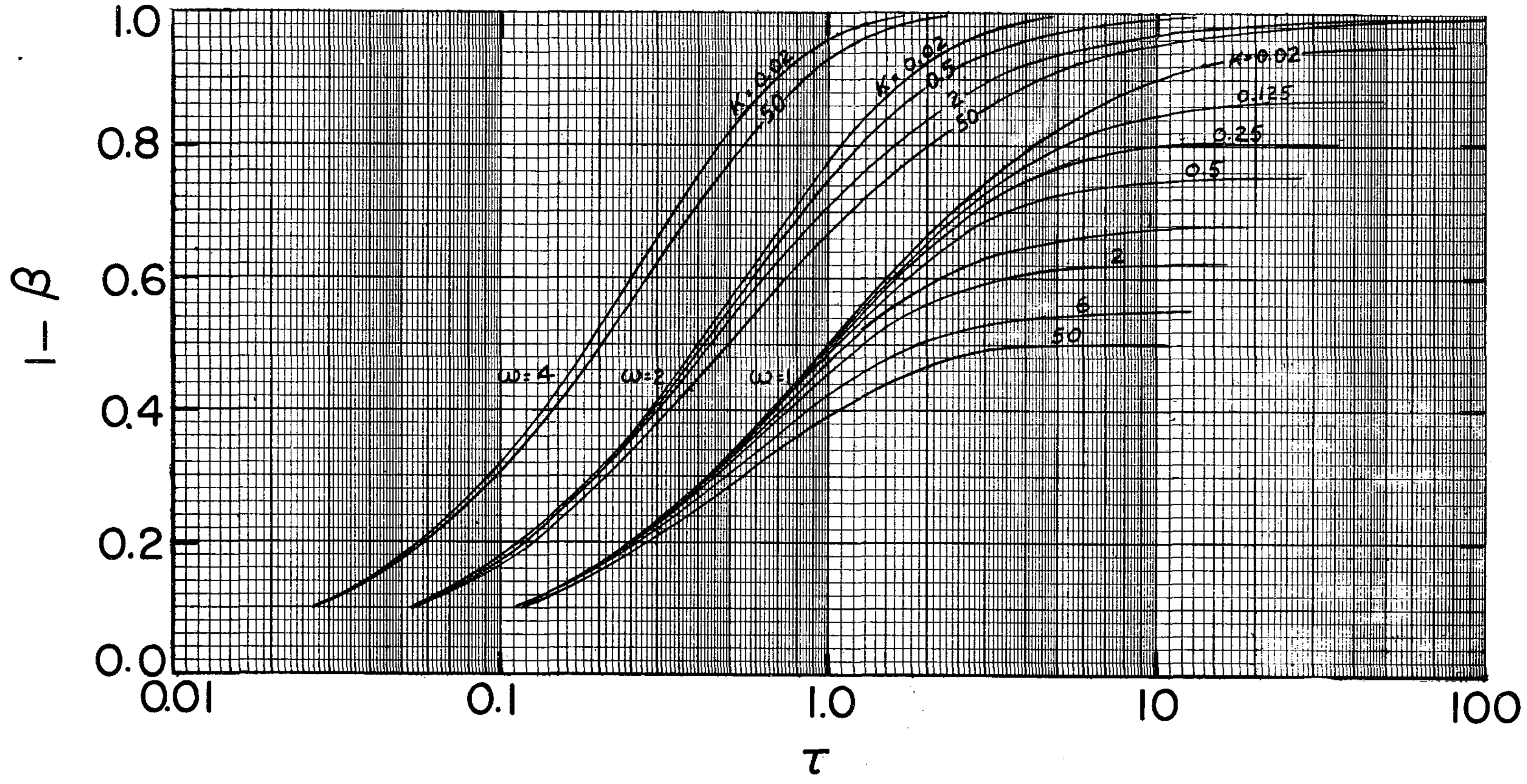

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Fig. 4. Fraction B reacted versus dimensionless time variable τ, for consecutive-competitive second-order reactions; batch or tubular-flow reactor; $\kappa = k_2/k_1$.

reacted to B reacted that are less than 2 (but still greater than 1). Hence there is less than the amount of excess B left unreacted and some intermediate C present. At $\omega = 1.0$, there is twice the equivalent amount of reactant B initially present. A conversion equal to one-half the conversion for the cases of equivalent amounts of reactants or excess A ($\omega \geqslant 2$) gives equal amounts of B reacted. Thus, the curves for $\omega = 1.0$ are to the right of the curves for $\omega \geqslant 2.0$.

4. Interpretation of Results

a. Effect of κ. The time to react to a given conversion of either A or B is, of course, dependent upon the two rate coefficients. A higher value of k_1 decreases the time to react to any conversion of either A or B at any value of κ. For lower values of κ, the dimensionless time τ is less for reacting to a given conversion of B, because the first reaction step is fast relative to the second step. However, for a given conversion of the coreactant A, τ is greater for low values of κ because the intermediate C builds up rapidly but reacts slowly with A.

As shown in Fig. 3, the yields of intermediate C and final product D depend upon the value of κ at any conversion of B. A low value of κ results in a greater yield of C at any given conversion of B or any given value of τ.

b. Effect of ω. An excess of reactant B(ω less than 2) increases the reaction rate of the first step and gives a greater yield of C at a given amount of B reacted. An excess of A(ω greater than 2) increases the rate of both steps equally and therefore does not favor either C or D at a given amount of either A or B reacted.

In all cases, the yield ratio of D to C is given by the following equation, obtained from Eqs. (11) and (12):

$$\frac{D}{C} = \frac{(1-\alpha)\omega - (1-\beta)}{2(1-\beta) - (1-\alpha)\omega} \quad . \tag{19}$$

An example of ratios of D to C, obtained at a given amount of B reacted, is shown below for $\kappa = 2$; we note that $k_1 t = \tau / B_0$.

ω	B_o	$1-\beta$	$(1-\alpha)\,\omega$	$1-\alpha$	D/C	τ	k_1t
2.0	1.0	0.80	1.45	0.72	4.34	1.60	1.60
4.0	1.0	0.80	1.45	0.36	4.34	0.50	0.50
1.0	2.0	0.40	0.56	0.56	0.67	0.76	0.38

At a given conversion of A, ratios of D to C obtained for $\kappa = 2$ are shown below.

ω	B_o	$1-\alpha$	$(1-\alpha)\omega$	$1-\beta$	D/C	τ	k_1t
2.0	1.0	0.80	1.60	0.86	6.17	2.30	2.30
4.0	1.0	0.40	1.60	0.86	6.17	0.62	0.62
1.0	2.0	0.80	0.80	0.52	1.17	1.46	0.73

An ω of 2.0 corresponds exactly to the equivalent amounts of A and B; $\omega = 4.0$ corresponds to twice as much A as the equivalent amount; and $\omega = 1.0$ corresponds to twice as much B as the equivalent amount. When there is initially twice the equivalent amount of a reactant, a conversion equal to half the conversion for the limiting or equivalent reactant cases gives equal amounts reacted.

The reaction time (shown above in the last column) for a given conversion of B is reduced more by using excess B ($\omega = 1$) than by excess A ($\omega = 4$); for a given conversion of A, excess A reduces the time more than excess B does. This results because A is a reactant for both reaction steps, whereas B is a reactant for just the first step.

As stated previously, excess A has no effect on the yield ratio of D to C at a given conversion of either A or B. However, at any finite reaction time, excess A favors production of the final product D. At k_1t (or τ/B_o) = 1, and $\kappa = 2$, the following values of D/C are obtained depending upon the value of ω.

ω	B_o	τ	k_1t	$1-\beta$	$(1-\alpha)\omega$	$1-\alpha$	D/C
2.0	1.0	1.0	1.0	0.71	1.22	0.61	2.55
4.0	1.0	1.0	1.0	0.94	1.83	0.46	17.80
1.0	2.0	2.0	1.0	0.56	0.88	0.88	1.33

At extremely high or low values of κ the yield ratio (D/C) is less dependent upon an excess of either reactant.

B. Continuous Stirred-Tank Reactor (CSTR)

1. Equations

By material balance, with substitution of previously defined dimensionless variables and parameters, we obtain

$$\alpha_n = \frac{\beta_{n-1} - \beta_n}{\omega \beta_n \bar{\tau}_n}, \tag{20}$$

and

$$\alpha_{n-1} - \alpha_n = \bar{\tau}_n \alpha_n \beta_n + \kappa \bar{\tau} \alpha_n (2 - 2\beta_n + \alpha_n \omega - \omega) \tag{21}$$

where subscripts n and n-1 designate values in (or leaving) tank n and tank n-1 respectively, and $\bar{\tau}$ is the dimensionless mean residence time in one tank. We substitute for α_n in Eq. (21), solve the resulting equation for $\bar{\tau}_n$, and obtain

$$\bar{\tau}_n = \frac{\left[1 + \kappa \left(\frac{\beta_{n-1} - \beta_n}{\beta_n}\right)\right]}{\alpha_{n-1}\left[\frac{\omega \beta_n}{\beta_{n-1} - \beta_n}\right] + \beta_n (2\kappa - 1) + \kappa(\omega - 2)} . \tag{22}$$

If 1.0 is substituted for α_{n-1} and β_{n-1} in the above equations, we have the equations for a single stirred-tank reactor, with a feed consisting entirely of reactants.

2. Interpretation of Results

Figures 5, 6, and 7 present the same type of yield structure graphs as given for the plug-flow reactor case, and Fig. 8 shows curves of conversion of B versus τ for a single CSTR. At a given conversion of B, the continuous stirred-tank reactor always favors production of final product D compared to the plug-flow reactor. This is easily seen by comparison of Figs. 3 and 7. Production of D is favored because the reactor composition is assumed to be at the exit

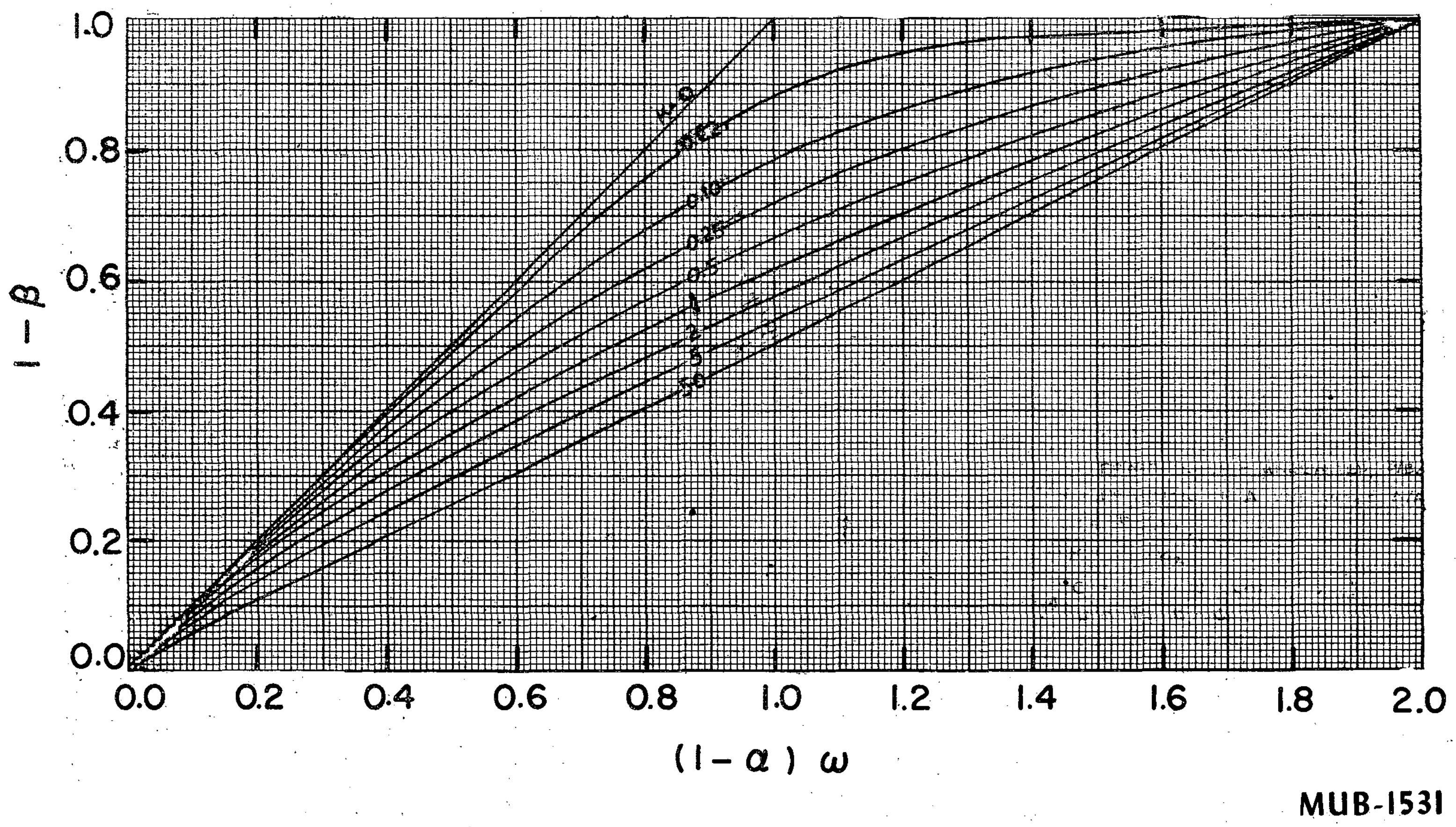

Fig. 5. Fraction B reacted versus moles A reacted/moles B in feed, for consecutive-competitive second order reactions; continuous stirred-tank reactor; $\kappa = k_2/k_1$.

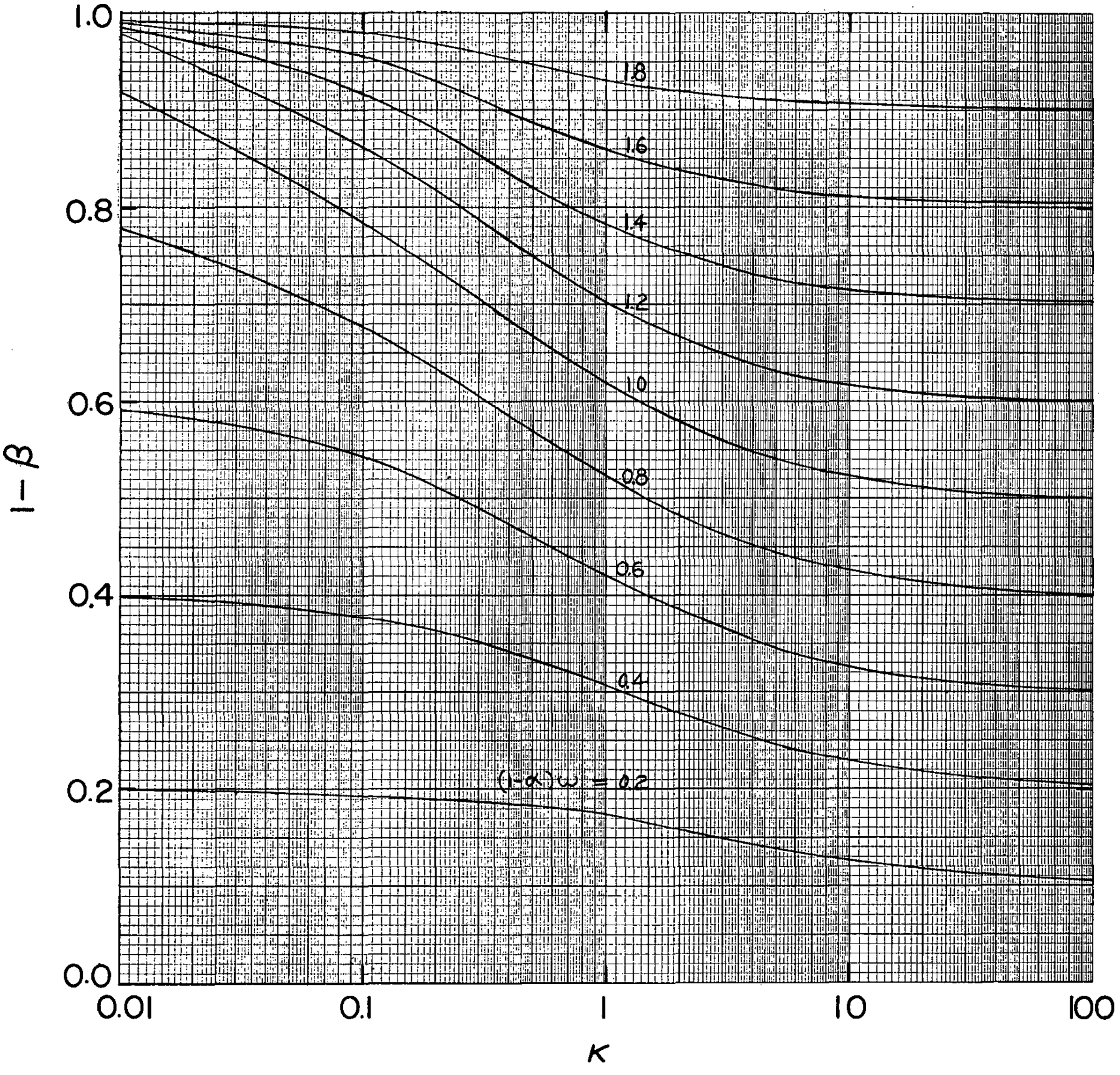

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Fig. 6. Fraction B reacted versus rate coefficient ratio κ for consecutive-competitive second order reactions; contours of constant (moles A reacted/moles B in feed); continuous stirred-tank reactor.

value; the intermediate C is continually present at its higher exit concentration, giving a greater reaction rate for the second step than the average rate of this step in the plug-flow reactor.

Excess reactants (either A or B) have the same respective directional effects on the yields of intermediate and final products as in the plug-flow reactor. However, at a given conversion of B, the incremental yield of C is greater when using excess B than it is in the plug-flow case. At a given time, the incremental yield of D is less when using excess A, and for C it is greater when using excess B. Also, for obtaining a given conversion of A or B, an excess of either reactant has a more pronounced effect in reducing the reaction time.

The general case consists of a number of continuous stirred-tank reactors in series. If the total volume of the reactor is divided into more and more separate tanks, the yield structure and the time to react to a given conversion approach that of a plug-flow reactor.

Given the volume of each tank in series, the compositions leaving each tank can be calculated by successive application of Eq. (21) and (22); it is necessary to solve a cubic equation to obtain the exit β of each tank.

C. Evaluation of Rate Coefficients

The rate coefficients can be evaluated by using the time-ratio method. Frost and Schwemer[1] and Burkhard [2] give tables of time ratios as a function of κ , and τ as a function of κ and α. Their tables are valid only for the case of equivalent amounts of reactants. The value of κ is determined from the measured time ratios. Knowing κ, values of τ are obtained for various values of α, and k_1 is calculated by dividing τ by $B_o t$.

French[9] reduces the two reaction steps to first order by introducing a new independent variable which is a combination of the concentration of the coreactant A and time; this allows integration of the rate equations. Letting $d\theta = A dt$ in Eqs. (1) and (2), we have

$$dA/d\theta = -k_1B - k_2C,$$

and

$$dB/d\theta = -k_1B.$$

The above equations integrate to

$$A = A_o - B_o\left[2 - 2e^{-k_1\theta} - \frac{k_1\left(e^{-k_2\theta} - e^{-k_1\theta}\right)}{k_1 - k_2}\right],$$

and

$$B = B_o e^{-k_1\theta}.$$

By plotting the experimental values of A as a function of time and graphically integrating values of θ as a function of time are obtained. The values of k_1 and k_2 can then be determined from the above equations.

Wideqvist[10] uses the same method as French, but in addition employs two graphical integrations to eliminate the transcendent parts of the equations.

The method of French or Wideqvist is not as rapid as the time-ratio method; however, it is not necessary that the reactants be present in equivalent amounts, and precalculation of the conversion-time grid is not required.

Powell[11] demonstrated the usefulness of α versus log τ plots for determining the rate coefficient and reaction mechanism. The dimensionless time and concentration are defined as

$$\tau = kA_o^{n-1}t$$

$$\alpha = A/A_o$$

where n is the reaction order and the other variables and parameters are defined as in the present study. Experimental values of α are plotted versus log time; the experimental curve should match the theoretical curve (α versus log τ) if the reaction mechanism is the same as the assumed mechanism except that the experimental curve is shifted by an amount $-\log kA_o^{n-1}$. The rate coefficient is then calculated from values of τ, A_o and time, at equal values of α on the theoretical and experimental curves.

From the data given in this work, the rate coefficients can be evaluated from just one data point (although more than one data point would be recommended). We obtain the value of κ from Figs. 1, 2, 3, or Eq. (10) by using the measured reactant concentrations. At κ and at the measured conversion of B and time, a value of τ is obtained from Fig. 4; k_1 is then calculated from τ. This method is not restricted to equivalent amounts of reactants, it is very rapid, and it is usually sufficiently accurate for obtaining rate coefficients to be used for reactor design purposes. However, like the Frost-Schwemer method, it requires precalculation of the entire conversion-time grid in order to evaluate the individual rate coefficients.

D. Applications

As mentioned in the Introduction, all calculations for preparation of the graphs were done with the restrictions of constant volume and temperature, and for idealized reactor behavior.

In liquid systems, changes in density during the reaction may cause changes in volume, but these changes are generally small. For gas-phase systems, a change in the total number of moles due to the reaction will cause a change in volume as a function of conversion. The graphs are valid for the following case where there is no change in the total moles:

$$A + B \rightarrow C + E ,$$

and

$$A + C \rightarrow D + F.$$

Because constant volume is assumed, the residence time in a plug-flow reactor is the same as the time in a batch reactor; therefore the charts for the plug-flow case are also applicable to the batch case. The following examples indicate the use of the graphs in solving problems with the above restrictions. The effect of an excess of either reactant on the required reactor volume for a given production rate of C or D is shown in Example 1. Example 2 is an optimization problem in which the best feed rate is found in order to obtain the maximum production rate of final product D. Example 3 is a calculation involving two CSTR's in series.

The charts can also be used to determine the rate coefficients for a reaction where the mechanism is known to be consecutive-competitive.

Example 1.

A consecutive-competitive reaction takes place at constant volume and temperature in an aqueous solution. A tubular (plug-flow) reactor with a volume of 10 ft^3 is used, under the following conditions ("mole" indicates lb molecular weight):

$$F = 10\ ft^3/sec\ \text{(feed rate)},$$
$$k_1 = 1.0\ ft^3/sec\ mole,$$
$$k_2 = 0.5\ ft^3/sec\ mole,$$
$$B_o = 1.0\ mole/ft^3,$$

and

$$\omega = 2.0\ .$$

a. What is the conversion and production rates of C and D?

$$\tau = B_o k_1 V/F = 1.0$$
$$1 - \beta = 0.75\ \text{(from Fig. 4)},$$
$$\omega(1-\alpha) = 1.00\ \text{(from Fig. 1); hence}\ 1 - \alpha = 0.50;$$
$$C = 2B_o(1-\beta) - A_o(1-\alpha) = 0.5\ mole/ft^3,$$
$$D = B_o(1-\beta) - C = 0.25\ mole/ft^3,$$
$$CF = 5\ mole/sec,$$

and

$$DF = 2.5\ mole/sec.$$

b. With $\omega = 1.0$, what reactor volume is required to obtain a production rate of C the same as in (a) above?

In this case $B_o = 2.0\ mole/ft^3$ and $A_o = 2.0\ mole/ft^3$. The concentration of C in the final reaction mix must be 0.5 $mole/ft^3$. Thus, we have

$$F = 5.0/C,$$

and

$$F = 10 - 5.0/[\,2B_o(1-\beta)-A_o(1-\alpha)]\ .$$

By trial and error, we find the volume at which the right side of the above equation is equal to 10. The following tabulation is made:

V	$\tau=(B_o k_1 V)/F$	$1-\beta$	$(1-\alpha)\omega$	$1-\alpha$	$5.0/[2B_o(1-\beta)-A_o(1-\alpha)]$
3.0	0.60	0.36	0.40	0.40	7.8
2.0	0.40	0.28	0.30	0.30	9.6
1.8	0.36	0.26	0.28	0.28	10.4

By interpolation, the required reactor volume is about 1.9 ft^3. Values of $1-\beta$ are obtained from Fig. 4 (at $\omega = 1.0$), and $(1-\alpha)\omega$ are obtained from Fig. 1.

c. With $\omega = 4.0$, what reactor volume will give a production rate of D the same as in (a) above?

In this case $B_o = 1.0$ mole/ft^3 and $A_o = 4.0$ mole/ft^3. Using excess A does not have an effect on the relative yields of D and C; therefore, the same conversion of B as in (a) above will give the required production rate of D.

At $\omega = 4.0$ and $(1-\beta) = 0.75$, $\tau = 0.42$ (from Fig. 4) and the reactor volume $V = 4.2$ ft^3.

Example 2.

Given the same data as in Example 1 except that $B_o = 2.0$ moles/ft^3, at $\omega = 2.0$, what feed rate will result in the maximum production rate of D? The following tabulation is made:

Feed rate (ft^3/sec)	$\tau = B_o k_1 \frac{V}{F}$	$1-\beta$	$\frac{D}{(1-\beta)B_o}$	D (mole/ft)	DF (mole/sec)
10	2.0	0.89	0.500	0.890	8.9
12	1.66	0.86	0.455	0.783	9.4
15	1.50	0.84	0.430	0.720	10.8
20	1.00	0.75	0.340	0.510	10.2

The values of $1-\beta$ are obtained from Fig. 4 at $\kappa = 0.5$ and $\omega = 2.0$, and values of $D/(1-\beta)B_o$ are obtained from Fig. 3. The maximum production rate of D is about 10.8 mole/sec at a feed rate of 15 ft^3/sec.

Example 3.

With two CSTR's in series, what are the production rates of C and D, based on the following information:

$$F = 1.0\ ft^3/min$$
$$k_1 = k_2 = 1.0\ ft^3/min\ mole$$
$$B = 1.0\ mole/ft^3$$

and

$$\omega = 2.0\ .$$

Volume of first CSTR: $V_1 = 7.0\ ft^3$.

Volume of second CSTR: $V_2 = 3.0\ ft^3$.

For the first CSTR:

$$\bar{\tau}_1 = B_o k_1 V_1/F = 7.0,$$
$$1-\beta_1\ 0.80 \text{ (from Fig. 8)},$$
$$(1-\alpha_1)\omega = 1.44 \text{ (from Fig. 5)},$$

and

$$1-\alpha_1 = 0.72.$$

For the second CSTR, Eqs. (20) and (22) are used to solve for the conversions of A and B, and the production rates of C and D:

$$\alpha_1 = 0.28,$$
$$\beta_1 = 0.20,$$

and

$$\bar{\tau}_2 = B_o k_1 V_2/F = 3.0\ .$$

Substituting α_1 and β_1 into Eq. (22) we solve for β_2 by trial and error and obtain $\beta_2 = 0.1$. We then use Eq. (20) to solve for α_2 and obtain $\alpha_2 = 0.167$. The concentrations of C and D are found as follows:

$$C_2 = 2B_o(1-\beta_2) - A_o(1-\alpha_2) = 0.134 \text{ mole/ft}^3,$$

and

$$D_2 = B_o(1-\beta_2) - C_2 = 0.766 \text{ mole/ft}^3.$$

And the production rates of products are

$$CF = 0.134 \text{ mole/min},$$

and

$$DF = 0.766 \text{ mole/min}.$$

III. CONSECUTIVE-REVERSIBLE REACTION MODEL

We now consider a group of consecutive-reversible reactions for which the general model is

$$aA \rightleftarrows bB$$

and

$$b'B \rightleftarrows cC \, .$$

The cases covered here will involve three of the four possible reactions, with all three reactions being first-order or with combinations of one second-order and two first-order reactions. If all the reaction steps are first-order, the differential equations are linear in the dependent variables (concentrations); successive differentiation yields a higher-order linear equation having a single dependent variable and constant coefficients which is easily solved analytically. For the second-order cases, the higher-order equation so obtained cannot be solved analytically except in the simplest cases. The second-order cases are solved numerically using a fourth-order Runge-Kutta method (due to Kutta).[8]

Eight cases are studied; two all-first-order, and six second-order—first-order cases. The results are presented in graphs or in tables of dimensionless concentrations as functions of dimensionless time with ratios of rate coefficients as parameters. Calculations were made for 25 ratios of rate coefficients for each model considered. The calculations were done on the IBM 650 Computer for the cases where it was possible to derive an algebraic equation, and the other cases were solved numerically on the IBM 7090 Computer. The Fortran statements for the 7090 program are given in Appendix C so that the program can be applied to cases involving four rate coefficients which are not covered in the present study.

Any stoichiometry may be applied to the reaction models because the calculated dimensionless-concentration values, as functions of the ratios of rate coefficients and dimensionless time, are dependent only upon the kinetic mechanism of the reaction model. Consider the above general reaction system; the material balance is

$$B = \frac{b}{a}(A_o - A) - \frac{b'}{c}\, C,$$

where A, B, and C are the concentrations and a, b, b', and c are the combining-proportion coefficients of the respective components. Normalizing the material balance by dividing through by bA_o/a we have

$$\alpha + \beta + \gamma = 1, \tag{23}$$

where the dimensionless concentrations are

$$\alpha = A/A_o, \tag{24}$$

$$\beta = aB/bA_o, \tag{25}$$

and

$$\gamma = ab'C/cbA_o . \tag{26}$$

In each of the models considered, both the stoichiometry and the mechanism are shown by chemical equations.

A. Model 1

We first consider the following model in which all the reaction steps are first-order; this is one of the cases treated by Lowry and John.[3]

$$\text{Mechanism}\begin{cases} A \xrightarrow{k_1} B \\ B \underset{k_3}{\overset{k_2}{\rightleftharpoons}} C \end{cases} \qquad \text{General stoichiometry}\begin{cases} aA \xrightarrow{k_1} bB \\ b'B \underset{k_3}{\overset{k_2}{\rightleftharpoons}} cC \end{cases}$$

In this reaction all of A is ultimately converted to an equilibrium mixture of B and C. The rate equations are

$$dA/dt = -k_1A, \tag{27}$$

$$dB/dt = [k_1b/a]A - k_2B + k_3C, \tag{28}$$

and

$$dC/dt = [k_2c/b']B - [k_3c/b']C . \tag{29}$$

In the above rate equations, k_1 is in terms of A molecules, and k_2 and k_3 are in terms of B molecules. Introducing the dimensionless concentrations α, β, and γ defined by Eqs. (24), (25), and (26) respectively, and dimensionless time, $\tau = k_1t$, we obtain

$$d\alpha/d\tau = -\alpha, \tag{30}$$

$$d\beta/d\tau = \alpha + \kappa_2\gamma - \kappa_1\beta, \tag{31}$$

and

$$d\gamma/d\tau = \kappa_1\beta - \kappa_2\gamma\ , \tag{32}$$

where

$$\kappa_2 = ck_3/b'k_1\ ,$$

and

$$\kappa_1 = k_2/k_1\ .$$

The case of the plug-flow reactor gives the following equations. Substituting $1-\alpha-\beta$ for γ in Eq. (31), we have

$$\frac{d\beta}{d\tau} = \alpha(1-\kappa_2) - (\kappa_1 + \kappa_2)\beta + \kappa_2\ . \tag{33}$$

Differentiating Eq. (33) with respect to τ, and substituting for $d\alpha/d\tau$ from Eq. (30), we obtain

$$\frac{d^2\beta}{d\tau^2} = -\ \alpha\ (1-\kappa_2) - (\kappa_1 + \kappa_2)\ \frac{d\beta}{d\tau}\ . \tag{34}$$

Solving Eq. (33) for $\alpha(1-\kappa_1)$, and substituting into Eq. (34), we have

$$\frac{d^2\beta}{d\tau^2} + (1 + \kappa_1 + \kappa_2)\ \frac{d\beta}{d\tau} + (\kappa_1 + \kappa_2)\beta = \kappa_2\ . \tag{35}$$

Equation (35) is a linear equation with constant coefficients, and its general solution is

$$\beta = C_1 + C_2\ e^{-\tau} + C_3 e^{-(\kappa_1+\kappa_2)\tau}\ . \tag{36}$$

The three constants C_1, C_2, and C_3, are found by using the following boundary conditions:

At $\tau = \infty$, we have $\beta + \gamma = 1$, and $\gamma = \dfrac{\kappa_1\beta}{\kappa_2}$;

therefore, we know $C_1 = \kappa_2/(\kappa_1 + \kappa_2)$.

At $\tau = 0$, we have $\beta = 0$; therefore we have $C_1 + C_2 + C_3 = 0$,
$\alpha = 1$, and, from Eq. (31), $d\beta/d\tau = 1$.

Differentiating Eq. (36) with respect to τ, setting $\tau = 0$, and substituting 1.0 for $d\beta/d\tau$, we have

$$C_2 = \frac{\kappa_2 - 1}{1-\kappa_1-\kappa_2} ,$$

and

$$C_3 = \frac{\kappa_1}{(\kappa_1+\kappa_2)(1-\kappa_1-\kappa_2)} .$$

Thus the final solution for the plug-flow case is

$$\beta = \frac{\kappa_2}{\kappa_1+\kappa_2} + \frac{\kappa_2-1}{(1-\kappa_1-\kappa_2)} e^{-\tau} + \frac{\kappa_1 e^{-(\kappa_1+\kappa_2)\tau}}{(\kappa_1+\kappa_2)(1-\kappa_1-\kappa_2)} , \tag{37}$$

and from inspection of Eq. (30) we have

$$\alpha = e^{-\tau} . \tag{38}$$

Figure 9 is a graph of γ as a function of τ, for five values of κ_1 each with five values of κ_2.

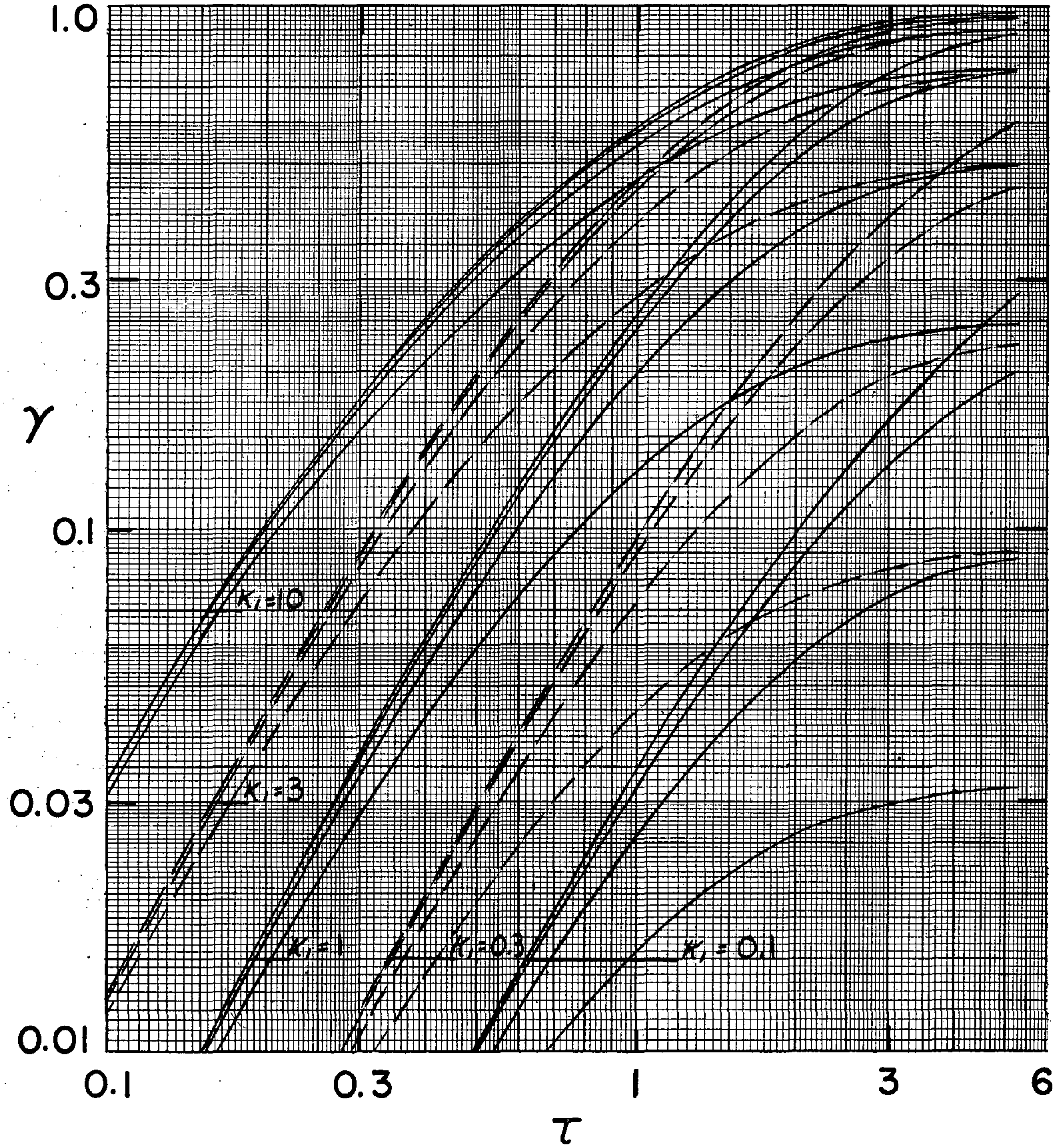
The general equations for the continuous stirred-tank reactor (CSTR) case are

$$\beta_n = \frac{(1+\overline{\tau}_n)(\beta_{n-1} + \kappa_2\overline{\tau}_n) + (1-\kappa_2)\overline{\tau}_n\alpha_{n-1}}{(1+\overline{\tau}_n)(1+\kappa_2\overline{\tau}_n+\kappa_1\overline{\tau}_n)} \tag{39}$$

and

$$\alpha_n = \frac{\alpha_{n-1}}{1+\overline{\tau}_n} . \tag{40}$$

The computations for the CSTR are based on the feed being all A so that $\alpha_{n-1} = 1$ and $\beta_{n-1} = 0$. Figures 10A and 10B are graphs of γ as a function of τ for a single CSTR. The same 25 combinations of κ_1 and κ_2 used for the plug-flow reactor were also used for the continuous stirred-tank reactor. We can compute cases consisting of two or more tanks in series by successively using Eqs. (39) and (40), if we are given the number of tanks in series, their volumes, and the volumetric feed rate.



MUB-1525

Fig. 9. Moles C produced/moles A in feed versus dimensionless time, for consecutive first-order reactions with second step reversible. Within each group of curves at a constant κ_1, values of κ_2 from left to right are 0.1, 0.3, 1.0, 3.0: Batch or tubular flow reactor.

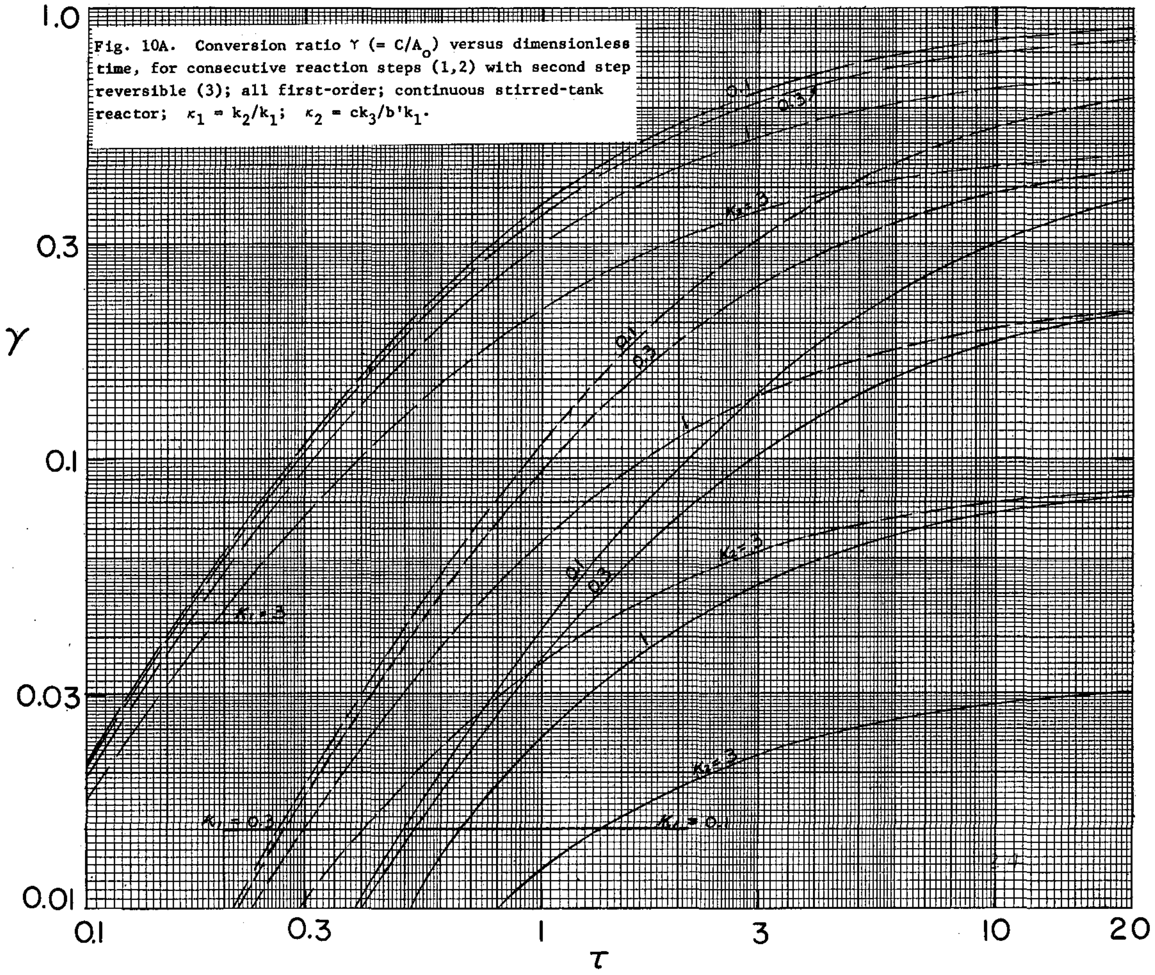


Fig. 10A. Conversion ratio γ (= C/A_o) versus dimensionless time, for consecutive reaction steps (1,2) with second step reversible (3); all first-order; continuous stirred-tank reactor; $\kappa_1 = k_2/k_1$; $\kappa_2 = ck_3/b'k_1$.

MUB-1549

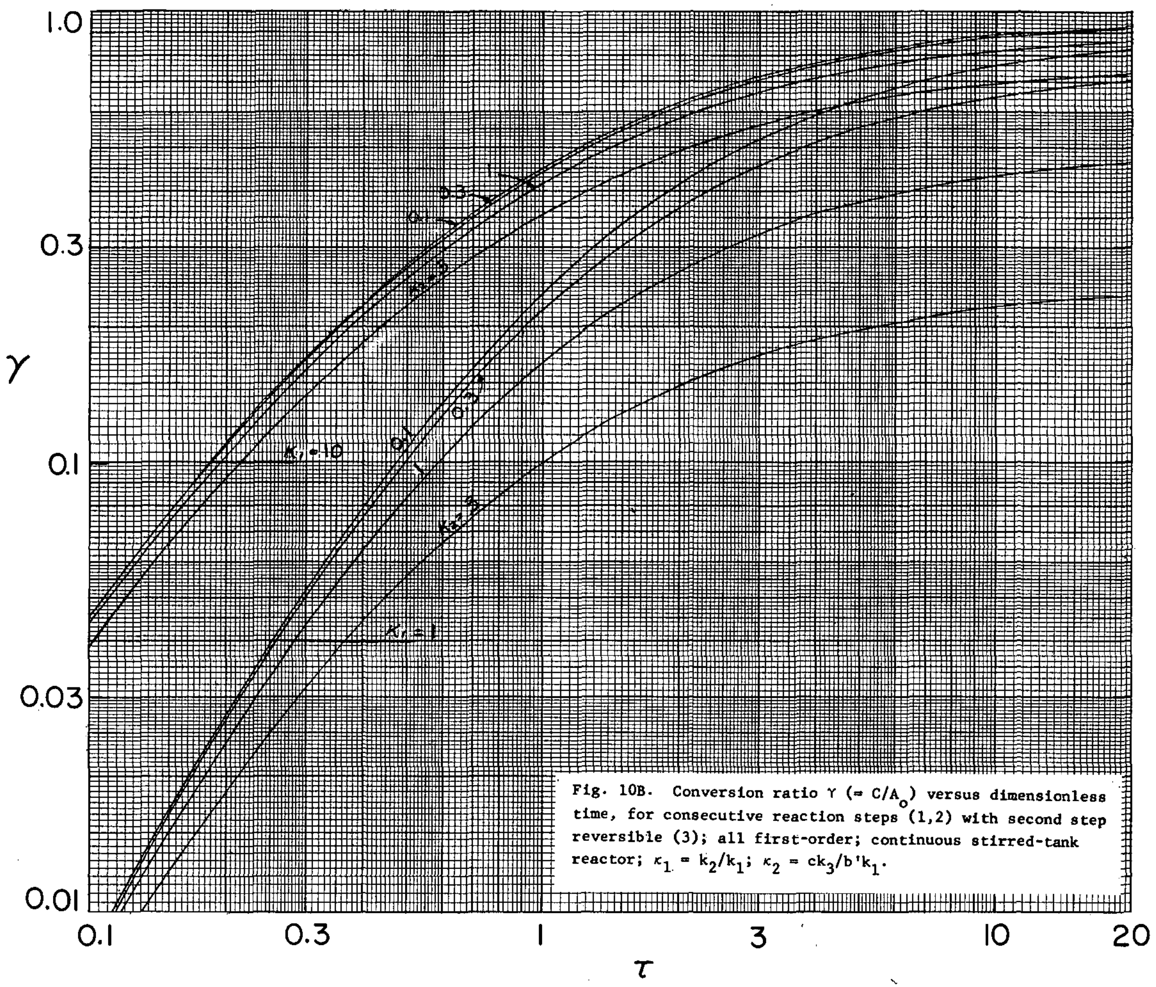


Fig. 10B. Conversion ratio γ ($= C/A_o$) versus dimensionless time, for consecutive reaction steps (1,2) with second step reversible (3); all first-order; continuous stirred-tank reactor; $\kappa_1 = k_2/k_1$; $\kappa_2 = ck_3/b'k_1$.

MUB-1548

For given values of κ_1 and κ_2, as the complete reaction of A is approached, it takes about four times longer to reach any given proportion of C in a CSTR as in a plug-flow reactor.

Since simple relations, Eqs. (38) and (40), are available for α as a function of τ, graphs only of γ versus τ are given for this reaction model.

B. Model 2

We now consider an all-first-order model where the first reaction step is reversible:

$$\text{Mechanism}\begin{cases} A \underset{k_3}{\overset{k_1}{\rightleftarrows}} B \\ B \xrightarrow{k_2} C \end{cases} \qquad \text{General stoichiometry}\begin{cases} aA \underset{k_3}{\overset{k_1}{\rightleftarrows}} bB \\ b'B \xrightarrow{k_2} cC \end{cases}$$

In this reaction all of A is ultimately converted to C. The rate equations are

$$dA/dt = -k_1A + k_3B, \tag{41}$$

$$dB/dt = [k_1b/a]A - [k_3b/a]B - k_2B, \tag{42}$$

and

$$dC/dt = [k_2c/b']B. \tag{43}$$

In the above rate equations k_1 and k_3 are in terms of A molecules, and k_2 is in terms of B molecules. As in Model 1, we introduce the dimensionless concentrations α, β, and γ, and the dimensionless time, $\tau = k_1 t$:

$$d\alpha/d\tau = -\alpha + \kappa_1\beta, \tag{44}$$

$$d\beta/d\tau = -\kappa_1\beta - \kappa_2\beta + \alpha, \tag{45}$$

and

$$d\gamma/d\tau = \kappa_2\beta, \tag{46}$$

where $\kappa_1 = bk_3/ak_1$ and $\kappa_2 = k_2/k_1$.

The above equations have been solved for the <u>plug-flow</u> case with the following results:[3]

$$\alpha = \frac{\lambda_2 - \kappa_2}{\lambda_2(\lambda_2-\lambda_3)} \, e^{-\lambda_2 \tau} + \frac{\kappa_2 - \lambda_3}{\lambda_3(\lambda_2-\lambda_3)} \, e^{-\lambda_3 \tau} , \tag{47}$$

and

$$\beta = \frac{1}{\lambda_2 - \lambda_3} \left[e^{-\lambda_3 \tau} - e^{-\lambda_2 \tau} \right] \tag{48}$$

where

$$\lambda_2 = \frac{1 + \kappa_1 + \kappa_2 + [(1+\kappa_1+\kappa_2)^2 - 4\,\kappa_2]^{1/2}}{2} ,$$

and

$$\lambda_3 = \frac{1 + \kappa_1 + \kappa_2 - [(1+\kappa_1+\kappa_2)^2 - 4\,\kappa_2]^{1/2}}{2}$$

Figures 11A and 11B are graphs of α versus τ, and Figs. 12A and 12B show γ as a function of τ.

By material balance, the general equations for the continuous stirred-tank reactor (as first derived in the present study) are

$$\alpha_n = \frac{\alpha_{n-1} + \kappa_2 \beta_n \bar{\tau}}{1 + \bar{\tau}} , \tag{49}$$

and

$$\beta_n = \frac{\beta_{n-1} (1 + \bar{\tau}) + \alpha_{n-1} \bar{\tau}}{(1+\bar{\tau}) \left[1 - \frac{\kappa_2 \bar{\tau}^2}{1+\bar{\tau}} + (\kappa_1+\kappa_2)\bar{\tau} \right]} \tag{50}$$

The computations for the CSTR are based on having the feed to the reactor entirely A, so that $\alpha_{n-1} = 1.0$ and $\beta_{n-1} = 0$. Figures 13A and 13B present graphs of α versus τ, and Figs. 14A and 14B are graphs of γ versus τ.

At a given conversion of A, the continuous stirred-tank reactor favors production of final product C, compared to the plug-flow reactor. Of course the time to reach a given conversion in a CSTR is much greater than for a plug-flow reactor.

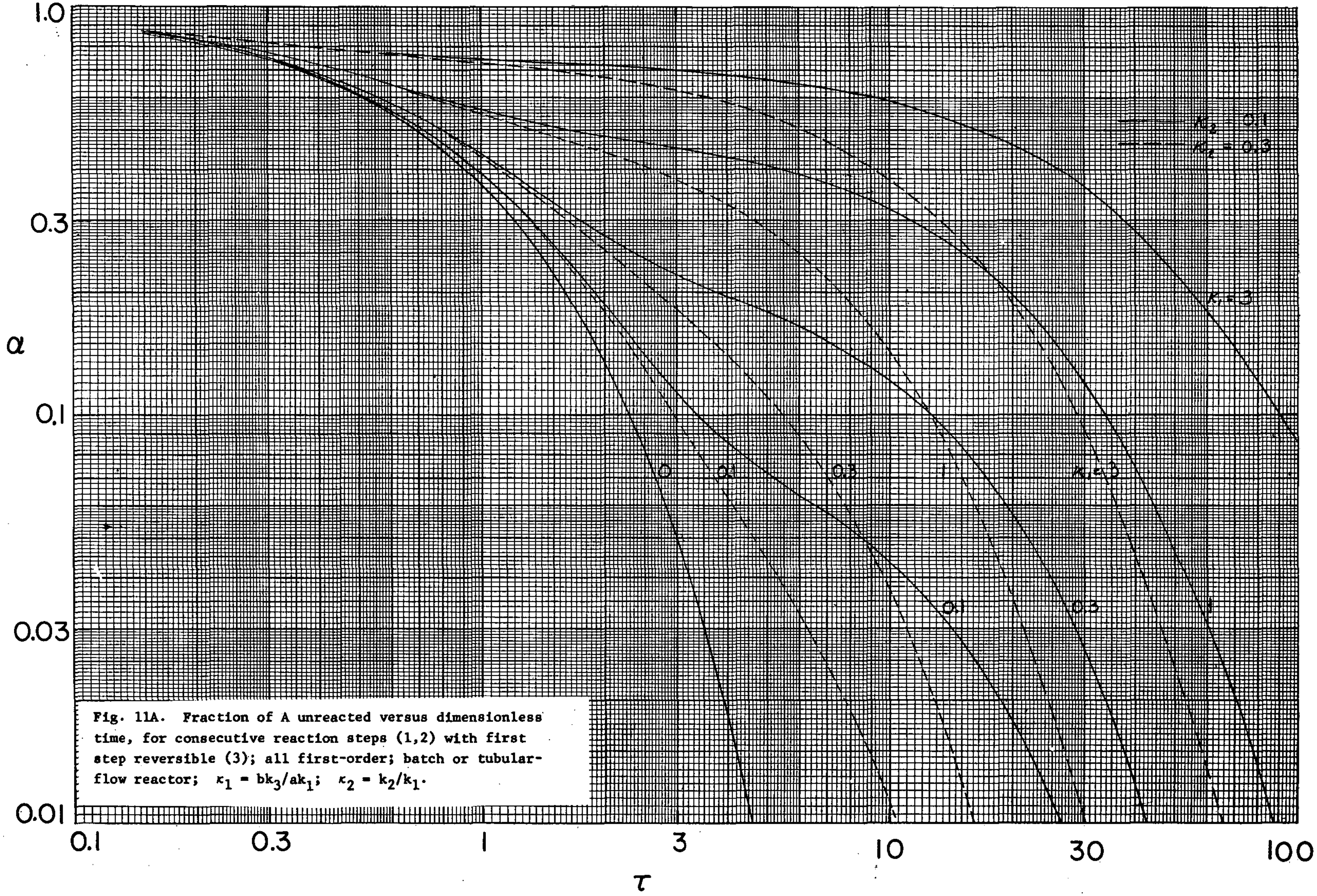


Fig. 11A. Fraction of A unreacted versus dimensionless time, for consecutive reaction steps (1,2) with first step reversible (3); all first-order; batch or tubular-flow reactor; $\kappa_1 = bk_3/ak_1$; $\kappa_2 = k_2/k_1$.

MUB-1547

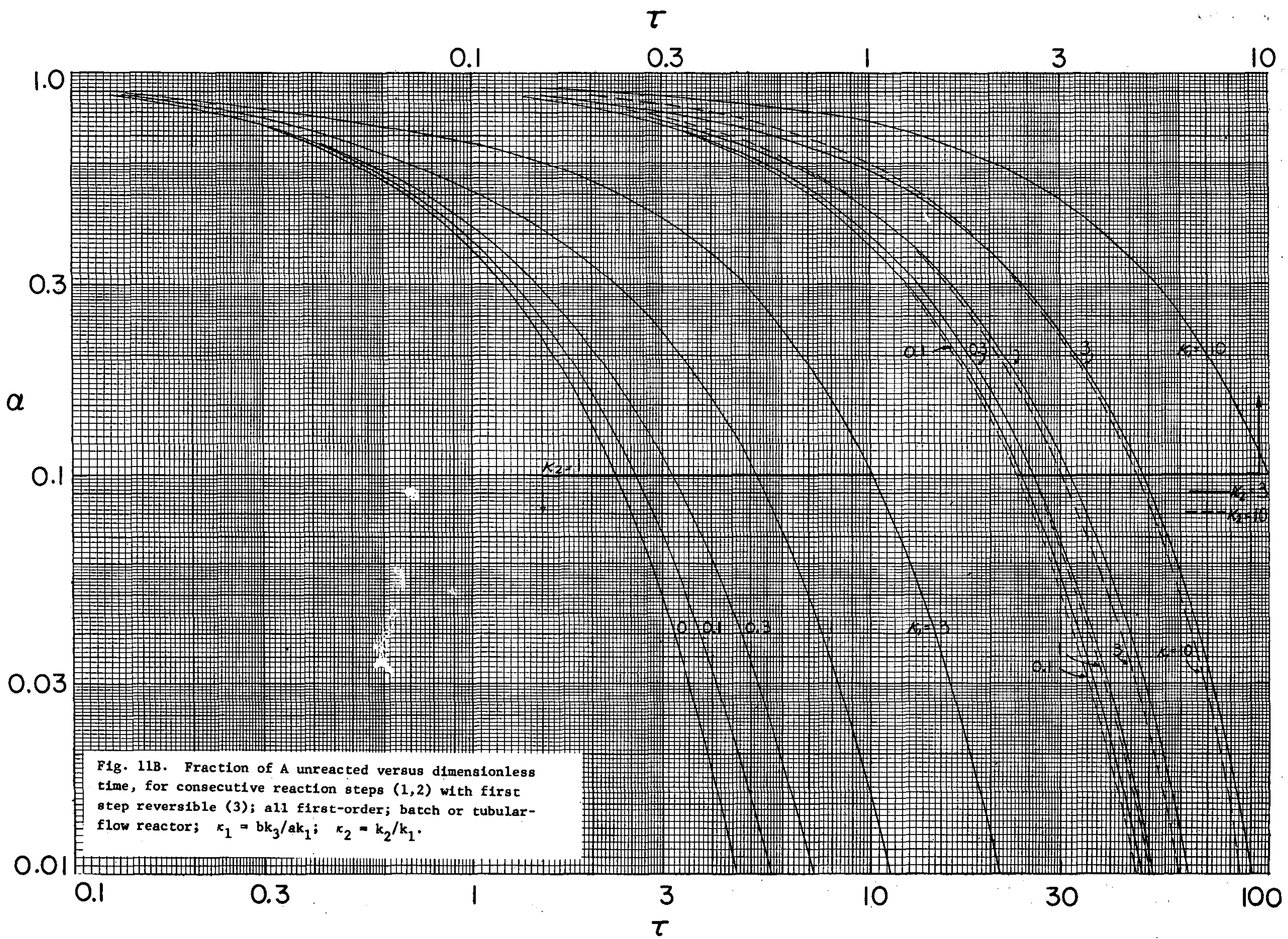


Fig. 11B. Fraction of A unreacted versus dimensionless time, for consecutive reaction steps (1,2) with first step reversible (3); all first-order; batch or tubular-flow reactor; $\kappa_1 = bk_3/ak_1$; $\kappa_2 = k_2/k_1$.

MUB-1546

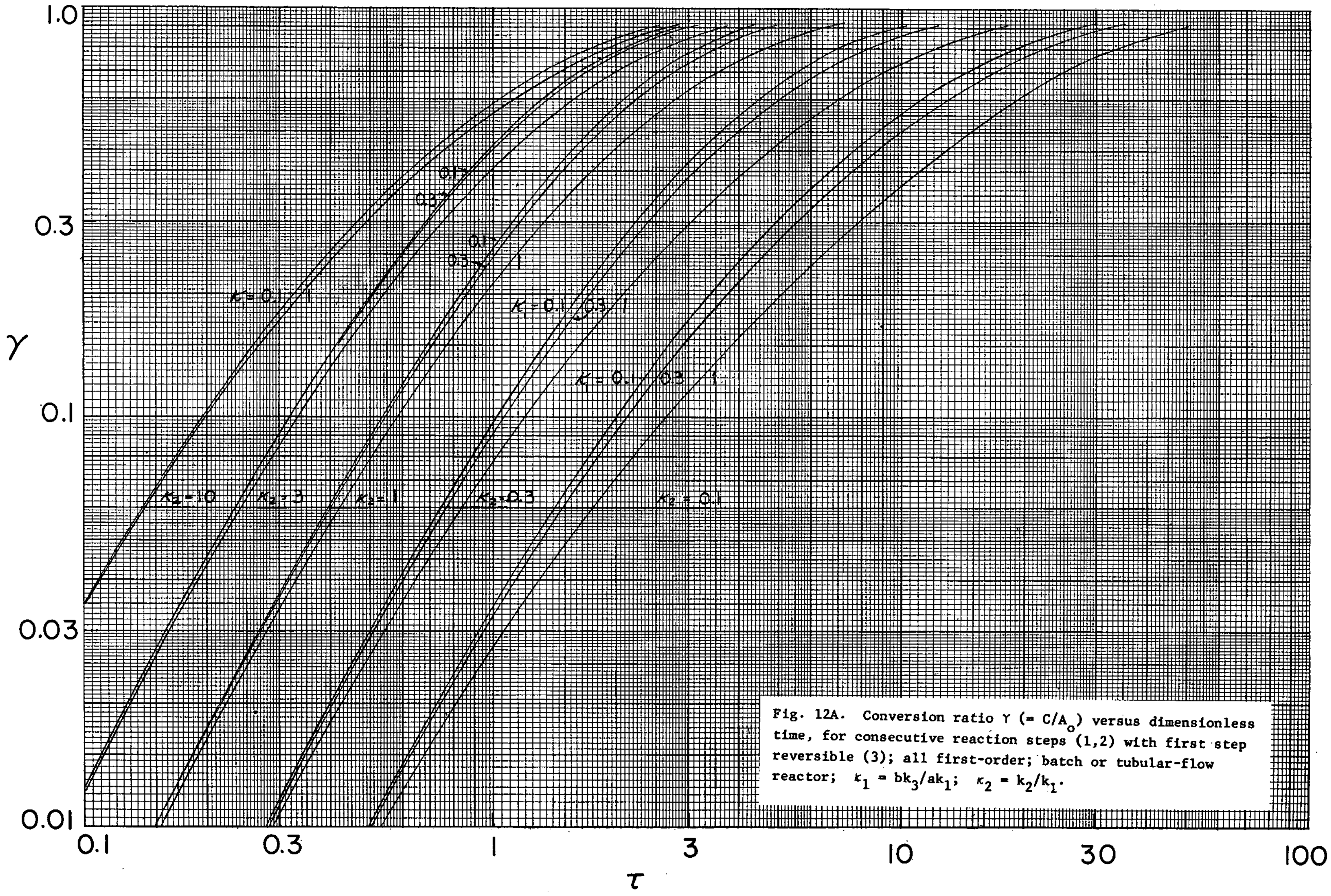


Fig. 12A. Conversion ratio γ (= C/A_o) versus dimensionless time, for consecutive reaction steps (1,2) with first step reversible (3); all first-order; batch or tubular-flow reactor; $\kappa_1 = bk_3/ak_1$; $\kappa_2 = k_2/k_1$.

MUB-1545

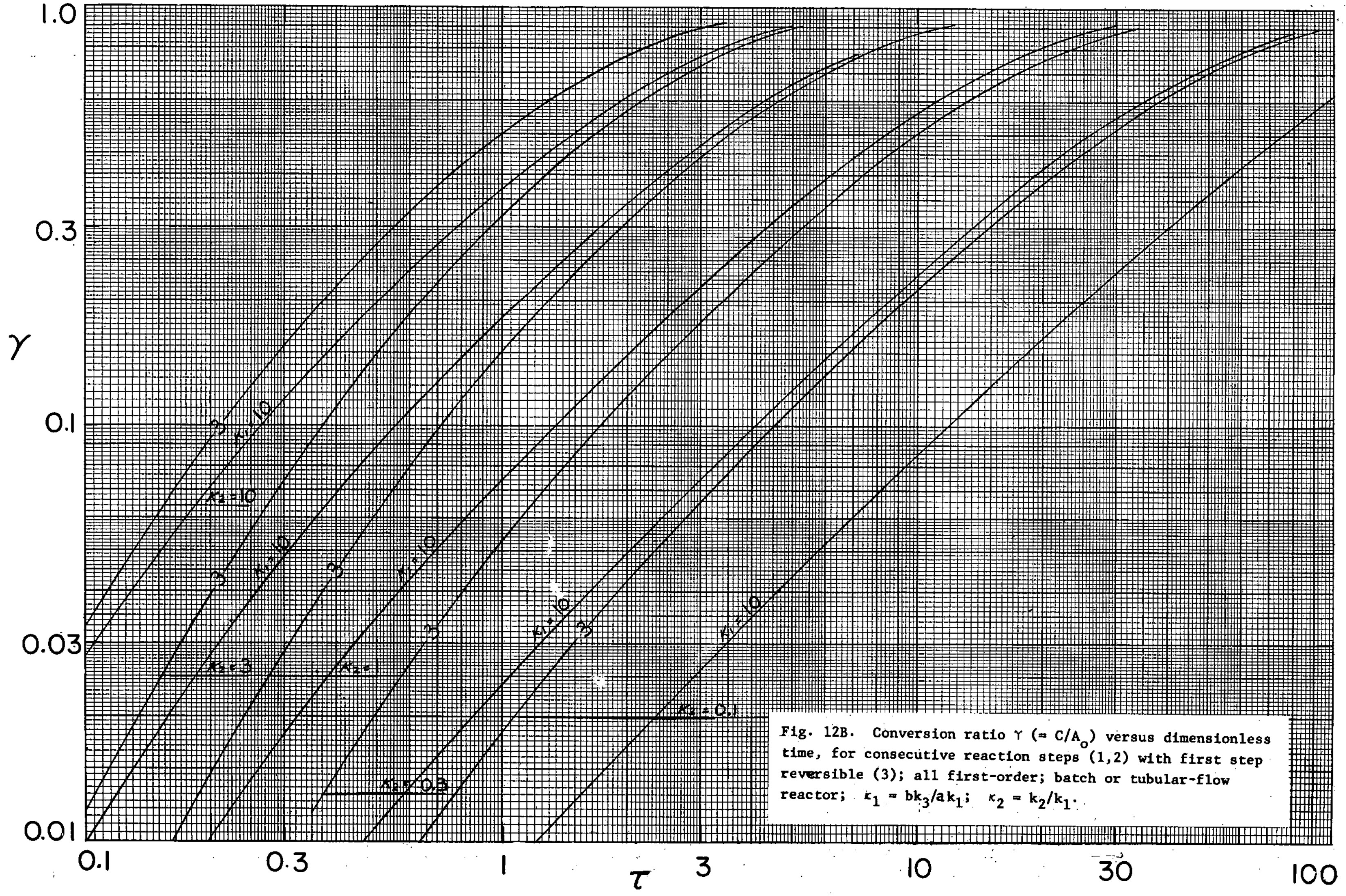


Fig. 12B. Conversion ratio Υ (= C/A_o) versus dimensionless time, for consecutive reaction steps (1,2) with first step reversible (3); all first-order; batch or tubular-flow reactor; $\kappa_1 = bk_3/ak_1$; $\kappa_2 = k_2/k_1$.

MUB-1544

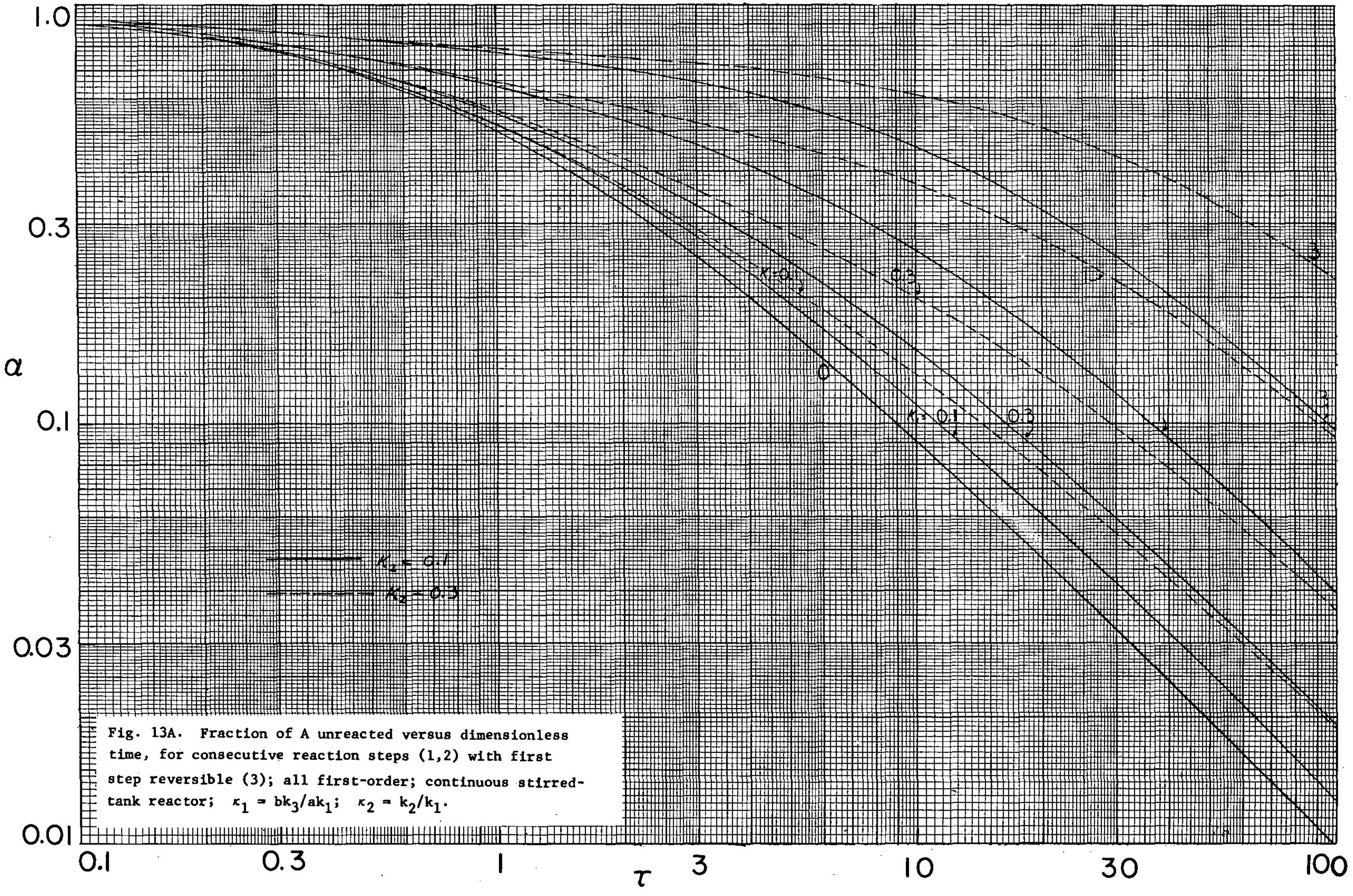


Fig. 13A. Fraction of A unreacted versus dimensionless time, for consecutive reaction steps (1,2) with first step reversible (3); all first-order; continuous stirred-tank reactor; $\kappa_1 = bk_3/ak_1$; $\kappa_2 = k_2/k_1$.

MUB-1543

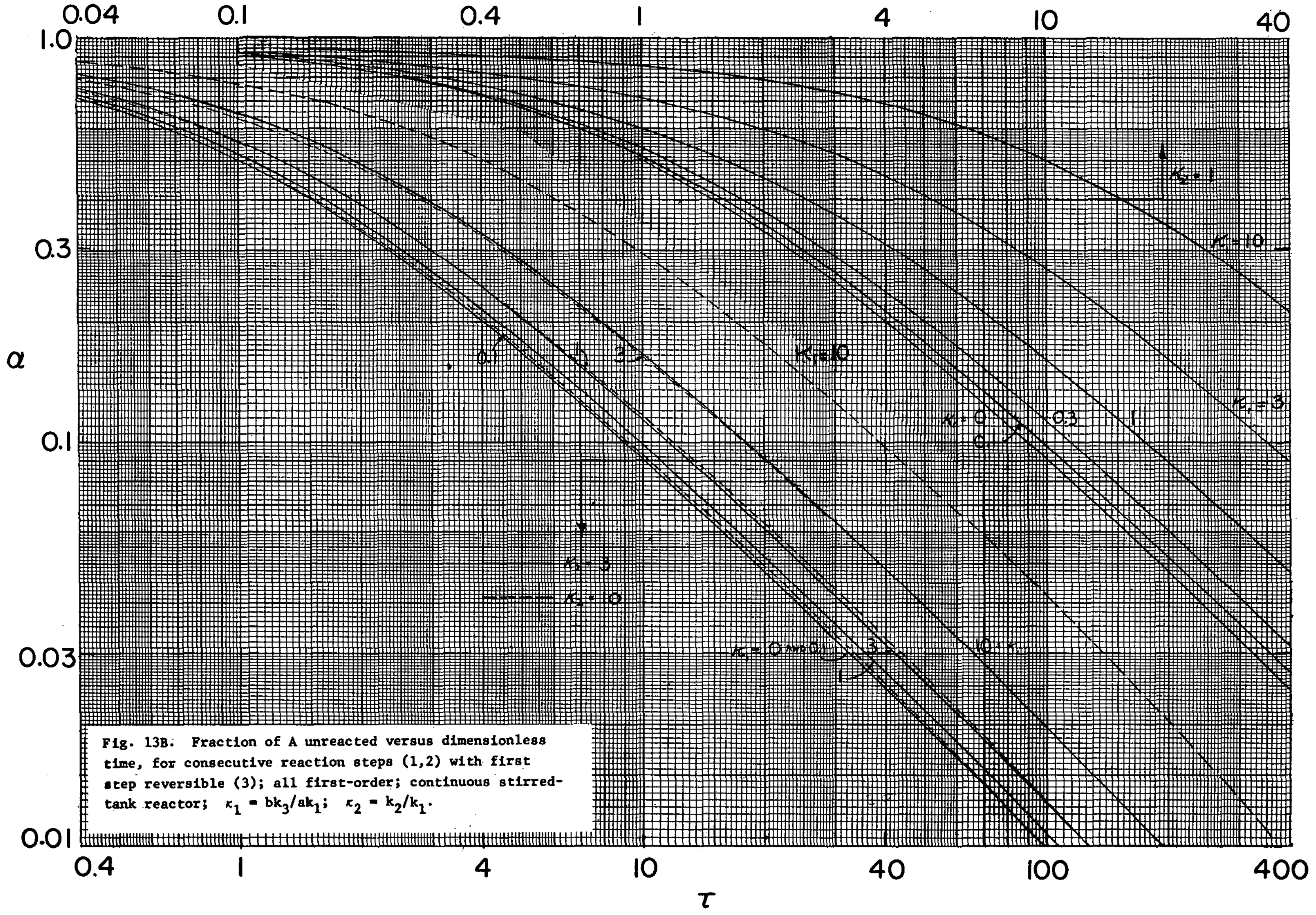


Fig. 13B. Fraction of A unreacted versus dimensionless time, for consecutive reaction steps (1,2) with first step reversible (3); all first-order; continuous stirred-tank reactor; $\kappa_1 = bk_3/ak_1$; $\kappa_2 = k_2/k_1$.

MUB-1542

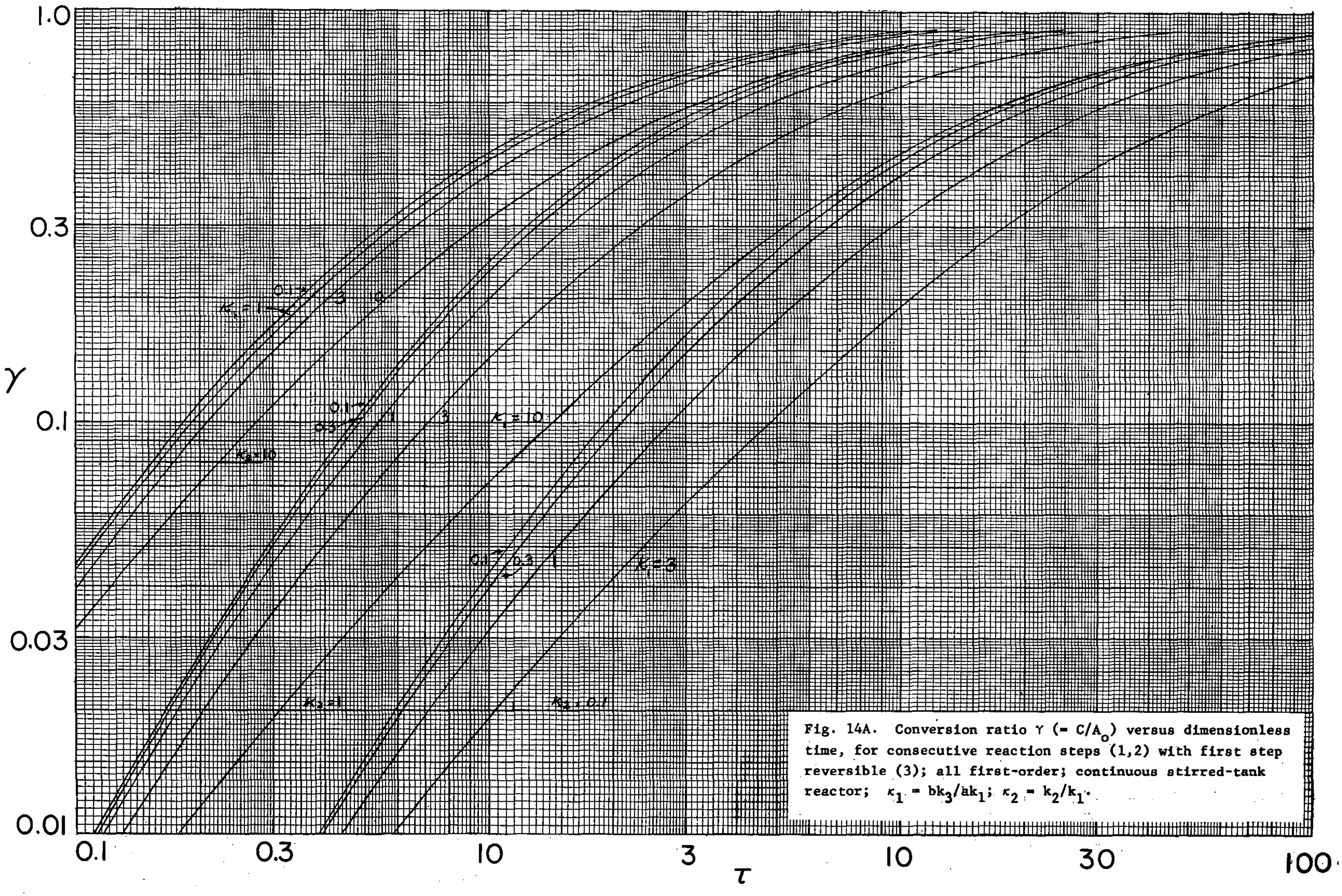


Fig. 14A. Conversion ratio γ (= C/A_0) versus dimensionless time, for consecutive reaction steps (1,2) with first step reversible (3); all first-order; continuous stirred-tank reactor; $\kappa_1 = bk_3/ak_1$; $\kappa_2 = k_2/k_1$.

MUB-1541

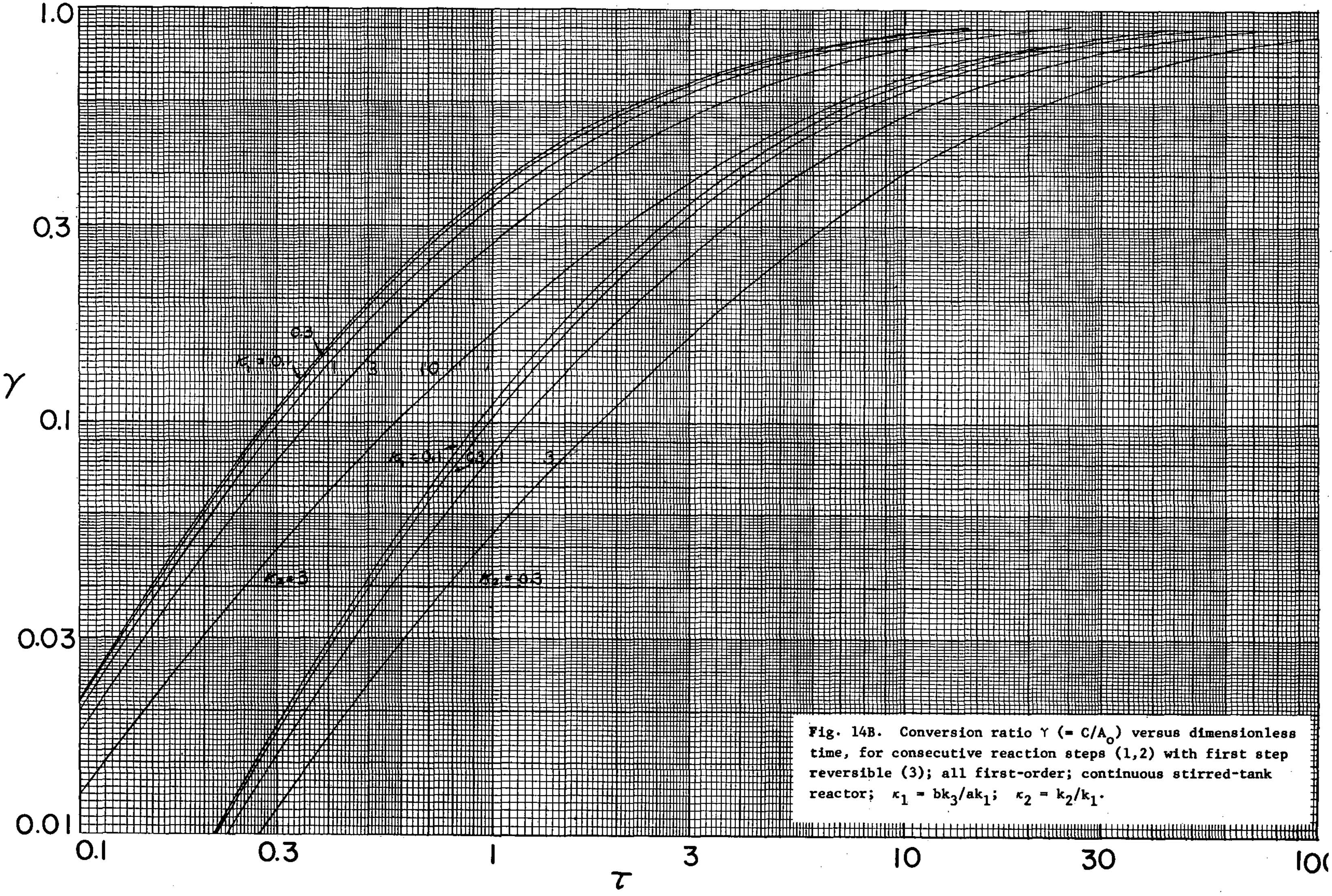


Fig. 14B. Conversion ratio Υ (= C/A_o) versus dimensionless time, for consecutive reaction steps (1,2) with first step reversible (3); all first-order; continuous stirred-tank reactor; $\kappa_1 = bk_3/ak_1$; $\kappa_2 = k_2/k_1$.

MUB-1540

C. Model 3

We next consider a more complicated case in which one of the reaction steps is second-order.

$$\text{Mechanism}\begin{cases} A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} 2B \\ B \xrightarrow{k_2} C \end{cases} \qquad \text{General stoichiometry}\begin{cases} aA \underset{k_3}{\overset{k_1}{\rightleftharpoons}} bB \\ b'B \xrightarrow{k_2} cC \end{cases} .$$

This reaction is the same as Model 2 except that the reverse step is second-order. As an example, this reaction model corresponds to a biologically important reaction in which glucose forms lactic acid as the intermediate and carbon dioxide as the final product.

1. Plug-flow or Batch Reactors

a. Equations. The rate equations based on the general stoichiometry are

$$dA/dt = k_3B^2 - k_1A, \tag{51}$$

$$dB/dt = [k_1b/a]\ A - [k_3b/a]\ B^2 - k_2B\ , \tag{52}$$

and

$$dC/dt = [k_2c/b']\ B, \tag{53}$$

where k_1 and k_3 are in terms of A molecules, and k_2 is in terms of B molecules. By introducing the dimensionless concentrations and dimensionless time, $\tau = k_1t$, we obtain

$$d\alpha/d\tau = \kappa_1\beta^2 - \alpha\ , \tag{54}$$

$$d\beta/d\tau = \alpha - \kappa_1\beta^2 - \kappa_2\beta\ , \tag{55}$$

and

$$d\gamma/d\tau = \kappa_2\beta\ , \tag{56}$$

where

$$\kappa_1 = b^2A_ok_3/a^2k_1\ ,$$

and

$$\kappa_2 = k_2/k_1\ ,$$

and α, β, and γ are defined by Eqs. (24), (25), and (26), respectively. Differentiating Eq. (55) with respect to τ, we have

$$\frac{d^2\beta}{d\tau^2} = \frac{d\alpha}{d\tau} - \kappa_2 \frac{d\beta}{d\tau} - 2\kappa_1\beta \frac{d\beta}{d\tau} . \tag{57}$$

Substituting for $d\alpha/d\tau$ from Eq. (54) we obtain

$$\frac{d^2\beta}{d\tau^2} = \kappa_1\beta^2 - \alpha - \kappa_2 \frac{d\beta}{d\tau} - 2\kappa_1\beta \frac{d\beta}{d\tau} . \tag{58}$$

After solving Eq. (55) for α and substituting for α in Eq. (58), we have

$$\frac{d^2\beta}{d\tau^2} + (1 + \kappa_2 + 2\kappa_1\beta) \frac{d\beta}{d\tau} + \kappa_2\beta = 0 . \tag{59}$$

Thus a differential equation in terms of just one dependent variable is obtained. It appears that this nonlinear equation can be solved only by an approximation method or by a numerical method.

b. Calculations. In this work Eqs. (54) and (55) are solved simultaneously by using a fourth-order Runge-Kutta method (due to Kutta)[8] on the IBM 7090 Computer.

The fourth-order Runge-Kutta method approximates the integral curve to fourth-order accuracy; the truncation error for a single interval is proportional to the fifth power of interval spacing. There are no errors in the coefficients up to the fourth-order. By contrast to some alternative methods, the evaluation of derivatives is not required. Also, the method does not require the use of function values at preceding times. A change in spacing can be easily made at any intermediate stage of the calculations. A description of how the Runge-Kutta method works along with a brief outline of the derivation of the coefficients which give fourth-order accuracy is given in the Appendix.

Values of α and β were calculated as a function of τ, and γ was obtained by material balance. Also, by linear interpolation of all the results, values of α and τ were obtained for values of γ in increments of 0.05 to $\gamma = 0.9$, and β was obtained by material balance.

c. Estimated Error. A small value of the spacing, $\Delta\tau$, is required both to minimize the culmulative truncation error and to maintain stability in the calculations. The value of $\Delta\tau$ was automatically decreased in the program until the calculations were stable.

The total truncation error is dependent on the size of $\Delta\tau$, the total τ, and the form of the function. To estimate the error in the Runge-Kutta method for Model 3, the analogous all-first-order reaction (Model 2) was solved analytically [using Eqs. (47) and (48)] and also numerically by the Runge-Kutta method. The total error in τ for Model 2 is less than 0.51% for the case which requires the longest time to reach a value of $\gamma = 0.9$. This error is probably all truncation error because rounding-off errors do not appear in the final significant figures retained. Since the equations for Model 2 and Model 3 are quite similar, the error computed for Model 2 is believed to be approximately the error for Model 3. The truncation error for Model 3 could not be estimated by performing the calculations at a given $\Delta\tau$ and at one-half the given $\Delta\tau$ because $\Delta\tau$ was continually decreased during the calculations in order to maintain stability.

d. Interpretation of Results for Model 3. Figures 15A and 15B present graphs of α versus τ, and Fig. 16 is a graph of γ as a function of τ. Obviously, the time to react to a given conversion is a function of the three rate coefficients.

At a given k_2/k_1 $(= \kappa_2)$, as k_3/k_1 $(= a^2\kappa_1/b^2A_o)$ is increased, the dimensionless time τ increases for a given conversion of reactant. This results because the rate for the reverse reaction of the first step is increased relative to that of the second reaction step.

Also, for a given set of rate coefficients, increasing the initial concentration of reactant A_o tends to increase τ for any given conversion because the reverse reaction of the first step is second-order. At higher values of A_o, the fractional conversion of A to B will be slower because of the increasing influence of the second-order back reaction (B → A). Moreover, the concentration of intermediate B at a

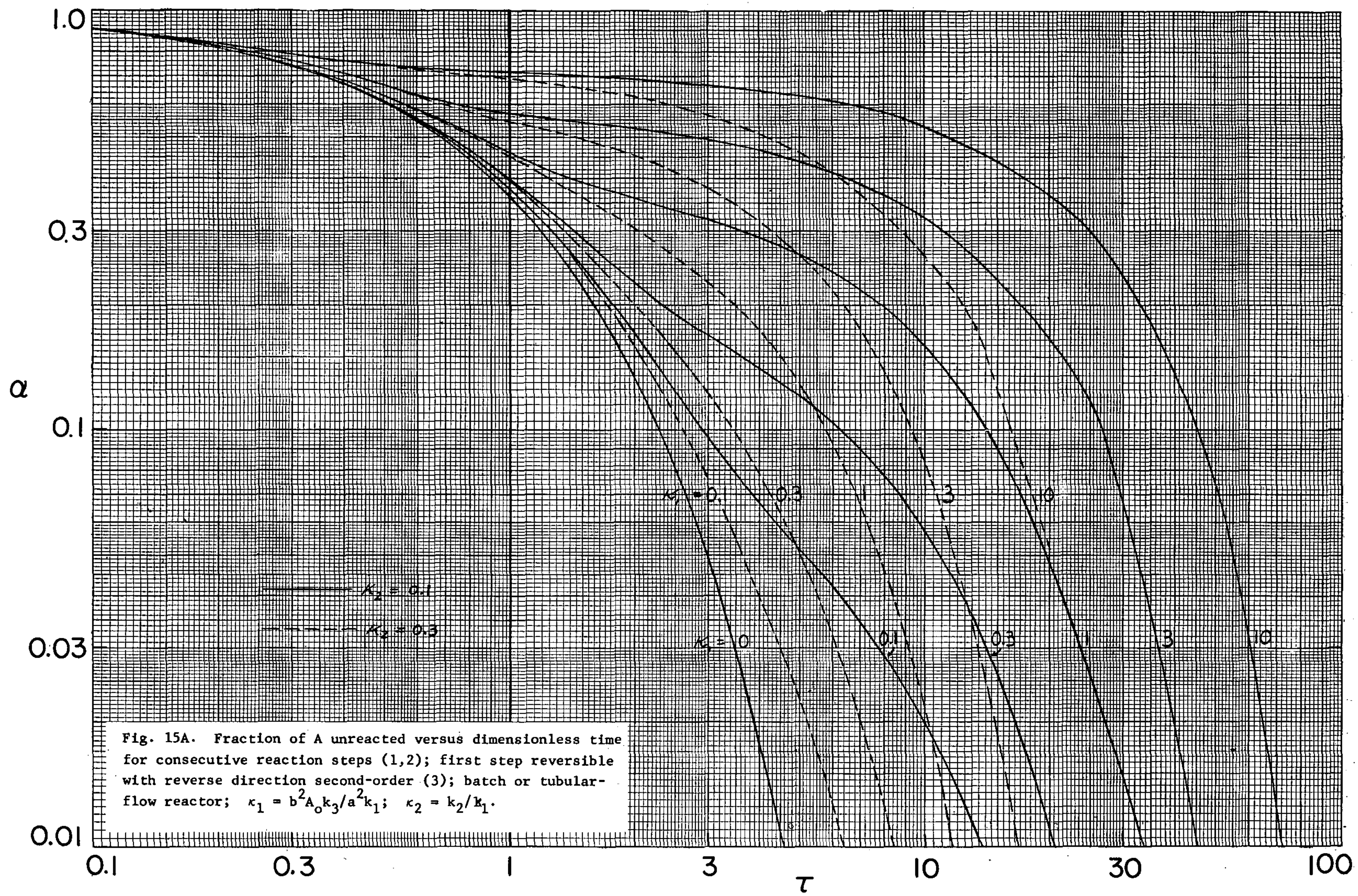


Fig. 15A. Fraction of A unreacted versus dimensionless time for consecutive reaction steps (1,2); first step reversible with reverse direction second-order (3); batch or tubular-flow reactor; $\kappa_1 = b^2 A_o k_3 / a^2 k_1$; $\kappa_2 = k_2/k_1$.

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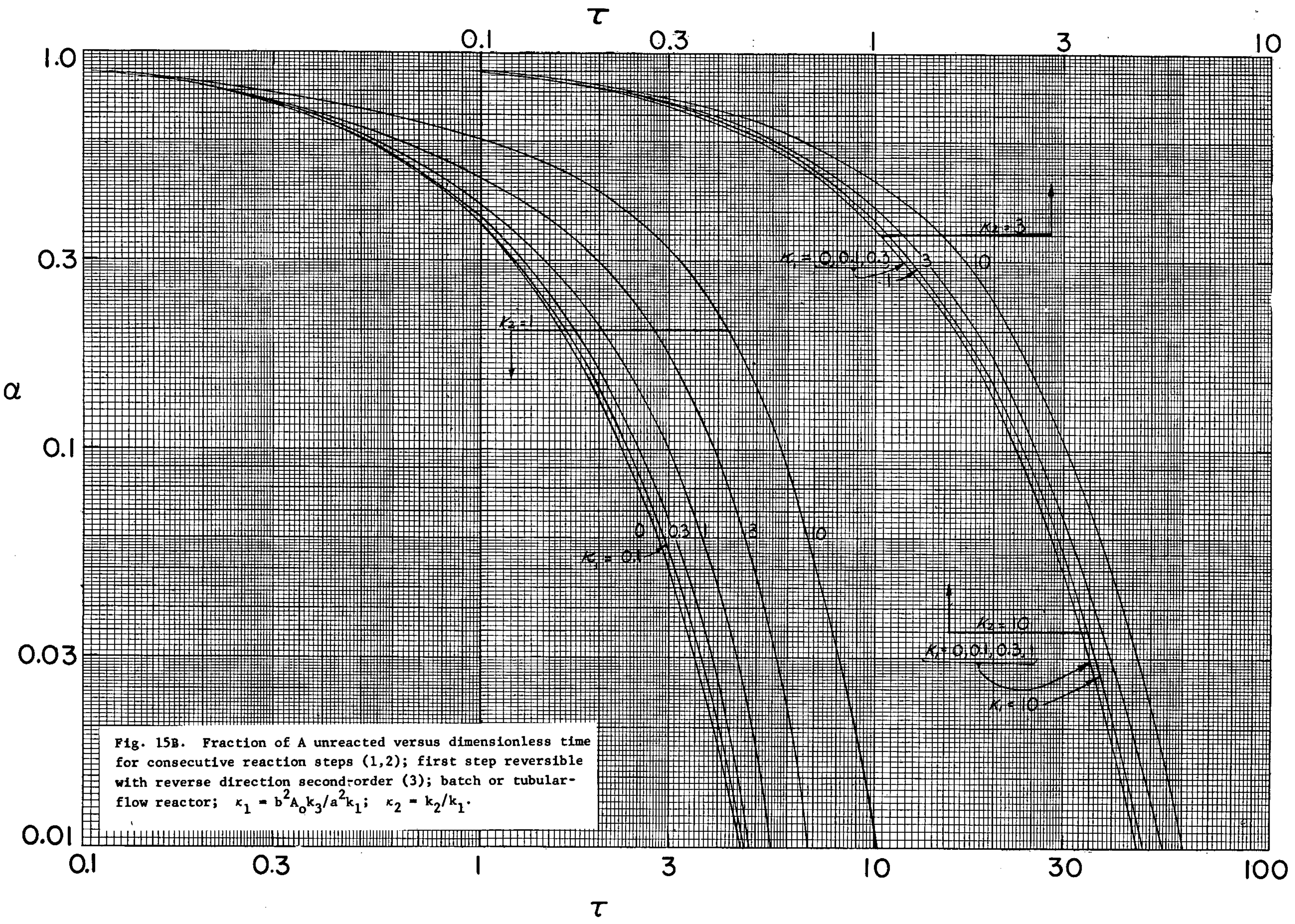

Fig. 15B. Fraction of A unreacted versus dimensionless time for consecutive reaction steps (1,2); first step reversible with reverse direction second-order (3); batch or tubular-flow reactor; $\kappa_1 = b^2A_0k_3/a^2k_1$; $\kappa_2 = k_2/k_1$.

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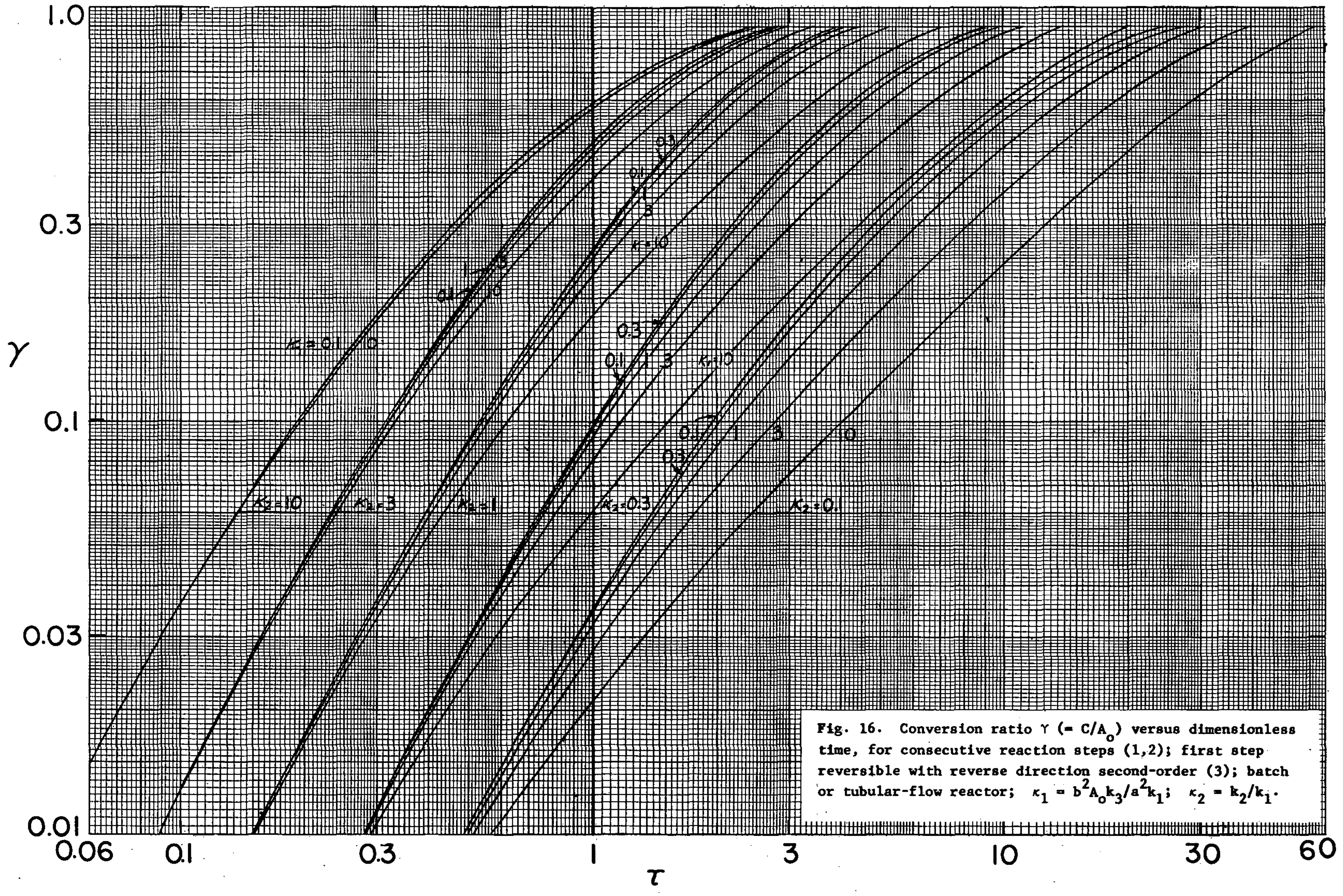

Fig. 16. Conversion ratio γ (= C/A_o) versus dimensionless time, for consecutive reaction steps (1,2); first step reversible with reverse direction second-order (3); batch or tubular-flow reactor; $\kappa_1 = b^2A_ok_3/a^2k_1$; $\kappa_2 = k_2/k_1$.

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given α is not directly proportional to A_o; thus, this lower relative concentration of B results in a slower second step (B → C).

All the cases for various values of the three rate coefficients are between the following reaction limits:

$$A \underset{k_3}{\overset{k_1}{\rightleftharpoons}} 2B$$

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \ .$$

For the first limit (where $k_2 = 0$), A_o has a pronounced effect on the time to react to a given conversion. At the second limit (where $k_3 = 0$), A_o has no effect on the time-conversion relationship.

This decrease in rate of conversion with higher values of A_o is seen from the graphs of α versus τ with parameters of κ_1, from Eq. (54) where the parameter κ_1 appears in the positive term, and from the fact that κ_1 is directly proportional to A_o.

e. Comparison of Model 2 and Model 3. In Model 2, all the reaction steps are first-order; thus the rate of conversion of A is independent of the initial concentration of reactant, A_o. Also, the values of α, β, and γ are independent of A_o. However, in Model 3 the time to react to a given conversion is a function of A_o as discussed above; therefore, at a given time, the values of α, β, and γ are dependent upon A_o. The yield ratio of intermediate B to final product C depends upon A_o at a given set of rate coefficients and elapsed time for Model 3 only.

As seen from the α versus τ graphs, the conversion $(1-\alpha)$ for Model 3 is greater than it is for Model 2 at the same values of κ_1, κ_2, and τ. However, for Model 3 the parameter κ_1 is a function of A_o, whereas for Model 2 it is not. If the value of A_o for Model 3 is increased, the value of κ_1 is proportionately increased, and the conversion is decreased at given rate coefficients and any time. Thus, the time to react to a given conversion for Model 3 may be greater than or less than that for Model 2 depending upon the value of A_o in Model 3.

2. Continuous Stirred-Tank Reactor (CSTR)

By material balance we obtain the general equations for the CSTR:

$$\alpha_{n-1} - \alpha_n = \alpha_n \bar{\tau}_n - \kappa_1 \beta_n^2 \bar{\tau}_n , \tag{60}$$

and

$$\beta_{n-1} - \beta_n = \kappa_2 \beta_n \bar{\tau}_n + \kappa_1 \beta_n^2 \bar{\tau}_n = \alpha_n \bar{\tau}_n . \tag{61}$$

The above equations are the counterparts of Eqs. (54) and (55), respectively. Solving Eq. (60) for α_n we have

$$\alpha_n = \frac{\alpha_{n-1} + \kappa_1 \beta_n^2 \bar{\tau}_n}{1 + \bar{\tau}_n} . \tag{62}$$

Substituting for α_n in Eq. (61) and solving for β_n we obtain

$$\beta_n = \frac{-(\kappa_2 \bar{\tau}_n + 1) + \left[(\kappa_2 \tau_n + 1)^2 \; \frac{4\kappa_1 \bar{\tau}_n}{1 + \bar{\tau}_n} \left(\beta_{n-1} + \frac{\alpha_{n-1} \bar{\tau}_n}{1 + \bar{\tau}_n} \right) \right]^{1/2}}{\frac{2 \kappa_1 \bar{\tau}_n}{1 + \bar{\tau}_n}} \tag{63}$$

Equations (62) and (63) may be applied to the case of any number of tanks in series. For a single CSTR with all the feed consisting of reactant A, $\alpha_{n-1} = 1.0$ and $\beta_{n-1} = 0$. Figures 17A and 17B are graphs of α versus τ, and Fig. 18 is a graph of γ as a function of τ. The factors influencing the conversion time are directionally the same as for the plug-flow case.

3. Evaluation of Rate Coefficients

The rate coefficients can be evaluated from experimental data by using the time-ratio method. Because there are three rate coefficients (two ratios of rate coefficients), two independent time ratios are required. These time ratios are used to evaluate κ_1 and κ_2. Additionally, we measure the time to obtain a given conversion to evaluate the rate coefficient for the forward reaction of the first step.

Figure 19 shows the ratio of times at $\alpha = 0.35$ and $\alpha = 0.7$, and Fig. 20 is a graph of the ratio of times at $\gamma = 0.5$ and $\gamma = 0.05$, as functions of κ_1 and κ_2. Figure 21 is a graph of τ at $\alpha = 0.35$ as a function of

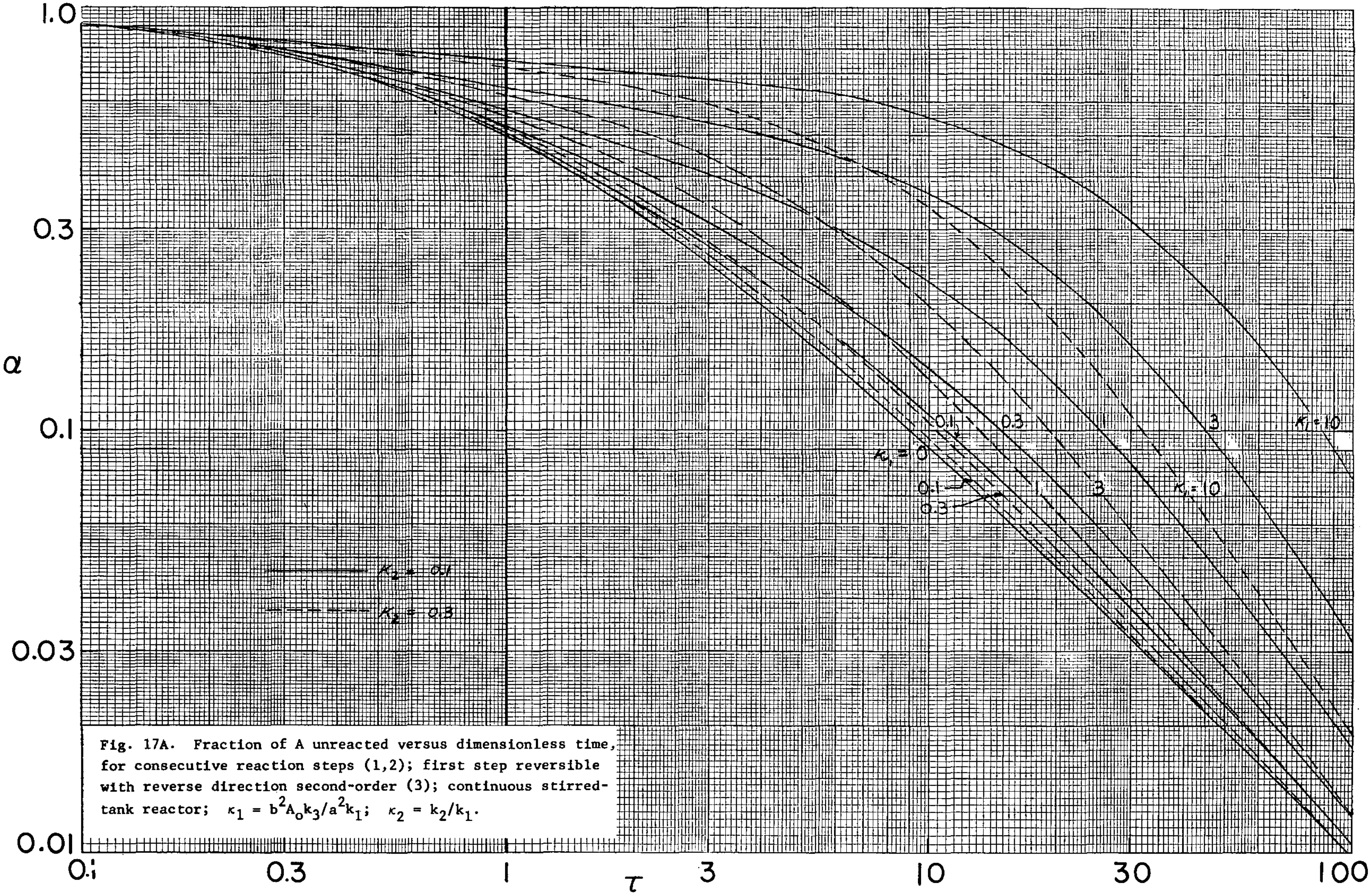

Fig. 17A. Fraction of A unreacted versus dimensionless time, for consecutive reaction steps (1,2); first step reversible with reverse direction second-order (3); continuous stirred-tank reactor; $\kappa_1 = b^2A_ok_3/a^2k_1$; $\kappa_2 = k_2/k_1$.

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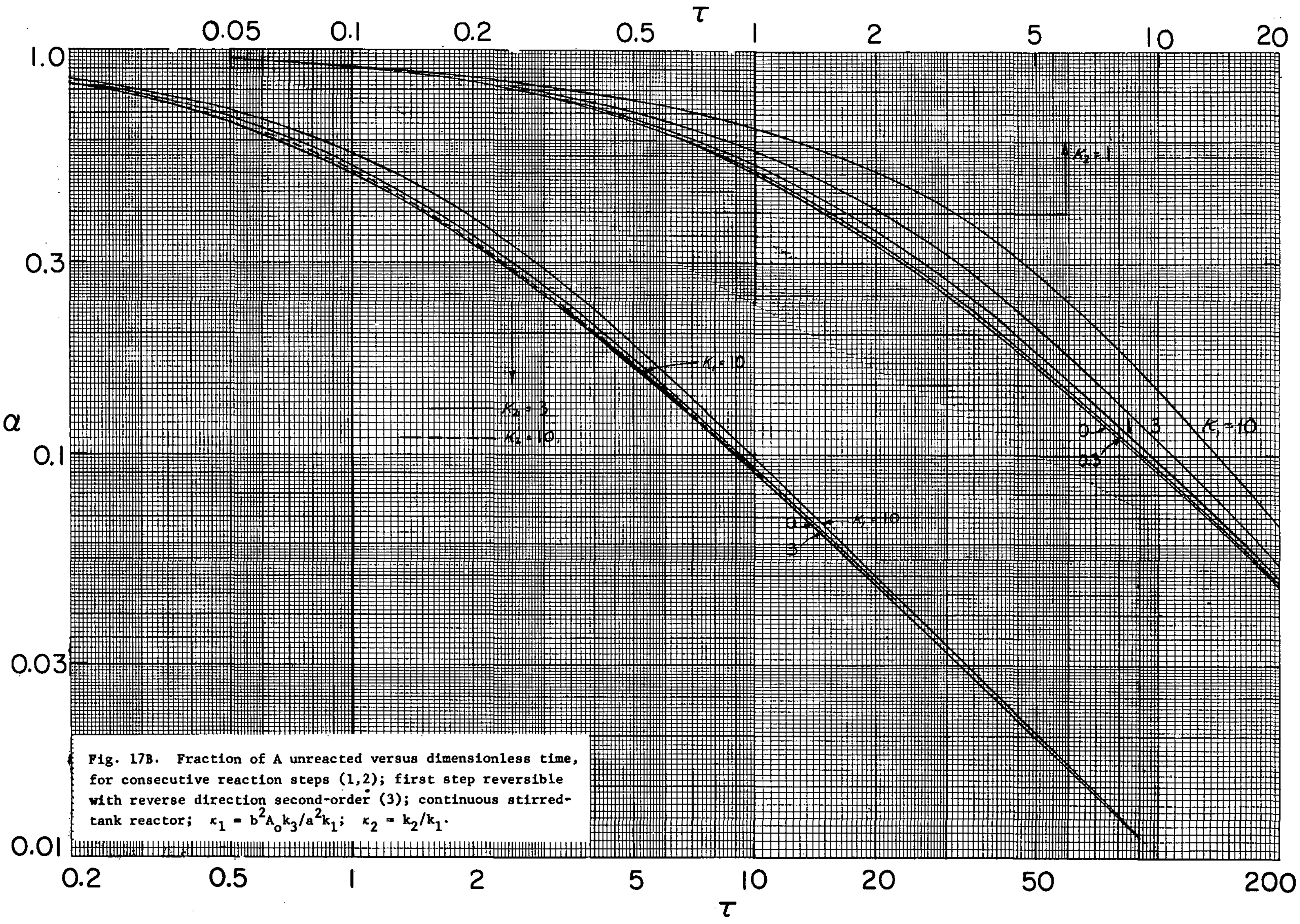

Fig. 17B. Fraction of A unreacted versus dimensionless time, for consecutive reaction steps (1,2); first step reversible with reverse direction second-order (3); continuous stirred-tank reactor; $\kappa_1 = b^2A_0k_3/a^2k_1$; $\kappa_2 = k_2/k_1$.

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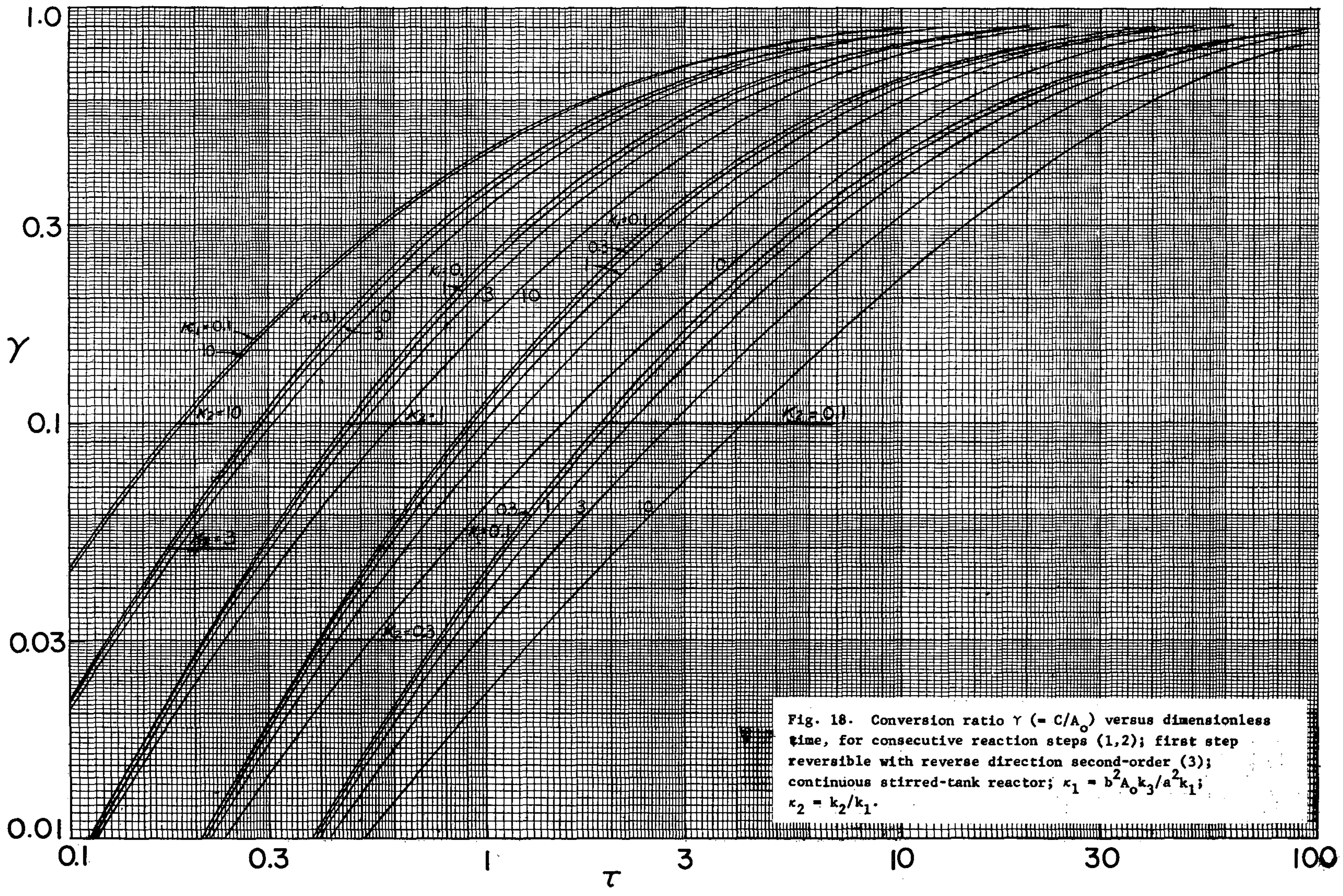

Fig. 18. Conversion ratio Υ (= C/A_o) versus dimensionless time, for consecutive reaction steps (1,2); first step reversible with reverse direction second-order (3); continuous stirred-tank reactor; $\kappa_1 = b^2A_ok_3/a^2k_1$; $\kappa_2 = k_2/k_1$.

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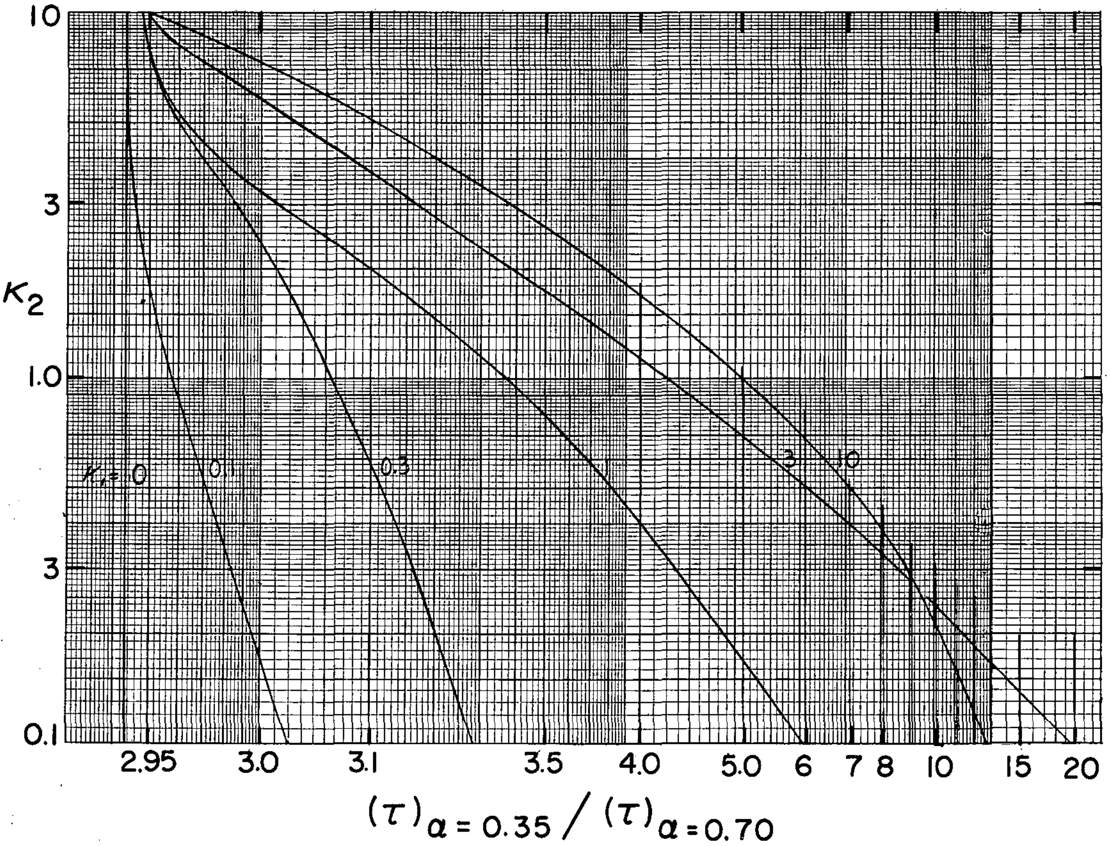

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Fig. 19. Time-ratio plot for given α values, in consecutive-reaction system with two first-order-forward steps and reverse of first step second-order; $\kappa_1 = (b^2 A_0 k_3)/(a^2 k_1)$; $\kappa_2 = k_2/k_1$.

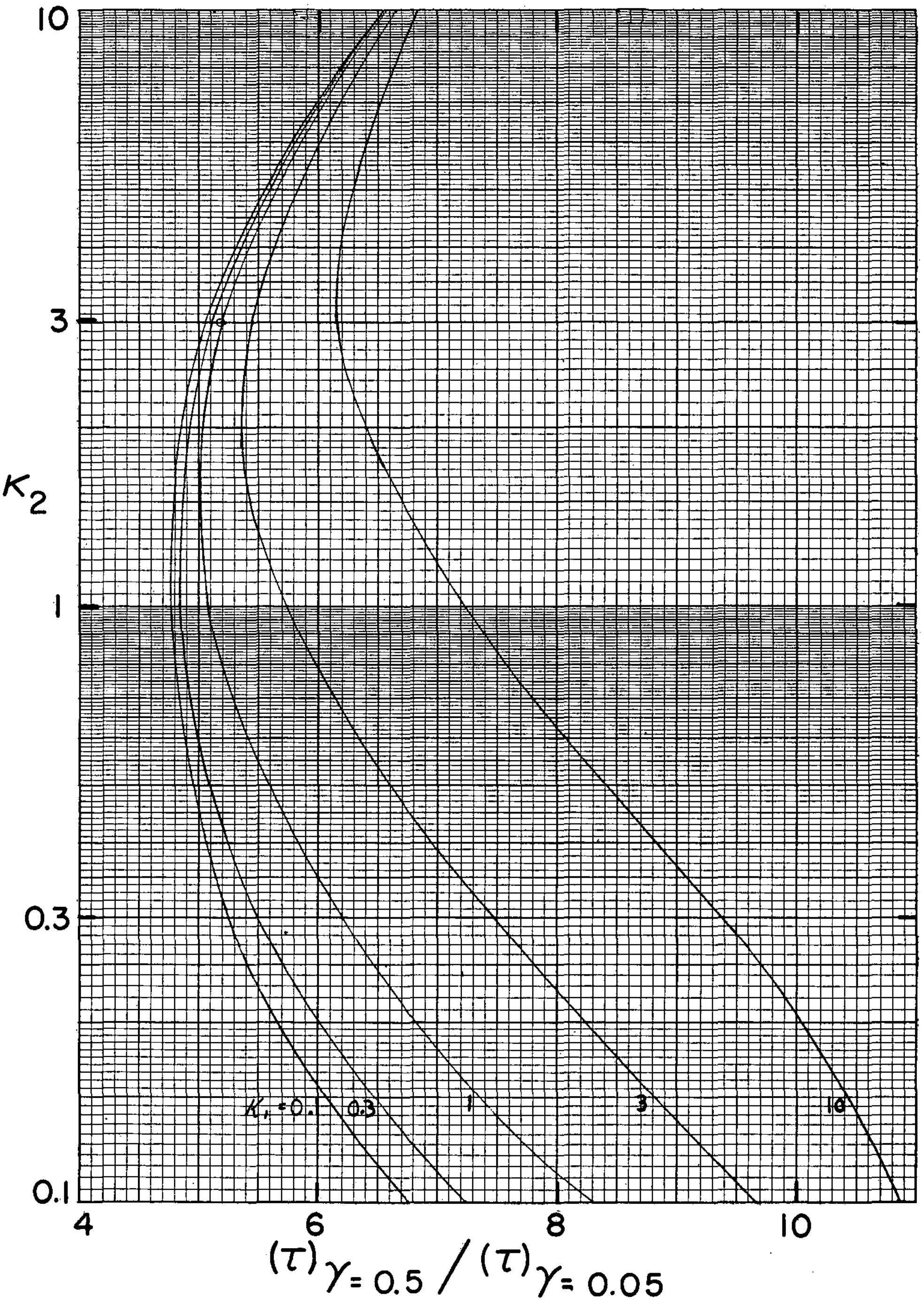

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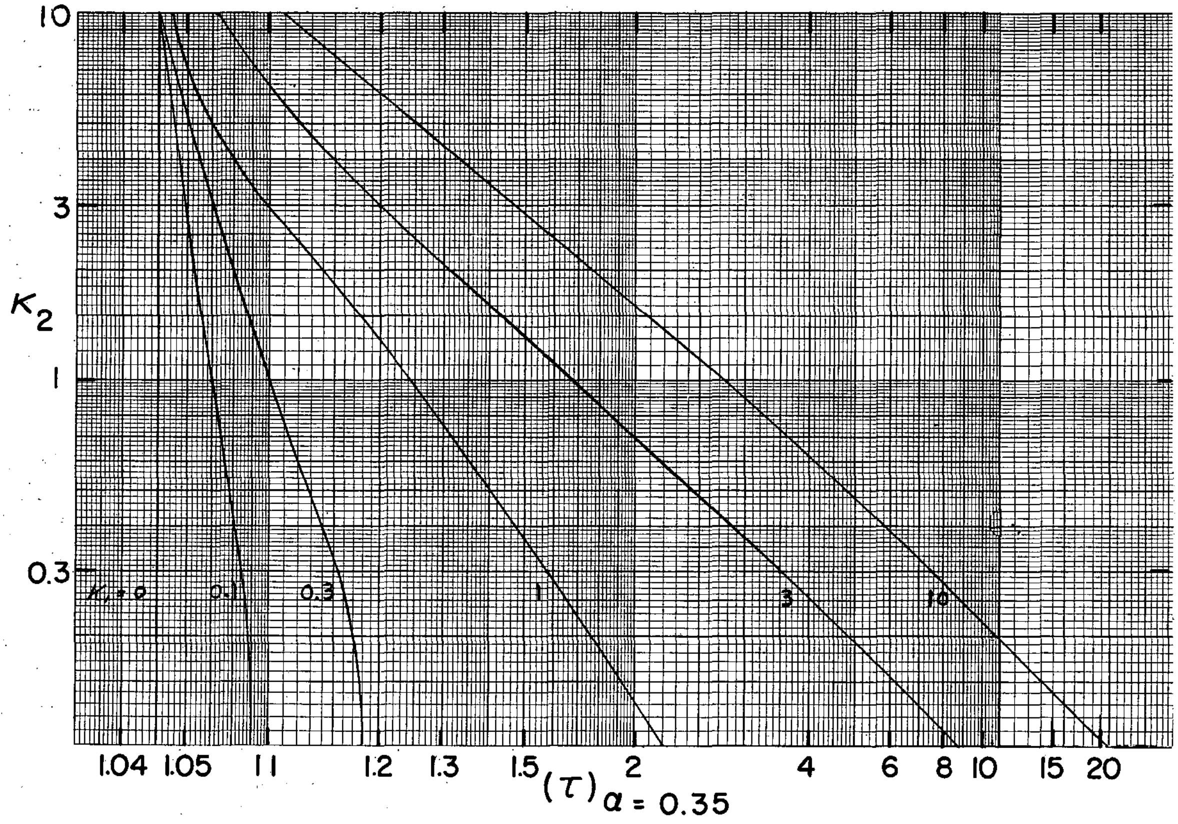
Fig. 20. Time-ratio plot for given γ values, in consecutive reaction system with two first-order forward steps and reverse of first step second-order; $\kappa_1 = (b^2 A_0 k_3)/(a^2 k_1)$; $\kappa_2 = k_2/k_1$.



MUB-1529

Fig. 21. Dimensionless-time plot for 35% of A unreacted, in consecutive reaction system with two first-order forward steps and reverse of first step second-order; $\kappa_1 = (b^2 A_0 k_3)/(a^2 k_1)$; $\kappa_2 = k_2/k_1$.

κ_1 and κ_2. The values of κ_1 and κ_2 which satisfy both time ratios are obtained from Figs. 19 and 20. Knowing κ_1 and κ_2, we obtain τ at $\alpha = 0.35$ from Fig. 21; from this, we calculate

$$k_1 = \left(\frac{\tau}{t}\right)_{\alpha = 0.35}.$$

The remaining rate coefficients are calculated from κ_1 and κ_2.

The rate coefficients can also be evaluated by fitting the data to graphs of computed results; in this way κ_1 and κ_2 are determined, and the rate coefficient for the first forward reaction is computed as above at any selected value of α.

D. Models A-I, A-II, A-III, A-IV, and A-V

Five additional consecutive-reversible reaction models were computed by the Runge-Kutta method (previously described) in the IBM 7090 Computer. The same five values for κ_1 and κ_2 used in previous models are also used here. Tables of results showing dimensionless time and concentrations are given in the Appendix. The following table shows the kinetic mechanism and general stoichiometry for the models, the dimensionless time τ, and the dimensionless parameters κ_1 and κ_2.

Appendix table	Reaction model		τ	κ_1	κ_2
	Kinetic mechanism	Stoichiometry			
A-I	$2A \underset{k_3}{\overset{k_1}{\rightleftharpoons}} B,\ B \xrightarrow{k_2} C$	$aA \rightleftharpoons bB,\ b'B \longrightarrow cC$	$k_1 A_o t$	$bk_3/aA_o k_1$	$k_2/A_o k_1$
A-II	$A \underset{k_3}{\overset{k_1}{\rightleftharpoons}} B,\ 2B \xrightarrow{k_2} C$	$aA \rightleftharpoons bB,\ b'B \longrightarrow cC$	$k_1 t$	bk_3/ak_1	$bA_o k_2/ak_1$
A-III	$A \xrightarrow{k_1} B,\ 2B \underset{k_3}{\overset{k_2}{\rightleftharpoons}} C$	$aA \longrightarrow bB,\ b'B \rightleftharpoons cC$	$k_1 t$	$bA_o k_2/ak_1$	$ck_3/b'k_1$
A-IV	$2A \xrightarrow{k_1} B,\ B \underset{k_3}{\overset{k_2}{\rightleftharpoons}} C$	$aA \longrightarrow bB,\ b'B \rightleftharpoons cC$	$k_1 A_o t$	$k_2/A_o k_1$	$ck_3/b'A_o k_1$
A-V	$A \xrightarrow{k_1} B,\ B \underset{k_3}{\overset{k_2}{\rightleftharpoons}} 2C$	$aA \longrightarrow bB,\ b'B \rightleftharpoons cC$	$k_1 t$	k_2/k_1	$\dfrac{c^2 bA_o k_3}{b'^2 a k_1}$

In Models A-I and A-II, k_1 and k_3 are in terms of A molecules, and k_2 is in terms of B molecules. In Models A-III, A-IV, and A-V, k_1 is in terms of A molecules, while k_2 and k_3 are in terms of B molecules. For all the models, α, β, and γ are defined by Eqs. (24), (25), and (26), respectively.

For us to use the computed results of these models, the reaction to be evaluated must have the same mechanism as the model. However, for Models A-I, A-IV, and A-V the second-order reaction step may involve two different compounds or species.

E. Applications

The graphs and tables for all the consecutive-reversible models are based on constant volume and temperature, and on idealized reactor behavior. Since constant volume is assumed, the calculated results for the plug-flow case and batch case are the same.

All the graphs and tables are applicable to liquid systems where changes in volume are usually small. For gas-phase reactions, the calculated results are valid if there is no change in total moles due to the reaction. Assuming the kinetics is the same as the stoichiometry, there is no change in total moles for the all first-order cases, but there is for all the first-order-second-order cases.

The following examples indicate the use of the graphs for solving problems with the above restrictions. Example 1 shows the effect of initial reactant concentration, in a first-order—second-order model, on the reactor volume required for a given production rate of final product C. Example 2 indicates that the conversion of A is independent of initial concentration of A for an all—first-order reaction. The solution of two CSTR's in series is given in Example 3.

Example 1.

A consecutive-reversible reaction with the following mechanism takes place in the liquid phase in a tubular-flow reactor at constant temperature and density:

$$A \underset{k_3}{\overset{k_1}{\rightleftharpoons}} 2B,$$

and

$$B \xrightarrow{k_2} C.$$

The following data are given:

$$k_1 = 1.0 \text{ min}^{-1},$$

$$k_3 = 0.75 \text{ ft}^3/\text{min-mole},$$

$$k_2 = 1.0 \text{ min}^{-1},$$

and

$$F = 5 \text{ ft}^3/\text{min}.$$

a. With an initial reactant concentration of 1.0 mole/ft^3, what reactor volume is required to produce 4.30 mole/min of product C? At this reactor volume, what is the conversion of A?

$$C = 4.30/5 = 0.86 \text{ mole/ft}^3,$$

$$\gamma = C/2A_o = 0.43,$$

$$\kappa_1 = 4A_o k_3/k_1 = 3,$$

$$\kappa_2 = k_2/k_1 = 1,$$

and

$$\tau = k_1 V/F = 1.8 \text{ (from Fig. 16).}$$

The reactor volume is $V = 9.0 \text{ ft}^3$.

The conversion is $1 - \alpha = 0.67$ ($\alpha = 0.33$ from Fig. 15B).

b. If $A_o = 3.33$ mole/ft^3, what is the reactor volume required for the same production rate of C as in (a) above? What is the conversion of A?

$$\kappa_1 = 10,$$

$$\gamma = 0.13,$$

and

$$\tau = 0.76 \text{ (from Fig. 16)}.$$

The reactor volume is $V = 3.8 \text{ ft}^3$.

The conversion is $1 - \alpha = 0.34$ ($\alpha = 0.66$ from Fig. 15B).

Example 2.

Given the following reaction and data

$$A \underset{k_3}{\overset{k_1}{\rightleftharpoons}} B,$$

and

$$B \xrightarrow{k_2} C,$$

where

$$k_1 = 1.0 \text{ min}^{-1} ,$$

$$k_3 = 0.75 \text{ min}^{-1} ,$$

$$k_2 = 1.0 \text{ min}^{-1} ,$$

$$F = 5 \text{ ft}^3/\text{min} ,$$

and

$$V = 9.0 \text{ ft}^3 ,$$

what is the conversion of A?

$$\kappa_1 = k_3/k_1 = 0.75,$$

$$\kappa_2 = k_2/k_1 = 1.00 ,$$

$$\tau = k_1 V/F = 1.8,$$

and

$$1-\alpha = 0.70 \ (\alpha = 0.30 \text{ from Fig. 11B}).$$

The conversion in this case is independent of the initial concentration of reactant, because all the reaction steps are first order. At this conversion, $\gamma = 0.45$ and $C = \gamma (A_o)$.

Example 3.

The reaction given in Example 2 occurs in two CSTR's in series. Given the following data, find the conversion of A and the value of final γ:

$$k_1 = 2.0 \text{ min}^{-1},$$

$$k_2 = k_3 = 6.0 \text{ min}^{-1} ,$$

$$\text{volume of first CSTR} = 10 \text{ ft}^3,$$

$$\text{volume of second CSTR} = 10 \text{ ft}^3 ,$$

and

$$\text{feed rate } F = 5 \text{ ft}^3/\text{min} .$$

For each CSTR $\kappa_1 = \kappa_2 = 3.0$ and $\overline{\tau}_1 = \overline{\tau}_2 = 4.0$. The first CSTR is solved by using the graphs. The second CSTR is solved using the results from the first CSTR, and Eqs. (49) and (50). For the first CSTR we have

$$\alpha_1 = 0.325 \text{ (from Fig. 13B)},$$
$$\gamma_1 = 0.620 \text{ (from Fig. 14B)},$$

and

$$\beta_1 = 1.0 - \alpha_1 - \gamma_1 = 0.055 .$$

Using these values of α_1 and β_1 in Eq. (50) we obtain

$$\beta_2 = 0.020.$$

Substituting for α_1 and β_2 in Eq. (49) we have

$$\alpha_2 = 0.114,$$
$$1-\alpha_2 = 0.886,$$

and

$$\gamma_2 = 1-\alpha_2 - \beta_2 = 0.866 .$$

IV. CONCLUSIONS

A. Consecutive-Competitive Reaction Model

(1) The following conclusions are made concerning the time to react to a given conversion:

(a) For a given conversion of B, the time is reduced more by using an excess of B than by using an excess of the co-reactant A.

(b) For a given conversion of A, the time is reduced more by using an excess of A than by using an excess of B.

(c) The time to react to a given conversion of B becomes less dependent on the value of κ as the initial concentration of A is increased.

(2) The following conclusions are made about the relative yields of intermediate and final products:

(a) At a given conversion of either A or B, excess B favors production of the intermediate C.

(b) Excess A favors neither C nor final product D at any given conversion of either A or B.

(c) At a given time, excess B favors production of C, and excess A favors production of D.

(3) The rate coefficients can be evaluated with sufficient accuracy for design purposes from just one data point (although more than one data point is recommended).

The reaction mechanism is easily checked by fitting the experimental curve of conversion versus time to the computed curve of conversion versus dimensionless time.

B. Consecutive-Reversible Reaction Models

(1) Consecutive-reversible reactions with second-order steps can be solved accurately by using a fourth-order Runge-Kutta method on a digital computer. Using the maximum spacing for stability, the truncation plus round-off error is about 0.5% maximum. A change in spacing can be easily made at an intermediate stage of the calculations; therefore, the maximum spacing for stability can be found during the course of the calculations.

(2) In models which contain a second-order step, the proportions of intermediate and final products are dependent upon the initial concentration of reactant regardless of which reaction step is second-order.

(3) A double time-ratio method can be used to determine the values of the three rate coefficients from experimental data. However, the rate coefficients are more easily determined by fitting the experimental curve of conversion versus time to the computed curves of conversion versus τ.

NOTATION

A, B, C, D	Designate components (in chemical equations)
A, B, C, D	Concentration of A, B, C, D in moles/unit volume
a, b, b', c	Combining-proportion coefficients for components A, B, and C
F	Volumetric feed rate
k	Rate Coefficient
Subscript n	Designates values in (or leaving) tank n
Subscript $n-1$	Designates values in (or leaving) tank $n-1$
Subscript o	Designates initial reactant concentrations
t	Designates time
V	Reactor volume
α, β, γ	Dimensionless concentration of A, B, C
$\Delta\beta$	Increment in β for numerical integration
κ	Dimensionless parameter of relative rate coefficients
τ	Dimensionless time
$\overline{\tau}$	Dimensionless mean residence time
$\Delta\tau$	Spacing interval in numerical calculations
ω	Ratio of initial reactant concentrations, A_o/B_o

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APPENDIX - CONSECUTIVE-REVERSIBLE REACTION MODELS

A. Fourth-Order Runge-Kutta Method

The following is a description of how the process works along with a brief outline of the derivation of the coefficients that give fourth-order accuracy.

1. Consider a first-order equation

$$dy/dx = f(x, y) \; .$$

2. Our starting point is $x = x_o$, $y = y_o$.
3. The slope is evaluated from the differential equation at x_o, y_o; the first approximation to the integral curve is a straight line between (x_o, y_o) and (x_o+h, y_o+k_o), where

$$k_o = hf\,(x_o, y_o) \; .$$

4. Now a fraction m of the spacing h is used to evaluate the next slope at $(x_o + mh, y_o + mk_o)$. A new move for y is obtained as

$$k_1 = hf\,(x_o + mh, y_o + mk_o) \; .$$

5. A third slope is estimated from moves k_o and k_1 at $[x_o + nh, y_o + (n-r)\,k_o + rk_1]$. The next estimate for the move in y is

$$k_2 = hf\,[x_o + nh, y_o + (n-r)\,k_o + rk_1] \; .$$

6. The process is continued to give a fourth estimate for the change in y as follows:

$$k_3 = hf\,[x_o + ph, y_o + (p-s-t)\,k_o + sk_1 + tk_2] \; .$$

Thus we have estimated the slope of the integral curve at four points in the interval; the calculation of each slope, after the first estimate, is based on the preceeding estimates of slopes, and the change in y is evaluated for each estimate of the slope. The move in the y direction is

$$y(x_o + h) - y(x_o) = ak_o + bk_1 + ck_2 + dk_3 \; ,$$

where

$$a+b+c+d = 1.0 \; .$$

The coefficients are now choosen to give accuracy to the fourth-order (correct as far as terms in h^4). To find the coefficients, we expand both sides of the above equation in a power series in h. Terms up to the fourth-order are equated to obtain the values of a, b, c, d, m, n, r, s, t, and p. When this is done, we obtain eight equations in ten unknowns. The equations imply that $p = 1.0$, and according to the Runge-Kutta rule, $m = 0.5$. These values of p and m are then used to obtain the remaining eight values which are:

$$a = 1/6, \quad b = 1/3, \quad c = 1/3, \quad d = 1/6,$$

and

$$r = h = 1/2, \quad s = 0, \quad t = 1.$$

With the above values of m, n, r, s, t, and p the independent variable assumes values only at the beginning, midpoint, and end of each interval. Thus the equations are

$$y(x_o + h) - y(x_o) = (1/6)\,k_o + (1/3)\,k_1 + (1/3)\,k_2 + (1/6)\,k_3$$

where

$$k_o = hf\,(x_o, y_o)\,,$$
$$k_1 = hf(x_o + \tfrac{1}{2}h,\ y_o + \tfrac{1}{2}k_o)\,,$$
$$k_2 = hf\,(x_o + \tfrac{1}{2}h,\ y_o + \tfrac{1}{2}k_1)\,,$$

and

$$k_3 = hf\,(x_o + h,\ y_o + k_2)\,.$$

The Runge-Kutta process can be applied to the solution of simultaneous equations such as Eqs. (54) and (55). With these equations, the slopes are functions only of the dependent variables,

$$d\alpha/d\tau = f'(\alpha, \beta)\,,$$

and

$$d\beta/d\tau = f\,(\alpha, \beta)\,.$$

The Runge-Kutta formulas are

$$\alpha_{i+1} - \alpha_i = (1/6)\,k_o + (1/3)k_1 + (1/3)k_2 + (1/6)\,k_3\,,$$

and

$$\beta_{i+1} - \beta_i = (1/6)\,j_o + (1/3)j_1 + (1/3)j_2 + (1/6)\,j_3\,,$$

where

$$\begin{aligned} k_o &= \Delta\tau f'(\alpha_i, \beta_i), & j_o &= \Delta\tau f(\alpha_i, \beta_i), \\ k_1 &= \Delta\tau f'(\alpha_i + \tfrac{1}{2} k_o, \beta_i + \tfrac{1}{2} j_o), & j_1 &= \Delta\tau f(\alpha_i + \tfrac{1}{2} k_o, \beta_i + \tfrac{1}{2} j_o), \\ k_2 &= \Delta\tau f'(\alpha_i + \tfrac{1}{2} k_1, \beta_i + \tfrac{1}{2} j_1), \quad \text{and} & j_2 &= \Delta\tau f(\alpha_i + \tfrac{1}{2} k_1, \beta_i + \tfrac{1}{2} j_1), \\ k_3 &= \Delta\tau f'(\alpha_i + k_2, \beta_i + j_2), & j_3 &= \Delta\tau f(\alpha_i + k_2, \beta_i + j_2), \end{aligned}$$

and i designates the ith iteration. The starting point for the calculations is

$$\alpha_o = 1 ,$$

and

$$\gamma_o = \beta_o = \tau_o = 0 .$$

B. Tables of α, β and γ versus τ

Table A-I. Composition vs. Time for Two Consecutive Reaction Steps with First Step Reversible ($2A \rightleftharpoons B$, $B \rightarrow C$).

K1 = 0.10 AND K2 = 0.10

τ	α	β	γ
0.050	0.9525	0.0474	0.0001
0.100	0.9095	0.0900	0.0005
0.150	0.8705	0.1285	0.0010
0.200	0.8349	0.1634	0.0017
0.250	0.8023	0.1951	0.0026
0.300	0.7724	0.2239	0.0037
0.350	0.7448	0.2503	0.0049
0.400	0.7193	0.2745	0.0062
0.450	0.6957	0.2967	0.0076
0.500	0.6738	0.3170	0.0092
1.050	0.5084	0.4605	0.0311
1.219	0.4755	0.4854	0.0391
1.438	0.4406	0.5094	0.0500
2.370	0.3489	0.5511	0.1000
3.278	0.3035	0.5465	0.1500
4.210	0.2758	0.5242	0.2000
5.192	0.2565	0.4935	0.2500
6.243	0.2415	0.4585	0.3000
7.380	0.2288	0.4212	0.3500
8.624	0.2170	0.3830	0.4000
10.000	0.2056	0.3444	0.4500
11.540	0.1941	0.3059	0.5000
13.286	0.1823	0.2677	0.5500
15.299	0.1699	0.2301	0.6000
17.668	0.1568	0.1932	0.6500
20.532	0.1427	0.1573	0.7000
24.125	0.1273	0.1227	0.7500
28.881	0.1104	0.0896	0.8000
35.736	0.0912	0.0588	0.8500
47.272	0.0686	0.0314	0.9000

K1 = 0.10 AND K2 = 0.30

0.050	0.9525	0.0471	0.0004
0.100	0.9095	0.0891	0.0014
0.150	0.8705	0.1265	0.0030
0.200	0.8349	0.1600	0.0052
0.250	0.8023	0.1900	0.0078
0.300	0.7723	0.2169	0.0108
0.350	0.7447	0.2410	0.0143
0.400	0.7192	0.2628	0.0181
0.450	0.6955	0.2823	0.0222
0.500	0.6736	0.2999	0.0265
0.735	0.5886	0.3614	0.0500
1.159	0.4846	0.4154	0.1000
1.552	0.4212	0.4288	0.1500
1.942	0.3762	0.4238	0.2000
2.341	0.3415	0.4085	0.2500
2.760	0.3134	0.3866	0.3000
3.206	0.2896	0.3604	0.3500
3.688	0.2688	0.3312	0.4000
4.217	0.2500	0.3000	0.4500
4.804	0.2325	0.2675	0.5000
5.470	0.2158	0.2342	0.5500
6.238	0.1994	0.2006	0.6000
7.147	0.1829	0.1671	0.6500
8.258	0.1658	0.1342	0.7000
9.678	0.1477	0.1023	0.7500
11.612	0.1278	0.0722	0.8000
14.529	0.1052	0.0448	0.8500
19.821	0.0782	0.0218	0.9000

K1 = 0.10 AND K2 = 1.0

τ	α	β	γ
0.050	0.9525	0.0463	0.0012
0.100	0.9095	0.0860	0.0045
0.150	0.8704	0.1199	0.0097
0.200	0.8348	0.1488	0.0164
0.250	0.8021	0.1734	0.0245
0.300	0.7721	0.1942	0.0337
0.350	0.7444	0.2118	0.0439
0.400	0.7187	0.2265	0.0548
0.450	0.6949	0.2386	0.0665
0.500	0.6727	0.2486	0.0787
0.583	0.6391	0.2609	0.1000
0.769	0.5757	0.2743	0.1500
0.951	0.5257	0.2743	0.2000
1.136	0.4837	0.2663	0.2500
1.328	0.4471	0.2529	0.3000
1.533	0.4142	0.2358	0.3500
1.754	0.3840	0.2160	0.4000
1.998	0.3557	0.1943	0.4500
2.272	0.3287	0.1713	0.5000
2.586	0.3025	0.1475	0.5500
2.956	0.2765	0.1235	0.6000
3.406	0.2504	0.0996	0.6500
3.977	0.2234	0.0766	0.7000
4.746	0.1949	0.0551	0.7500
5.867	0.1641	0.0359	0.8000
7.716	0.1297	0.0203	0.8500
11.416	0.0910	0.0090	0.9000

K1 = 0.10 AND K2 = 3.00

0.050	0.9525	0.0441	0.0034
0.100	0.9095	0.0778	0.0127
0.150	0.8704	0.1033	0.0264
0.200	0.8346	0.1220	0.0433
0.250	0.8018	0.1355	0.0627
0.300	0.7716	0.1447	0.0838
0.350	0.7436	0.1504	0.1059
0.400	0.7177	0.1535	0.1288
0.450	0.6936	0.1545	0.1519
0.500	0.6711	0.1539	0.1750
0.554	0.6483	0.1517	0.2000
0.667	0.6058	0.1442	0.2500
0.787	0.5664	0.1336	0.3000
0.918	0.5288	0.1212	0.3500
1.063	0.4925	0.1075	0.4000
1.230	0.4568	0.0932	0.4500
1.424	0.4211	0.0789	0.5000
1.656	0.3850	0.0650	0.5500
1.943	0.3482	0.0518	0.6000
2.311	0.3102	0.0398	0.6500
2.800	0.2708	0.0292	0.7000
3.486	0.2298	0.0202	0.7500
4.517	0.1871	0.0129	0.8000
6.240	0.1427	0.0073	0.8500
9.688	0.0968	0.0032	0.9000

Table A-I, continued. Composition vs. Time for Two Consecutive Reaction Steps with First Step Reversible ($2A \rightleftharpoons B$, $B \rightarrow C$).

K1 = 0.30 AND K2 = 3.00

τ	α	β	γ
0.050	0.9527	0.0438	0.0034
0.100	0.9103	0.0771	0.0126
0.150	0.8719	0.1019	0.0261
0.200	0.8371	0.1200	0.0429
0.250	0.8053	0.1328	0.0619
0.300	0.7761	0.1414	0.0825
0.350	0.7492	0.1466	0.1041
0.400	0.7243	0.1493	0.1264
0.450	0.7012	0.1500	0.1488
0.500	0.6796	0.1491	0.1713
0.565	0.6538	0.1462	0.2000
0.682	0.6120	0.1380	0.2500
0.807	0.5729	0.1271	0.3000
0.945	0.5356	0.1144	0.3500
1.100	0.4991	0.1009	0.4000
1.278	0.4630	0.0870	0.4500
1.487	0.4268	0.0732	0.5000
1.738	0.3900	0.0600	0.5500
2.049	0.3522	0.0478	0.6000
2.447	0.3133	0.0367	0.6500
2.977	0.2730	0.0270	0.7000
3.717	0.2312	0.0188	0.7500
4.827	0.1880	0.0120	0.8000
6.675	0.1432	0.0068	0.8500
10.363	0.0970	0.0030	0.9000

K1 = 0.30 AND K2 = 10.00

0.050	0.9527	0.0370	0.0103
0.100	0.9100	0.0559	0.0341
0.150	0.8713	0.0642	0.0645
0.200	0.8359	0.0667	0.0974
0.250	0.8033	0.0660	0.1307
0.300	0.7732	0.0636	0.1631
0.350	0.7453	0.0605	0.1942
0.400	0.7194	0.0570	0.2236
0.450	0.6952	0.0536	0.2512
0.500	0.6726	0.0502	0.2771
0.547	0.6527	0.0473	0.3000
0.661	0.6091	0.0409	0.3500
0.793	0.5651	0.0349	0.4000
0.949	0.5206	0.0294	0.4500
1.136	0.4757	0.0243	0.5000
1.365	0.4304	0.0196	0.5500
1.651	0.3845	0.0155	0.6000
2.020	0.3381	0.0119	0.6500
2.511	0.2913	0.0087	0.7000
3.198	0.2439	0.0061	0.7500
4.229	0.1961	0.0039	0.8000
5.947	0.1478	0.0022	0.8500
9.382	0.0990	0.0010	0.9000

K1 = 1.00 AND K2 = 0.10

τ	α	β	γ
0.050	0.9535	0.0463	0.0001
0.100	0.9133	0.0862	0.0005
0.150	0.8784	0.1206	0.0010
0.200	0.8480	0.1504	0.0017
0.250	0.8214	0.1762	0.0025
0.300	0.7980	0.1986	0.0034
0.350	0.7774	0.2181	0.0045
0.400	0.7592	0.2352	0.0056
0.450	0.7432	0.2500	0.0068
0.500	0.7289	0.2630	0.0081
1.050	0.6438	0.3313	0.0249
1.789	0.6082	0.3418	0.0500
3.294	0.5796	0.3204	0.1000
4.921	0.5556	0.2944	0.1500
6.698	0.5312	0.2688	0.2000
8.651	0.5062	0.2438	0.2500
10.812	0.4805	0.2195	0.3000
13.223	0.4542	0.1958	0.3500
15.939	0.4271	0.1729	0.4000
19.035	0.3992	0.1508	0.4500
22.610	0.3704	0.1296	0.5000
26.807	0.3406	0.1094	0.5500
31.836	0.3097	0.0903	0.6000
38.019	0.2776	0.0724	0.6500
45.880	0.2442	0.0558	0.7000
56.343	0.2092	0.0408	0.7500
71.208	0.1724	0.0276	0.8000
94.572	0.1335	0.0165	0.8500
138.403	0.0922	0.0078	0.9000

K1 = 1.00 AND K2 = 0.30

0.050	0.9535	0.0461	0.0004
0.100	0.9133	0.0853	0.0013
0.150	0.8783	0.1188	0.0029
0.200	0.8478	0.1473	0.0049
0.250	0.8210	0.1717	0.0073
0.300	0.7974	0.1926	0.0100
0.350	0.7765	0.2104	0.0130
0.400	0.7580	0.2257	0.0163
0.450	0.7415	0.2387	0.0198
0.500	0.7268	0.2497	0.0235
0.824	0.6610	0.2890	0.0500
1.387	0.6045	0.2955	0.1000
1.966	0.5715	0.2785	0.1500
2.590	0.5443	0.2557	0.2000
3.274	0.5181	0.2319	0.2500
4.032	0.4916	0.2084	0.3000
4.880	0.4646	0.1854	0.3500
5.838	0.4368	0.1632	0.4000
6.933	0.4082	0.1418	0.4500
8.202	0.3786	0.1214	0.5000
9.699	0.3480	0.1020	0.5500
11.501	0.3162	0.0838	0.6000
13.729	0.2833	0.0667	0.6500
16.579	0.2489	0.0511	0.7000
20.400	0.2129	0.0371	0.7500
25.877	0.1751	0.0249	0.8000
34.575	0.1353	0.0147	0.8500
51.101	0.0931	0.0069	0.9000

Table A-I, continued. Composition vs. Time for Two Consecutive Reaction Steps with First Step Reversible ($2A \rightleftharpoons B$, $B \rightarrow C$).

K1 = 0.10 AND K2 = 10.00

τ	α	β	γ
0.050	0.9525	0.0372	0.0103
0.100	0.9094	0.0563	0.0343
0.150	0.8702	0.0649	0.0649
0.200	0.8342	0.0676	0.0982
0.250	0.8011	0.0669	0.1320
0.300	0.7706	0.0645	0.1649
0.350	0.7423	0.0613	0.1964
0.400	0.7160	0.0578	0.2262
0.450	0.6915	0.0543	0.2542
0.500	0.6687	0.0509	0.2805
0.540	0.6517	0.0483	0.3000
0.651	0.6081	0.0419	0.3500
0.780	0.5643	0.0357	0.4000
0.933	0.5200	0.0300	0.4500
1.116	0.4752	0.0248	0.5000
1.340	0.4299	0.0201	0.5500
1.620	0.3841	0.0159	0.6000
1.981	0.3379	0.0121	0.6500
2.461	0.2911	0.0089	0.7000
3.134	0.2438	0.0062	0.7500
4.144	0.1960	0.0040	0.8000
5.828	0.1478	0.0022	0.8500
9.195	0.0990	0.0010	0.9000

K1 = 0.30 AND K2 = 0.10

0.050	0.9527	0.0471	0.0001
0.100	0.9104	0.0891	0.0005
0.150	0.8723	0.1267	0.0010
0.200	0.8379	0.1603	0.0017
0.250	0.8068	0.1906	0.0026
0.300	0.7784	0.2179	0.0036
0.350	0.7526	0.2426	0.0048
0.400	0.7290	0.2650	0.0060
0.450	0.7073	0.2852	0.0074
0.500	0.6874	0.3037	0.0089
1.050	0.5456	0.4249	0.0295
1.282	0.5115	0.4489	0.0396
1.509	0.4862	0.4638	0.0500
2.560	0.4233	0.4767	0.1000
3.631	0.3952	0.4548	0.1500
4.769	0.3763	0.4237	0.2000
5.998	0.3599	0.3901	0.2500
7.339	0.3439	0.3561	0.3000
8.814	0.3276	0.3224	0.3500
10.452	0.3109	0.2891	0.4000
12.287	0.2934	0.2566	0.4500
14.368	0.2753	0.2247	0.5000
16.763	0.2563	0.1937	0.5500
19.568	0.2363	0.1637	0.6000
22.931	0.2152	0.1348	0.6500
27.084	0.1927	0.1073	0.7000
32.430	0.1687	0.0813	0.7500
39.733	0.1426	0.0574	0.8000
50.689	0.1140	0.0360	0.8500
70.107	0.0818	0.0182	0.9000

K1 = 0.30 AND K2 = 0.30

τ	α	β	γ
0.050	0.9527	0.0469	0.0004
0.100	0.9104	0.0882	0.0014
0.150	0.8723	0.1247	0.0030
0.200	0.8379	0.1570	0.0051
0.250	0.8067	0.1857	0.0077
0.300	0.7782	0.2111	0.0107
0.350	0.7523	0.2337	0.0140
0.400	0.7286	0.2538	0.0177
0.450	0.7068	0.2716	0.0216
0.500	0.6867	0.2875	0.0258
0.753	0.6059	0.3441	0.0500
1.205	0.5156	0.3844	0.1000
1.635	0.4633	0.3867	0.1500
2.073	0.4269	0.3731	0.2000
2.533	0.3988	0.3512	0.2500
3.025	0.3751	0.3249	0.3000
3.562	0.3539	0.2961	0.3500
4.156	0.3338	0.2662	0.4000
4.820	0.3141	0.2359	0.4500
5.576	0.2942	0.2058	0.5000
6.451	0.2738	0.1762	0.5500
7.483	0.2524	0.1476	0.6000
8.734	0.2298	0.1202	0.6500
10.298	0.2058	0.0942	0.7000
12.346	0.1799	0.0701	0.7500
15.204	0.1517	0.0483	0.8000
19.620	0.1207	0.0293	0.8500
27.770	0.0859	0.0141	0.9000

K1 = 0.30 AND K2 = 1.00

0.050	0.9527	0.0461	0.0012
0.100	0.9104	0.0852	0.0045
0.150	0.8722	0.1182	0.0096
0.200	0.8377	0.1461	0.0162
0.250	0.8063	0.1696	0.0241
0.300	0.7776	0.1893	0.0331
0.350	0.7514	0.2056	0.0430
0.400	0.7272	0.2191	0.0536
0.450	0.7050	0.2301	0.0649
0.500	0.6844	0.2390	0.0766
0.595	0.6492	0.2508	0.1000
0.790	0.5898	0.2602	0.1500
0.983	0.5431	0.2569	0.2000
1.181	0.5038	0.2462	0.2500
1.390	0.4693	0.2307	0.3000
1.616	0.4379	0.2121	0.3500
1.864	0.4086	0.1914	0.4000
2.141	0.3805	0.1695	0.4500
2.458	0.3530	0.1470	0.5000
2.827	0.3255	0.1245	0.5500
3.269	0.2977	0.1023	0.6000
3.817	0.2688	0.0812	0.6500
4.524	0.2385	0.0615	0.7000
5.486	0.2062	0.0438	0.7500
6.895	0.1713	0.0287	0.8000
9.198	0.1336	0.0164	0.8500
13.721	0.0926	0.0074	0.9000

Table A-I, continued. Composition vs. Time for Two Consecutive Reaction Steps with First Step Reversible ($2A \rightleftharpoons B$, $B \rightarrow C$).

K1 = 1.00 AND K2 = 1.00

τ	α	β	γ
0.050	0.9535	0.0453	0.0012
0.100	0.9132	0.0824	0.0044
0.150	0.8780	0.1127	0.0093
0.200	0.8471	0.1373	0.0156
0.250	0.8198	0.1573	0.0229
0.300	0.7955	0.1733	0.0312
0.350	0.7737	0.1861	0.0402
0.400	0.7541	0.1961	0.0498
0.450	0.7364	0.2038	0.0598
0.500	0.7202	0.2097	0.0701
0.639	0.6819	0.2181	0.1000
0.868	0.6333	0.2167	0.1500
1.104	0.5944	0.2056	0.2000
1.357	0.5603	0.1897	0.2500
1.634	0.5284	0.1716	0.3000
1.942	0.4973	0.1527	0.3500
2.292	0.4662	0.1338	0.4000
2.694	0.4347	0.1153	0.4500
3.165	0.4023	0.0977	0.5000
3.727	0.3689	0.0811	0.5500
4.412	0.3344	0.0656	0.6000
5.272	0.2985	0.0515	0.6500
6.390	0.2612	0.0388	0.7000
7.918	0.2224	0.0276	0.7500
10.154	0.1819	0.0181	0.8000
13.787	0.1396	0.0104	0.8500
20.872	0.0952	0.0048	0.9000

K1 = 1.00 AND K2 = 3.00

0.050	0.9535	0.0431	0.0034
0.100	0.9130	0.0747	0.0124
0.150	0.8773	0.0974	0.0254
0.200	0.8455	0.1133	0.0412
0.250	0.8169	0.1240	0.0591
0.300	0.7910	0.1308	0.0782
0.350	0.7673	0.1345	0.0982
0.400	0.7455	0.1360	0.1185
0.450	0.7252	0.1359	0.1389
0.500	0.7064	0.1344	0.1592
0.603	0.6711	0.1289	0.2000
0.738	0.6309	0.1191	0.2500
0.885	0.5926	0.1074	0.3000
1.049	0.5550	0.0950	0.3500
1.238	0.5176	0.0824	0.4000
1.457	0.4798	0.0702	0.4500
1.717	0.4414	0.0586	0.5000
2.032	0.4022	0.0478	0.5500
2.422	0.3620	0.0380	0.6000
2.922	0.3207	0.0293	0.6500
3.583	0.2783	0.0217	0.7000
4.503	0.2349	0.0151	0.7500
5.874	0.1902	0.0098	0.8000
8.144	0.1445	0.0055	0.8500
12.657	0.0975	0.0025	0.9000

K1 = 1.00 AND K2 = 10.00

τ	α	β	γ
0.050	0.9534	0.0364	0.0102
0.100	0.9122	0.0543	0.0335
0.150	0.8752	0.0619	0.0628
0.200	0.8416	0.0639	0.0945
0.250	0.8107	0.0630	0.1263
0.300	0.7821	0.0607	0.1573
0.350	0.7555	0.0576	0.1869
0.400	0.7307	0.0544	0.2149
0.450	0.7075	0.0512	0.2413
0.500	0.6857	0.0482	0.2661
0.574	0.6560	0.0440	0.3000
0.696	0.6120	0.0380	0.3500
0.838	0.5675	0.0325	0.4000
1.006	0.5227	0.0273	0.4500
1.207	0.4774	0.0226	0.5000
1.454	0.4317	0.0183	0.5500
1.761	0.3855	0.0145	0.6000
2.156	0.3389	0.0111	0.6500
2.682	0.2919	0.0081	0.7000
3.419	0.2443	0.0057	0.7500
4.523	0.1964	0.0036	0.8000
6.361	0.1480	0.0020	0.8500
10.035	0.0991	0.0009	0.9000

K1 = 3.00 AND K2 = 0.10

0.050	0.9557	0.0442	0.0001
0.100	0.9211	0.0785	0.0004
0.150	0.8938	0.1053	0.0009
0.200	0.8723	0.1262	0.0015
0.250	0.8552	0.1426	0.0021
0.300	0.8417	0.1555	0.0029
0.350	0.8308	0.1655	0.0037
0.400	0.8221	0.1734	0.0045
0.450	0.8151	0.1795	0.0054
0.500	0.8094	0.1843	0.0063
1.050	0.7845	0.1985	0.0170
1.817	0.7730	0.1948	0.0322
2.747	0.7611	0.1889	0.0500
5.517	0.7275	0.1725	0.1000
8.558	0.6933	0.1567	0.1500
11.918	0.6587	0.1413	0.2000
15.656	0.6234	0.1266	0.2500
19.847	0.5876	0.1124	0.3000
24.591	0.5512	0.0988	0.3500
30.015	0.5141	0.0859	0.4000
36.294	0.4763	0.0737	0.4500
43.672	0.4377	0.0623	0.5000
52.495	0.3984	0.0516	0.5500
63.278	0.3583	0.0417	0.6000
76.824	0.3173	0.0327	0.6500
94.458	0.2754	0.0246	0.7000
118.539	0.2325	0.0175	0.7500
153.740	0.1885	0.0115	0.8000
205.725	0.0698	0.0802	0.8500
291.830	0.0752	0.0248	0.9000

Table A-I, continued. Composition vs. Time for Two Consecutive Reaction Steps with First Step Reversible ($2A \rightleftharpoons B$, $B \rightarrow C$).

K1 = 3.00 AND K2 = 0.30

τ	α	β	γ
0.050	0.9557	0.0439	0.0003
0.100	0.9210	0.0777	0.0013
0.150	0.8936	0.1038	0.0026
0.200	0.8718	0.1239	0.0044
0.250	0.8544	0.1393	0.0063
0.300	0.8403	0.1512	0.0085
0.350	0.8289	0.1603	0.0109
0.400	0.8195	0.1672	0.0133
0.450	0.8117	0.1724	0.0159
0.500	0.8052	0.1763	0.0185
1.075	0.7677	0.1823	0.0500
2.027	0.7326	0.1674	0.1000
3.072	0.6981	0.1519	0.1500
4.228	0.6631	0.1369	0.2000
5.515	0.6275	0.1225	0.2500
6.959	0.5914	0.1086	0.3000
8.596	0.5546	0.0954	0.3500
10.470	0.5171	0.0829	0.4000
12.642	0.4790	0.0710	0.4500
15.197	0.4401	0.0599	0.5000
18.258	0.4005	0.0495	0.5500
22.004	0.3601	0.0399	0.6000
26.719	0.3187	0.0313	0.6500
32.868	0.2765	0.0235	0.7000
41.283	0.2333	0.0167	0.7500
53.611	0.1891	0.0109	0.8000
73.664	0.1437	0.0063	0.8500
112.764	0.0971	0.0029	0.9000

K1 = 3.00 AND K2 = 1.00

0.050	0.9557	0.0432	0.0011
0.100	0.9207	0.0751	0.0041
0.150	0.8928	0.0987	0.0085
0.200	0.8701	0.1160	0.0139
0.250	0.8515	0.1285	0.0200
0.300	0.8359	0.1374	0.0267
0.350	0.8226	0.1436	0.0337
0.400	0.8112	0.1478	0.0410
0.450	0.8011	0.1505	0.0485
0.500	0.7920	0.1519	0.0560
0.790	0.7515	0.1485	0.1000
1.141	0.7136	0.1364	0.1500
1.527	0.6771	0.1229	0.2000
1.958	0.6404	0.1096	0.2500
2.442	0.6031	0.0969	0.3000
2.994	0.5652	0.0848	0.3500
3.627	0.5266	0.0734	0.4000
4.364	0.4874	0.0626	0.4500
5.235	0.4474	0.0526	0.5000
6.283	0.4067	0.0433	0.5500
7.572	0.3652	0.0348	0.6000
9.202	0.3229	0.0271	0.6500
11.339	0.2798	0.0202	0.7000
14.280	0.2357	0.0143	0.7500
18.616	0.1907	0.0093	0.8000
25.715	0.1447	0.0053	0.8500
39.658	0.0976	0.0024	0.9000

K1 = 3.00 AND K2 = 3.00

τ	α	β	γ
0.050	0.9556	0.0411	0.0033
0.100	0.9200	0.0683	0.0117
0.150	0.8907	0.0859	0.0233
0.200	0.8660	0.0969	0.0371
0.250	0.8445	0.1033	0.0522
0.300	0.8254	0.1066	0.0680
0.350	0.8082	0.1078	0.0841
0.400	0.7923	0.1075	0.1002
0.450	0.7776	0.1062	0.1163
0.500	0.7637	0.1043	0.1320
0.558	0.7484	0.1016	0.1500
0.730	0.7075	0.0925	0.2000
0.921	0.6675	0.0825	0.2500
1.136	0.6274	0.0726	0.3000
1.382	0.5868	0.0632	0.3500
1.666	0.5457	0.0543	0.4000
2.000	0.5040	0.0460	0.4500
2.396	0.4617	0.0383	0.5000
2.877	0.4187	0.0313	0.5500
3.473	0.3751	0.0249	0.6000
4.234	0.3307	0.0193	0.6500
5.239	0.2857	0.0143	0.7000
6.634	0.2400	0.0100	0.7500
8.710	0.1936	0.0064	0.8000
12.141	0.1463	0.0037	0.8500
18.944	0.0984	0.0016	0.9000

K1 = 3.00 AND K2 = 10.00

0.050	0.9553	0.0348	0.0099
0.100	0.9180	0.0502	0.0318
0.150	0.8854	0.0560	0.0586
0.200	0.8560	0.0570	0.0870
0.250	0.8290	0.0557	0.1152
0.300	0.8039	0.0535	0.1426
0.350	0.7804	0.0509	0.1687
0.400	0.7582	0.0483	0.1935
0.450	0.7373	0.0457	0.2170
0.500	0.7175	0.0432	0.2392
0.652	0.6632	0.0368	0.3000
0.799	0.6182	0.0318	0.3500
0.969	0.5729	0.0271	0.4000
1.170	0.5272	0.0228	0.4500
1.411	0.4811	0.0189	0.5000
1.705	0.4347	0.0153	0.5500
2.071	0.3879	0.0121	0.6000
2.542	0.3407	0.0093	0.6500
3.168	0.2932	0.0068	0.7000
4.043	0.2452	0.0048	0.7500
5.353	0.1969	0.0031	0.8000
7.533	0.1483	0.0017	0.8500
11.886	0.0992	0.0008	0.9000

Table A-I, continued. Composition vs. Time for Two Consecutive Reaction Steps with First Step Reversible ($2A \rightleftharpoons B$, $B \rightarrow C$).

K1 = 10.00 AND K2 = 0.10

τ	α	β	γ
0.050	0.9624	0.0375	0.0001
0.100	0.9416	0.0580	0.0003
0.150	0.9300	0.0693	0.0007
0.200	0.9235	0.0755	0.0010
0.250	0.9197	0.0789	0.0014
0.300	0.9175	0.0807	0.0018
0.350	0.9161	0.0817	0.0022
0.400	0.9152	0.0822	0.0026
0.450	0.9145	0.0825	0.0030
0.500	0.9140	0.0826	0.0035
1.050	0.9099	0.0821	0.0080
2.993	0.8966	0.0797	0.0237
6.376	0.8742	0.0758	0.0500
13.313	0.8315	0.0685	0.1000
21.006	0.7884	0.0616	0.1500
29.592	0.7450	0.0550	0.2000
39.246	0.7013	0.0487	0.2500
50.190	0.6572	0.0428	0.3000

K1 = 10.00 AND K2 = 0.30

0.050	0.9624	0.0373	0.0003
0.100	0.9414	0.0575	0.0010
0.150	0.9295	0.0685	0.0020
0.200	0.9226	0.0744	0.0031
0.250	0.9183	0.0775	0.0042
0.300	0.9155	0.0791	0.0054
0.350	0.9135	0.0800	0.0066
0.400	0.9119	0.0803	0.0078
0.450	0.9106	0.0804	0.0090
0.500	0.9094	0.0804	0.0102
1.050	0.8980	0.0786	0.0233
2.210	0.8753	0.0747	0.0500
4.556	0.8324	0.0676	0.1000
7.158	0.7893	0.0607	0.1500
10.063	0.7458	0.0542	0.2000
13.330	0.7020	0.0480	0.2500
17.035	0.6578	0.0422	0.3000
21.275	0.6134	0.0366	0.3500
26.183	0.5685	0.0315	0.4000
31.936	0.5233	0.0267	0.4500
38.782	0.4778	0.0222	0.5000
47.082	0.4319	0.0181	0.5500
57.377	0.3841	0.0159	0.6000

K1 = 10.00 AND K2 = 1.00

τ	α	β	γ
0.050	0.9623	0.0367	0.0010
0.100	0.9408	0.0558	0.0034
0.150	0.9279	0.0657	0.0065
0.200	0.9195	0.0707	0.0099
0.250	0.9135	0.0730	0.0135
0.300	0.9088	0.0740	0.0172
0.350	0.9048	0.0743	0.0209
0.400	0.9012	0.0742	0.0246
0.450	0.8978	0.0739	0.0283
0.500	0.8945	0.0735	0.0320
0.749	0.8789	0.0711	0.0500
1.489	0.8357	0.0643	0.1000
2.309	0.7923	0.0577	0.1500
3.226	0.7485	0.0515	0.2000
4.258	0.7044	0.0456	0.2500
5.429	0.6600	0.0400	0.3000
6.770	0.6153	0.0347	0.3500
8.324	0.5702	0.0298	0.4000
10.147	0.5248	0.0252	0.4500
12.318	0.4790	0.0210	0.5000
14.952	0.4329	0.0171	0.5500
18.219	0.3863	0.0137	0.6000
22.388	0.3395	0.0105	0.6500
27.904	0.2922	0.0078	0.7000
35.567	0.2445	0.0055	0.7500
46.970	0.1965	0.0035	0.8000

K1 = 10.00 AND K2 = 3.00

0.050	0.9620	0.0350	0.0030
0.100	0.9391	0.0513	0.0096
0.150	0.9235	0.0586	0.0180
0.200	0.9116	0.0615	0.0270
0.250	0.9015	0.0622	0.0363
0.300	0.8923	0.0620	0.0456
0.350	0.8838	0.0613	0.0549
0.400	0.8755	0.0604	0.0640
0.450	0.8675	0.0595	0.0730
0.500	0.8597	0.0584	0.0818
0.606	0.8437	0.0563	0.1000
0.918	0.7995	0.0505	0.1500
1.268	0.7550	0.0450	0.2000
1.662	0.7103	0.0397	0.2500
2.110	0.6652	0.0348	0.3000
2.624	0.6198	0.0302	0.3500
3.221	0.5741	0.0259	0.4000
3.922	0.5282	0.0218	0.4500
4.759	0.4818	0.0182	0.5000
5.776	0.4352	0.0148	0.5500
7.040	0.3882	0.0118	0.6000
8.657	0.3410	0.0090	0.6500
10.799	0.2933	0.0067	0.7000
13.782	0.2453	0.0047	0.7500
18.230	0.1970	0.0030	0.8000
25.599	0.1483	0.0017	0.8500
40.252	0.0992	0.0008	0.9000

K1 = 10.00 AND K2 = 10.00

0.050	0.9612	0.0296	0.0091
0.100	0.9341	0.0390	0.0269
0.150	0.9118	0.0411	0.0471
0.200	0.8917	0.0407	0.0676
0.250	0.8728	0.0395	0.0877
0.300	0.8549	0.0380	0.1071
0.350	0.8377	0.0365	0.1257
0.400	0.8212	0.0351	0.1436
0.450	0.8054	0.0338	0.1608
0.500	0.7901	0.0325	0.1774
0.572	0.7693	0.0307	0.2000
0.745	0.7229	0.0271	0.2500
0.942	0.6763	0.0237	0.3000
1.170	0.6296	0.0204	0.3500
1.434	0.5825	0.0175	0.4000
1.746	0.5353	0.0147	0.4500
2.119	0.4878	0.0122	0.5000
2.574	0.4401	0.0099	0.5500
3.142	0.3922	0.0078	0.6000
3.870	0.3440	0.0060	0.6500
4.838	0.2956	0.0044	0.7000
6.189	0.2469	0.0031	0.7500
8.212	0.1980	0.0020	0.8000
11.574	0.1489	0.0011	0.8500
18.281	0.0995	0.0005	0.9000

Table A-II. Composition vs. Time for Two Consecutive Reaction Steps with First Step Reversible ($A \rightleftharpoons B$, $2B \rightarrow C$).

K1 = 0.10 AND K2 = 0.10

τ	α	β	γ
0.050	0.9513	0.0486	0.0000
0.099	0.9053	0.0946	0.0000
0.149	0.8617	0.1381	0.0000
0.199	0.8204	0.1793	0.0002
0.249	0.7814	0.2181	0.0004
0.299	0.7444	0.2548	0.0007
0.349	0.7094	0.2894	0.0010
0.399	0.6763	0.3220	0.0015
0.449	0.6450	0.3528	0.0021
0.499	0.6153	0.3818	0.0027
0.550	0.5876	0.4086	0.0036
1.050	0.3772	0.6054	0.0172
1.550	0.2551	0.7056	0.0392
2.050	0.1836	0.7503	0.0660
2.550	0.1413	0.7638	0.0948
3.050	0.1157	0.7602	0.1239
3.550	0.0998	0.7476	0.1524
4.050	0.0896	0.7305	0.1797
4.550	0.0827	0.7115	0.2057
5.471	0.0745	0.6754	0.2500
6.642	0.0679	0.6320	0.3000
7.987	0.0623	0.5876	0.3500
9.554	0.0572	0.5427	0.4000
11.407	0.0522	0.4977	0.4500
13.624	0.0472	0.4527	0.5000
16.335	0.0423	0.4076	0.5500
19.718	0.0375	0.3624	0.6000
24.064	0.0326	0.3173	0.6500
29.857	0.0279	0.2720	0.7000
37.957	0.0231	0.2268	0.7500
50.099	0.0184	0.1815	0.8000
70.319	0.0137	0.1362	0.8500
110.728	0.0091	0.0908	0.9000

K1 = 0.10 AND K2 = 0.30

0.050	0.9513	0.0486	0.0000
0.100	0.9053	0.0946	0.0000
0.150	0.8617	0.1379	0.0002
0.200	0.8204	0.1788	0.0006
0.250	0.7814	0.2173	0.0012
0.300	0.7444	0.2534	0.0021
0.350	0.7094	0.2873	0.0032
0.400	0.6763	0.3190	0.0045
0.450	0.6449	0.3487	0.0062
0.500	0.6153	0.3764	0.0082
1.051	0.3807	0.5692	0.0500
1.505	0.2612	0.6387	0.1000
1.901	0.1969	0.6530	0.1500
2.295	0.1540	0.6459	0.2000
2.706	0.1235	0.6264	0.2500
3.149	0.1012	0.5987	0.3000
3.641	0.0844	0.5655	0.3500
4.198	0.0716	0.5283	0.4000
4.844	0.0616	0.4883	0.4500
5.608	0.0535	0.4464	0.5000
6.533	0.0466	0.4033	0.5500
7.682	0.0404	0.3595	0.6000
9.152	0.0348	0.3151	0.6500
11.106	0.0293	0.2706	0.7000
13.833	0.0241	0.2258	0.7500
17.912	0.0190	0.1809	0.8000
24.691	0.0141	0.1358	0.8500
38.213	0.0093	0.0906	0.9000

K1 = 0.10 AND K2 = 1.00

τ	α	β	γ
0.050	0.9513	0.0486	0.0000
0.100	0.9053	0.0943	0.0003
0.150	0.8617	0.1372	0.0009
0.200	0.8204	0.1773	0.0022
0.250	0.7814	0.2144	0.0041
0.300	0.7444	0.2487	0.0068
0.350	0.7094	0.2802	0.0103
0.400	0.6762	0.3090	0.0147
0.450	0.6448	0.3352	0.0199
0.500	0.6150	0.3589	0.0259
0.632	0.5527	0.3972	0.0500
0.904	0.4172	0.4827	0.1000
1.108	0.3550	0.4949	0.1500
1.310	0.2999	0.5000	0.2000
1.511	0.2544	0.4955	0.2500
1.719	0.2158	0.4841	0.3000
1.939	0.1825	0.4674	0.3500
2.178	0.1534	0.4465	0.4000
2.443	0.1278	0.4221	0.4500
2.743	0.1052	0.3947	0.5000
3.090	0.0855	0.3644	0.5500
3.503	0.0683	0.3316	0.6000
4.011	0.0535	0.2964	0.6500
4.661	0.0410	0.2589	0.7000
5.541	0.0308	0.2191	0.7500
6.824	0.0224	0.1775	0.8000
8.918	0.0156	0.1343	0.8500
13.044	0.0098	0.0901	0.9000

K1 = 0.10 AND K2 = 3.00

0.050	0.9513	0.0485	0.0001
0.100	0.9053	0.0937	0.0009
0.150	0.8617	0.1353	0.0029
0.200	0.8204	0.1730	0.0065
0.250	0.7813	0.2066	0.0119
0.300	0.7443	0.2363	0.0193
0.350	0.7092	0.2620	0.0286
0.400	0.6759	0.2841	0.0399
0.450	0.6444	0.3026	0.0528
0.500	0.6145	0.3181	0.0673
0.592	0.5680	0.3319	0.1000
0.685	0.4830	0.3669	0.1500
0.819	0.4363	0.3636	0.2000
0.956	0.3922	0.3577	0.2500
1.097	0.3504	0.3495	0.3000
1.242	0.3105	0.3394	0.3500
1.393	0.2723	0.3276	0.4000
1.555	0.2364	0.3135	0.4500
1.734	0.2027	0.2972	0.5000
1.935	0.1710	0.2789	0.5500
2.166	0.1413	0.2586	0.6000
2.438	0.1135	0.2364	0.6500
2.770	0.0878	0.2121	0.7000
3.192	0.0643	0.1856	0.7500
3.764	0.0436	0.1563	0.8000
4.623	0.0263	0.1236	0.8500
6.168	0.0134	0.0865	0.9000

Table A-II, continued. Composition vs. Time for Two Consecutive Reaction Steps with First Step Reversible ($A \rightleftarrows B$, $2B \rightarrow C$).

K1 = 0.10 AND K2 = 10.00

τ	α	β	γ
0.050	0.9513	0.0482	0.0003
0.100	0.9052	0.0917	0.0029
0.150	0.8616	0.1291	0.0091
0.200	0.8203	0.1598	0.0197
0.250	0.7812	0.1841	0.0346
0.300	0.7440	0.2025	0.0534
0.350	0.7087	0.2158	0.0754
0.400	0.6752	0.2249	0.0997
0.450	0.6434	0.2307	0.1257
0.500	0.6132	0.2339	0.1528
0.586	0.5686	0.2313	0.2000
0.392	0.5746	0.1753	0.2500
0.548	0.5150	0.1849	0.3000
0.701	0.4609	0.1890	0.3500
0.854	0.4107	0.1892	0.4000
1.010	0.3637	0.1862	0.4500
1.171	0.3190	0.1809	0.5000
1.339	0.2763	0.1736	0.5500
1.515	0.2351	0.1648	0.6000
1.712	0.1960	0.1539	0.6500
1.941	0.1588	0.1411	0.7000
2.220	0.1233	0.1266	0.7500
2.578	0.0898	0.1101	0.8000
3.072	0.0586	0.0913	0.8500
3.858	0.0309	0.0690	0.9000

K1 = 0.30 AND K2 = 0.10

0.050	0.9515	0.0484	0.0000
0.550	0.6075	0.3889	0.0034
1.050	0.4267	0.5578	0.0153
1.550	0.3305	0.6359	0.0335
2.050	0.2779	0.6670	0.0549
2.550	0.2480	0.6744	0.0775
3.050	0.2298	0.6699	0.1002
3.550	0.2178	0.6597	0.1223
4.050	0.2092	0.6470	0.1436
4.550	0.2024	0.6333	0.1641
5.481	0.1922	0.6077	0.2000
6.923	0.1793	0.5706	0.2500
8.565	0.1669	0.5330	0.3000
10.459	0.1546	0.4953	0.3500
12.665	0.1423	0.4576	0.4000
15.268	0.1302	0.4197	0.4500
18.387	0.1180	0.3819	0.5000
22.193	0.1060	0.3439	0.5500
26.943	0.0940	0.3059	0.6000
33.042	0.0820	0.2679	0.6500
41.163	0.0701	0.2298	0.7000
52.515	0.0583	0.1916	0.7500
69.520	0.0465	0.1534	0.8000
97.822	0.0348	0.1151	0.8500
54.344	0.0231	0.0768	0.9000

K1 = 0.30 AND K2 = 0.30

τ	α	β	γ
0.050	0.9515	0.0483	0.0000
0.099	0.9062	0.0936	0.0000
0.149	0.8637	0.1359	0.0002
0.199	0.8238	0.1754	0.0006
0.249	0.7865	0.2122	0.0012
0.299	0.7515	0.2464	0.0020
0.349	0.7187	0.2782	0.0030
0.399	0.6879	0.3076	0.0043
0.449	0.6591	0.3349	0.0058
0.499	0.6320	0.3602	0.0077
0.550	0.6073	0.3824	0.0102
1.116	0.4114	0.5385	0.0500
1.632	0.3150	0.5849	0.1000
2.112	0.2620	0.5879	0.1500
2.606	0.2278	0.5721	0.2000
3.138	0.2031	0.5468	0.2500
3.729	0.1836	0.5163	0.3000
4.396	0.1669	0.4830	0.3500
5.164	0.1518	0.4481	0.4000
6.063	0.1377	0.4122	0.4500
7.141	0.1241	0.3758	0.5000
8.448	0.1108	0.3391	0.5500
10.071	0.0977	0.3022	0.6000
12.153	0.0849	0.2650	0.6500
14.913	0.0722	0.2277	0.7000
18.759	0.0597	0.1902	0.7500
24.500	0.0474	0.1525	0.8000
34.027	0.0353	0.1146	0.8500
52.998	0.0233	0.0766	0.9000

K1 = 0.30 AND K2 = 1.00

0.050	0.9515	0.0483	0.0000
0.100	0.9062	0.0934	0.0003
0.150	0.8637	0.1353	0.0009
0.200	0.8238	0.1739	0.0021
0.250	0.7864	0.2094	0.0040
0.300	0.7514	0.2419	0.0065
0.350	0.7185	0.2715	0.0098
0.400	0.6876	0.2983	0.0139
0.450	0.6586	0.3225	0.0187
0.500	0.6314	0.3442	0.0243
0.653	0.5679	0.3820	0.0500
0.944	0.4456	0.4543	0.1000
1.177	0.3853	0.4646	0.1500
1.407	0.3348	0.4651	0.2000
1.642	0.2936	0.4563	0.2500
1.890	0.2587	0.4412	0.3000
2.159	0.2283	0.4216	0.3500
2.456	0.2012	0.3987	0.4000
2.791	0.1768	0.3731	0.4500
3.179	0.1545	0.3454	0.5000
3.636	0.1340	0.3159	0.5500
4.191	0.1151	0.2848	0.6000
4.886	0.0974	0.2525	0.6500
5.789	0.0809	0.2190	0.7000
7.026	0.0655	0.1844	0.7500
8.843	0.0509	0.1490	0.8000
11.816	0.0372	0.1127	0.8500
17.658	0.0241	0.0758	0.9000

Table A-II, continued. Composition vs. Time for Two Consecutive Reaction Steps with First Step Reversible ($A \rightleftharpoons B$, $2B \rightarrow C$).

K1 = 0.30 AND K2 = 3.00

τ	α	β	γ
0.050	0.9515	0.0482	0.0001
0.100	0.9062	0.0928	0.0008
0.150	0.8636	0.1334	0.0028
0.200	0.8237	0.1698	0.0063
0.250	0.7863	0.2021	0.0115
0.300	0.7511	0.2302	0.0185
0.350	0.7180	0.2544	0.0274
0.400	0.6869	0.2750	0.0379
0.450	0.6575	0.2923	0.0500
0.500	0.6299	0.3065	0.0635
0.610	0.5805	0.3194	0.1000
0.713	0.5038	0.3461	0.1500
0.862	0.4571	0.3428	0.2000
1.014	0.4132	0.3367	0.2500
1.171	0.3714	0.3285	0.3000
1.332	0.3316	0.3183	0.3500
1.503	0.2942	0.3057	0.4000
1.690	0.2592	0.2907	0.4500
1.899	0.2262	0.2737	0.5000
2.138	0.1950	0.2549	0.5500
2.416	0.1654	0.2345	0.6000
2.750	0.1374	0.2125	0.6500
3.165	0.1111	0.1888	0.7000
3.704	0.0866	0.1633	0.7500
4.453	0.0642	0.1357	0.8000
5.610	0.0442	0.1057	0.8500
7.757	0.0269	0.0730	0.9000

K1 = 1.00 AND K2 = 0.10

τ	α	β	γ
0.050	0.9524	0.0475	0.0000
0.550	0.6693	0.3276	0.0029
1.050	0.5613	0.4280	0.0105
1.550	0.5178	0.4614	0.0206
2.050	0.4982	0.4701	0.0315
2.550	0.4873	0.4699	0.0426
3.050	0.4798	0.4664	0.0536
3.550	0.4736	0.4619	0.0643
4.050	0.4680	0.4570	0.0749
4.550	0.4626	0.4520	0.0852
5.282	0.4550	0.4449	0.1000
7.954	0.4295	0.4204	0.1500
10.957	0.4039	0.3960	0.2000
14.356	0.3785	0.3714	0.2500
18.236	0.3530	0.3469	0.3000
22.706	0.3276	0.3223	0.3500
27.915	0.3022	0.2977	0.4000
34.063	0.2768	0.2731	0.4500
41.432	0.2515	0.2484	0.5000
50.428	0.2262	0.2237	0.5500
61.657	0.2009	0.1990	0.6000
76.077	0.1757	0.1742	0.6500
95.280	0.1505	0.1494	0.7000
122.130	0.1253	0.1246	0.7500
162.354	0.1002	0.0997	0.8000
229.309	0.0751	0.0748	0.8500
363.049	0.0500	0.0499	0.9000

K1 = 0.30 AND K2 = 10.00

0.050	0.9515	0.0480	0.0003
0.100	0.9062	0.0908	0.0029
0.150	0.8636	0.1273	0.0089
0.200	0.8235	0.1571	0.0192
0.250	0.7859	0.1805	0.0335
0.300	0.7503	0.1980	0.0516
0.350	0.7167	0.2106	0.0725
0.400	0.6849	0.2193	0.0957
0.450	0.6547	0.2247	0.1204
0.500	0.6261	0.2277	0.1460
0.604	0.5766	0.2233	0.2000
0.434	0.5836	0.1663	0.2500
0.600	0.5231	0.1768	0.3000
0.762	0.4684	0.1815	0.3500
0.923	0.4180	0.1819	0.4000
1.088	0.3708	0.1791	0.4500
1.256	0.3261	0.1738	0.5000
1.432	0.2832	0.1667	0.5500
1.622	0.2426	0.1573	0.6000
1.839	0.2041	0.1458	0.6500
2.097	0.1672	0.1327	0.7000
2.415	0.1318	0.1181	0.7500
2.830	0.0982	0.1017	0.8000
3.417	0.0667	0.0832	0.8500
4.383	0.0384	0.0615	0.9000

K1 = 1.00 AND K2 = 0.30

0.050	0.9524	0.0475	0.0000
0.550	0.6688	0.3223	0.0087
1.050	0.5570	0.4124	0.0304
1.404	0.5214	0.4285	0.0500
2.292	0.4698	0.4301	0.1000
3.232	0.4391	0.4108	0.1500
4.277	0.4120	0.3879	0.2000
5.454	0.3855	0.3644	0.2500
6.797	0.3591	0.3408	0.3000
8.339	0.3329	0.3170	0.3500
10.129	0.3067	0.2932	0.4000
12.240	0.2806	0.2693	0.4500
14.762	0.2546	0.2453	0.5000
17.833	0.2287	0.2212	0.5500
21.657	0.2029	0.1970	0.6000
26.554	0.1772	0.1727	0.6500
33.060	0.1516	0.1483	0.7000
42.135	0.1261	0.1238	0.7500
55.694	0.1007	0.0992	0.8000
78.207	0.0754	0.0745	0.8500
123.059	0.0501	0.0498	0.9000

Table A-II, continued. Composition vs. Time for Two Consecutive Reaction Steps with First Step Reversible ($A \rightleftharpoons B$, $2B \rightarrow C$).

K1 = 1.00 AND K2 = 1.00

τ	α	β	γ
0.050	0.9524	0.0475	0.0000
0.100	0.9093	0.0903	0.0002
0.150	0.8703	0.1287	0.0008
0.200	0.8350	0.1629	0.0019
0.250	0.8030	0.1933	0.0035
0.300	0.7739	0.2202	0.0057
0.350	0.7475	0.2440	0.0084
0.400	0.7235	0.2647	0.0116
0.450	0.7016	0.2829	0.0154
0.500	0.6816	0.2987	0.0196
0.750	0.6169	0.3330	0.0500
1.137	0.5298	0.3701	0.1000
1.501	0.4813	0.3686	0.1500
1.880	0.4438	0.3561	0.2000
2.294	0.4110	0.3389	0.2500
2.755	0.3805	0.3194	0.3000
3.278	0.3510	0.2989	0.3500
3.880	0.3221	0.2778	0.4000
4.582	0.2936	0.2563	0.4500
5.413	0.2654	0.2345	0.5000
6.416	0.2375	0.2124	0.5500
7.654	0.2099	0.1900	0.6000
9.225	0.1826	0.1673	0.6500
11.293	0.1556	0.1443	0.7000
14.151	0.1288	0.1211	0.7500
18.383	0.1024	0.0975	0.8000
25.347	0.0764	0.0735	0.8500
39.095	0.0506	0.0493	0.9000

K1 = 1.00 AND K2 = 3.00

0.050	0.9524	0.0474	0.0001
0.100	0.9093	0.0898	0.0008
0.150	0.8703	0.1270	0.0026
0.200	0.8348	0.1593	0.0057
0.250	0.8026	0.1870	0.0102
0.300	0.7732	0.2105	0.0162
0.350	0.7462	0.2301	0.0235
0.400	0.7215	0.2464	0.0320
0.450	0.6986	0.2596	0.0417
0.500	0.6775	0.2702	0.0522
0.685	0.6209	0.2790	0.1000
0.838	0.5656	0.2843	0.1500
1.049	0.5177	0.2822	0.2000
1.263	0.4731	0.2768	0.2500
1.488	0.4326	0.2673	0.3000
1.732	0.3954	0.2545	0.3500
2.005	0.3599	0.2400	0.4000
2.314	0.3258	0.2241	0.4500
2.672	0.2925	0.2074	0.5000
3.095	0.2599	0.1900	0.5500
3.604	0.2280	0.1719	0.6000
4.236	0.1967	0.1532	0.6500
5.049	0.1662	0.1337	0.7000
6.144	0.1363	0.1136	0.7500
7.726	0.1073	0.0926	0.8000
10.262	0.0791	0.0708	0.8500
15.139	0.0518	0.0481	0.9000

K1 = 1.00 AND K2 = 10.00

τ	α	β	γ
0.050	0.9524	0.0003	0.0472
0.100	0.9092	0.0027	0.0879
0.150	0.8700	0.0083	0.1215
0.200	0.8342	0.0175	0.1481
0.250	0.8013	0.0301	0.1684
0.300	0.7708	0.0457	0.1833
0.350	0.7424	0.0636	0.1939
0.400	0.7159	0.0831	0.2009
0.450	0.6909	0.1038	0.2052
0.500	0.6672	0.1251	0.2075
0.984	0.4847	0.1652	0.3500
1.174	0.4358	0.1641	0.4000
1.367	0.3899	0.1600	0.4500
1.570	0.3470	0.1529	0.5000
1.797	0.3065	0.1434	0.5500
2.060	0.2675	0.1324	0.6000
2.373	0.2295	0.1204	0.6500
2.758	0.1924	0.1075	0.7000
3.253	0.1562	0.0937	0.7500
3.929	0.1212	0.0787	0.8000
4.945	0.0877	0.0622	0.8500
6.755	0.0559	0.0440	0.9000

K1 = 3.00 AND K2 = 0.10

0.050	0.9547	0.0453	0.0000
0.100	0.9176	0.0824	0.0000
0.150	0.8872	0.1127	0.0001
0.200	0.8623	0.1375	0.0002
0.250	0.8419	0.1578	0.0003
0.300	0.8252	0.1744	0.0004
0.350	0.8115	0.1879	0.0006
0.400	0.8003	0.1990	0.0008
0.450	0.7910	0.2080	0.0010
0.500	0.7835	0.2154	0.0012
0.950	0.7538	0.2425	0.0036
4.515	0.7324	0.2426	0.0250
8.736	0.7645	0.1855	0.0500
13.668	0.7229	0.1998	0.0772
30.468	0.6322	0.1963	0.1714
41.775	0.5882	0.1912	0.2206
63.865	0.5266	0.1734	0.3000
80.672	0.4886	0.1614	0.3500
86.522	0.4769	0.1581	0.3650
93.698	0.4643	0.1532	0.3825
110.244	0.4534	0.1109	0.4357
124.054	0.4295	0.0969	0.4736
153.131	0.3879	0.0809	0.5312
169.052	0.3654	0.0792	0.5554
204.726	0.3287	0.0728	0.5985
253.533	0.2883	0.0673	0.6443

Table A-II, continued. Composition vs. Time for Two Consecutive Reaction Steps with First Step Reversible ($A \rightleftharpoons B$, $2B \rightarrow C$).

K1 = 3.00 AND K2 = 0.30

τ	α	β	γ
0.050	0.9546	0.0453	0.0000
0.550	0.8180	0.1733	0.0085
1.050	0.7661	0.2174	0.0163
1.550	0.7436	0.2316	0.0246
2.050	0.7315	0.2353	0.0330
2.550	0.7231	0.2353	0.0414
3.050	0.7162	0.2340	0.0497
3.550	0.7097	0.2323	0.0579
4.050	0.7036	0.2304	0.0659
4.550	0.6976	0.2285	0.0738
6.268	0.6778	0.2221	0.1000
9.839	0.6400	0.2100	0.1500
13.852	0.6022	0.1977	0.2000
18.393	0.5644	0.1855	0.2500
23.576	0.5267	0.1732	0.3000
29.548	0.4889	0.1610	0.3500
36.506	0.4512	0.1487	0.4000
44.717	0.4135	0.1364	0.4500
54.557	0.3758	0.1241	0.5000
66.567	0.3382	0.1117	0.5500
81.559	0.3005	0.0994	0.6000
100.807	0.2629	0.0870	0.6500
126.435	0.2253	0.0746	0.7000
162.264	0.1877	0.0622	0.7500
215.933	0.1501	0.0498	0.8000
305.253	0.1125	0.0374	0.8500
483.639	0.0750	0.0249	0.9000

K1 = 3.00 AND K2 = 3.00

τ	α	β	γ
0.050	0.9546	0.0452	0.0001
0.099	0.9175	0.0817	0.0007
0.149	0.8869	0.1108	0.0021
0.199	0.8616	0.1338	0.0044
0.249	0.8406	0.1518	0.0075
0.299	0.8229	0.1657	0.0113
0.349	0.8078	0.1764	0.0157
0.399	0.7949	0.1844	0.0206
0.449	0.7835	0.1905	0.0258
0.499	0.7735	0.1949	0.0314
0.648	0.7543	0.1956	0.0500
1.018	0.7190	0.1809	0.1000
1.490	0.6614	0.1885	0.1500
1.978	0.6196	0.1803	0.2000
2.520	0.5797	0.1702	0.2500
3.133	0.5401	0.1598	0.3000
3.831	0.5006	0.1493	0.3500
4.636	0.4613	0.1386	0.4000
5.575	0.4221	0.1278	0.4500
6.689	0.3830	0.1169	0.5000
8.033	0.3440	0.1059	0.5500
9.693	0.3052	0.0947	0.6000
11.799	0.2665	0.0834	0.6500
14.571	0.2279	0.0720	0.7000
18.402	0.1895	0.0604	0.7500
24.071	0.1513	0.0486	0.8000
33.393	0.1132	0.0367	0.8500

K1 = 3.00 AND K2 = 1.00

0.050	0.9546	0.0452	0.0000
0.550	0.8178	0.1524	0.0296
1.050	0.7523	0.1939	0.0536
1.550	0.7147	0.2079	0.0772
2.050	0.6890	0.2105	0.1004
2.550	0.6685	0.2085	0.1228
3.050	0.6506	0.2048	0.1444
3.550	0.6342	0.2006	0.1650
4.050	0.6189	0.1962	0.1847
4.550	0.6043	0.1919	0.2036
5.884	0.5687	0.1812	0.2500
7.510	0.5304	0.1695	0.3000
9.382	0.4922	0.1577	0.3500
11.551	0.4540	0.1459	0.4000
14.107	0.4159	0.1340	0.4500
17.160	0.3778	0.1221	0.5000
20.875	0.3398	0.1101	0.5500
25.495	0.3018	0.0981	0.6000
31.411	0.2639	0.0860	0.6500
39.262	0.2260	0.0739	0.7000
50.202	0.1882	0.0617	0.7500
66.537	0.1504	0.0495	0.8000
93.636	0.1127	0.0372	0.8500
147.578	0.0751	0.0248	0.9000

K1 = 3.00 AND K2 = 10.00

0.050	0.9546	0.0449	0.0003
0.100	0.9174	0.0801	0.0024
0.150	0.8864	0.1066	0.0068
0.200	0.8603	0.1259	0.0137
0.250	0.8378	0.1395	0.0225
0.300	0.8181	0.1488	0.0330
0.350	0.8004	0.1548	0.0446
0.400	0.7844	0.1586	0.0569
0.450	0.7695	0.1607	0.0696
0.500	0.7556	0.1616	0.0827
1.445	0.5660	0.1339	0.3000
1.736	0.5222	0.1277	0.3500
2.062	0.4800	0.1199	0.4000
2.436	0.4383	0.1116	0.4500
2.870	0.3969	0.1030	0.5000
3.385	0.3557	0.0942	0.5500
4.007	0.3148	0.0851	0.6000
4.780	0.2741	0.0758	0.6500
5.775	0.2338	0.0661	0.7000
7.118	0.1937	0.0562	0.7500
9.055	0.1541	0.0458	0.8000
12.157	0.1149	0.0350	0.8500
18.103	0.0761	0.0238	0.9000

Table A-II, continued. Composition vs. Time for Two Consecutive Reaction Steps with First Step Reversible (A $\rightleftharpoons$ B, 2B $\rightarrow$ C).

K1 = 10.00 AND K2 = 0.10

τ	α	β	γ
0.050	0.9616	0.0384	0.0000
0.100	0.9394	0.0606	0.0000
0.150	0.9266	0.0734	0.0000
0.200	0.9192	0.0808	0.0001
0.250	0.9149	0.0850	0.0001
0.300	0.9124	0.0875	0.0001
0.350	0.9109	0.0889	0.0002
0.400	0.9101	0.0897	0.0002
0.450	0.9096	0.0902	0.0003
0.500	0.9093	0.0904	0.0003
1.050	0.9085	0.0908	0.0008
2.008	0.9078	0.0907	0.0015
3.840	0.9064	0.0906	0.0030
5.445	0.9052	0.0904	0.0044
8.115	0.9032	0.0902	0.0065
10.413	0.9015	0.0901	0.0084
12.712	0.8998	0.0899	0.0103
15.519	0.8978	0.0897	0.0125
18.024	0.8959	0.0895	0.0145
20.933	0.8938	0.0893	0.0169
25.554	0.8905	0.0890	0.0205
29.679	0.8875	0.0887	0.0238
34.469	0.8841	0.0883	0.0276
40.032	0.8802	0.0879	0.0319
46.494	0.8757	0.0875	0.0368
51.371	0.8723	0.0872	0.0406

K1 = 10.00 AND K2 = 0.30

τ	α	β	γ
0.050	0.9616	0.0384	0.0000
0.100	0.9394	0.0606	0.0000
0.150	0.9265	0.0733	0.0001
0.200	0.9191	0.0807	0.0002
0.250	0.9148	0.0849	0.0003
0.300	0.9122	0.0874	0.0004
0.350	0.9107	0.0887	0.0005
0.400	0.9098	0.0895	0.0007
0.450	0.9092	0.0900	0.0008
0.500	0.9088	0.0903	0.0009
1.050	0.9072	0.0905	0.0023
1.489	0.9063	0.0904	0.0033
2.451	0.9041	0.0902	0.0057
5.180	0.8981	0.0896	0.0123
7.720	0.8926	0.0890	0.0184
10.946	0.8857	0.0884	0.0260
15.519	0.8760	0.0874	0.0366
20.933	0.8649	0.0863	0.0488
29.679	0.8475	0.0846	0.0680
40.032	0.8277	0.0826	0.0897
56.759	0.7977	0.0796	0.1227

K1 = 10.00 AND K2 = 1.00

τ	α	β	γ
0.050	0.9616	0.0384	0.0000
0.100	0.9394	0.0605	0.0002
0.150	0.9265	0.0732	0.0004
0.200	0.9189	0.0804	0.0007
0.250	0.9144	0.0845	0.0010
0.300	0.9117	0.0869	0.0014
0.350	0.9100	0.0882	0.0018
0.400	0.9088	0.0890	0.0022
0.450	0.9080	0.0894	0.0026
0.500	0.9074	0.0896	0.0030
1.050	0.9030	0.0896	0.0074
2.332	0.8938	0.0887	0.0176
4.688	0.8772	0.0870	0.0358
6.596	0.8642	0.0858	0.0500
13.770	0.8187	0.0813	0.1000
21.783	0.7732	0.0768	0.1500
30.790	0.7277	0.0723	0.2000
40.990	0.6822	0.0678	0.2500
52.639	0.6367	0.0633	0.3000

K1 = 10.00 AND K2 = 3.00

τ	α	β	γ
0.050	0.9616	0.0383	0.0001
0.100	0.9393	0.0602	0.0005
0.150	0.9262	0.0726	0.0012
0.200	0.9184	0.0796	0.0020
0.250	0.9134	0.0835	0.0030
0.300	0.9102	0.0857	0.0041
0.350	0.9079	0.0868	0.0052
0.400	0.9062	0.0875	0.0064
0.450	0.9047	0.0878	0.0075
0.500	0.9034	0.0879	0.0087
1.050	0.8916	0.0871	0.0213
1.565	0.8810	0.0861	0.0329
2.347	0.8654	0.0846	0.0500
4.804	0.8198	0.0802	0.1000
7.543	0.7742	0.0758	0.1500
10.618	0.7285	0.0715	0.2000
14.096	0.6829	0.0671	0.2500
18.062	0.6373	0.0627	0.3000
22.629	0.5918	0.0582	0.3500
27.945	0.5462	0.0538	0.4000
34.213	0.5006	0.0494	0.4500
41.719	0.4550	0.0450	0.5000
50.873	0.4095	0.0405	0.5500

K1 = 10.00 AND K2 = 10.00

τ	α	β	γ
0.050	0.9615	0.0382	0.0003
0.100	0.9390	0.0594	0.0016
0.150	0.9254	0.0709	0.0037
0.200	0.9165	0.0770	0.0065
0.250	0.9102	0.0802	0.0096
0.300	0.9054	0.0817	0.0129
0.350	0.9013	0.0825	0.0163
0.400	0.8976	0.0827	0.0197
0.450	0.8942	0.0827	0.0231
0.500	0.8909	0.0826	0.0265
0.851	0.8691	0.0809	0.0500
1.655	0.8231	0.0769	0.1000
2.548	0.7772	0.0728	0.1500
3.546	0.7312	0.0688	0.2000
4.670	0.6853	0.0647	0.2500
5.946	0.6394	0.0606	0.3000
7.408	0.5936	0.0564	0.3500
9.103	0.5477	0.0523	0.4000
11.092	0.5019	0.0481	0.4500
13.464	0.4561	0.0439	0.5000
16.342	0.4104	0.0396	0.5500
19.916	0.3647	0.0353	0.6000
24.478	0.3190	0.0310	0.6500
30.518	0.2733	0.0267	0.7000
38.914	0.2277	0.0223	0.7500
51.418	0.1821	0.0179	0.8000
66.880	0.1451	0.0049	0.8500

Table A-III. Composition vs. Time for Two Consecutive Reaction Steps with Second Step Reversible (A → B, 2B ⇌ C).

K1 = 0.10 AND K2 = 0.10

τ	α	β	γ
0.050	0.9512	0.0488	0.0000
0.100	0.9048	0.0951	0.0000
0.150	0.8607	0.1392	0.0001
0.200	0.8187	0.1810	0.0002
0.250	0.7788	0.2208	0.0004
0.300	0.7408	0.2585	0.0007
0.350	0.7047	0.2942	0.0011
0.400	0.6703	0.3281	0.0016
0.450	0.6376	0.3602	0.0022
0.500	0.6065	0.3906	0.0028
0.550	0.5769	0.4194	0.0037
0.600	0.5488	0.4466	0.0046
0.650	0.5220	0.4724	0.0056
0.700	0.4966	0.4967	0.0067
0.750	0.4724	0.5196	0.0080
0.800	0.4493	0.5413	0.0094
0.850	0.4274	0.5617	0.0108
0.900	0.4066	0.5810	0.0124
0.950	0.3867	0.5992	0.0141
1.551	0.2120	0.7474	0.0406
1.727	0.1780	0.7720	0.0500
2.595	0.0748	0.8252	0.1000
3.496	0.0304	0.8196	0.1500
4.553	0.0106	0.7894	0.2000
5.930	0.0027	0.7473	0.2500
7.979	0.0003	0.6997	0.3000
12.095	0.0000	0.6500	0.3500

K1 = 0.10 AND K2 = 1.00

τ	α	β	γ
0.050	0.9512	0.0488	0.0000
0.100	0.9048	0.0951	0.0000
0.150	0.8607	0.1392	0.0001
0.200	0.8187	0.1811	0.0002
0.250	0.7788	0.2208	0.0004
0.300	0.7408	0.2585	0.0007
0.350	0.7047	0.2943	0.0010
0.400	0.6703	0.3282	0.0014
0.450	0.6376	0.3604	0.0019
0.500	0.6065	0.3909	0.0025
0.550	0.5769	0.4198	0.0032
0.600	0.5488	0.4472	0.0040
0.650	0.5220	0.4731	0.0048
0.700	0.4966	0.4977	0.0057
0.750	0.4724	0.5209	0.0067
0.800	0.4493	0.5429	0.0078
0.850	0.4274	0.5637	0.0089
0.900	0.4066	0.5834	0.0101
0.950	0.3867	0.6020	0.0113
1.551	0.2120	0.7598	0.0283
2.527	0.0799	0.8664	0.0537
4.116	0.0163	0.9085	0.0752

K1 = 0.10 AND K2 = 0.30

0.050	0.9512	0.0488	0.0000
0.100	0.9048	0.0951	0.0000
0.150	0.8607	0.1392	0.0001
0.200	0.8187	0.1810	0.0002
0.250	0.7788	0.2208	0.0004
0.300	0.7408	0.2585	0.0007
0.350	0.7047	0.2942	0.0011
0.400	0.6703	0.3281	0.0015
0.450	0.6376	0.3603	0.0021
0.500	0.6065	0.3907	0.0028
0.550	0.5769	0.4195	0.0035
0.600	0.5488	0.4468	0.0044
0.650	0.5220	0.4725	0.0054
0.700	0.4966	0.4969	0.0065
0.750	0.4724	0.5199	0.0077
0.800	0.4493	0.5417	0.0090
0.850	0.4274	0.5622	0.0103
0.900	0.4066	0.5816	0.0118
0.950	0.3867	0.5999	0.0134
1.551	0.2120	0.7508	0.0372
1.8	0.1611	0.7889	0.0500
2.921	0.0539	0.8461	0.1000
4.425	0.0120	0.8380	0.1500
8.690	0.0002	0.7998	0.2000

K1 = 0.10 AND K2 = 3.00

0.050	0.9512	0.0488	0.0000
0.100	0.9048	0.0951	0.0000
0.150	0.8607	0.1392	0.0001
0.200	0.8187	0.1811	0.0002
0.250	0.7788	0.2208	0.0004
0.300	0.7408	0.2586	0.0006
0.350	0.7047	0.2945	0.0009
0.400	0.6703	0.3285	0.0012
0.450	0.6376	0.3608	0.0016
0.500	0.6065	0.3915	0.0020
0.550	0.5769	0.4205	0.0025
0.600	0.5488	0.4482	0.0030
0.650	0.5220	0.4744	0.0036
0.700	0.4966	0.4992	0.0042
0.750	0.4724	0.5228	0.0048
0.800	0.4493	0.5452	0.0055
0.850	0.4274	0.5664	0.0062
0.900	0.4066	0.5866	0.0068
0.950	0.3867	0.6057	0.0075
1.551	0.2120	0.7723	0.0158
2.527	0.0799	0.8954	0.0247

Table A-III, continued. Composition vs. Time for Two Consecutive Reaction Steps with Second Step Reversible ($A \rightarrow B$, $2B \rightleftarrows C$).

K1 = 0.10 AND K2 = 10.00

τ	α	β	γ
0.050	0.9512	0.0488	0.0000
0.100	0.9048	0.0951	0.0001
0.150	0.8607	0.1390	0.0003
0.200	0.8187	0.1806	0.0007
0.250	0.7788	0.2199	0.0013
0.300	0.7408	0.2571	0.0021
0.350	0.7047	0.2921	0.0033
0.400	0.6703	0.3250	0.0047
0.450	0.6376	0.3560	0.0064
0.500	0.6065	0.3851	0.0084
0.550	0.5769	0.4123	0.0107
0.600	0.5488	0.4378	0.0134
0.650	0.5220	0.4616	0.0164
0.700	0.4966	0.4838	0.0196
0.750	0.4724	0.5045	0.0232
0.800	0.4493	0.5237	0.0270
0.850	0.4274	0.5415	0.0311
0.900	0.4066	0.5579	0.0355
0.950	0.3867	0.5732	0.0401
1.050	0.3499	0.6001	0.0500
1.480	0.2276	0.6724	0.1000
1.868	0.1545	0.6955	0.1500
2.258	0.1046	0.6954	0.2000
2.675	0.0690	0.6810	0.2500
3.144	0.0432	0.6568	0.3000
3.695	0.0249	0.6251	0.3500
4.385	0.0125	0.5875	0.4000
5.324	0.0049	0.5451	0.4500
6.821	0.0011	0.4989	0.5000
10.700	0.0000	0.4500	0.5500

K1 = 0.30 AND K2 = 0.30

τ	α	β	γ
0.050	0.9512	0.0488	0.0000
0.100	0.9048	0.0951	0.0001
0.150	0.8607	0.1390	0.0003
0.200	0.8187	0.1806	0.0007
0.250	0.7788	0.2199	0.0013
0.300	0.7408	0.2571	0.0021
0.350	0.7047	0.2921	0.0032
0.400	0.6703	0.3251	0.0046
0.450	0.6376	0.3561	0.0062
0.500	0.6065	0.3853	0.0082
0.550	0.5769	0.4126	0.0104
0.600	0.5488	0.4382	0.0130
0.650	0.5220	0.4621	0.0158
0.700	0.4966	0.4845	0.0189
0.750	0.4724	0.5054	0.0223
0.800	0.4493	0.5248	0.0259
0.850	0.4274	0.5428	0.0298
0.900	0.4066	0.5596	0.0338
0.950	0.3867	0.5751	0.0381
1.078	0.3403	0.6097	0.0500
1.549	0.2125	0.6875	0.1000
1.999	0.1355	0.7145	0.1500
2.491	0.0829	0.7171	0.2000
3.086	0.0457	0.7043	0.2500
3.909	0.0201	0.6799	0.3000
5.449	0.0043	0.6457	0.3500
6.705	0.0012	0.6312	0.3676
10.921	0.0000	0.6189	0.3811
17.790	0.0000	0.6180	0.3820

K1 = 0.30 AND K2 = 0.10

0.050	0.9512	0.0488	0.0000
0.100	0.9048	0.0951	0.0000
0.150	0.8607	0.1392	0.0001
0.200	0.8187	0.1811	0.0001
0.250	0.7788	0.2209	0.0003
0.300	0.7408	0.2588	0.0004
0.350	0.7047	0.2948	0.0005
0.400	0.6703	0.3290	0.0007
0.450	0.6376	0.3615	0.0009
0.500	0.6065	0.3924	0.0011
0.550	0.5769	0.4217	0.0013
0.600	0.5488	0.4496	0.0016
0.650	0.5220	0.4762	0.0018
0.700	0.4966	0.5014	0.0020
0.750	0.4724	0.5254	0.0023
0.800	0.4493	0.5482	0.0025
0.850	0.4274	0.5698	0.0028
0.900	0.4066	0.5904	0.0030
0.950	0.3867	0.6100	0.0032
1.551	0.2120	0.7823	0.0058
2.527	0.0799	0.9119	0.0082

K1 = 0.30 AND K2 = 1.00

0.050	0.9512	0.0488	0.0000
0.100	0.9048	0.0951	0.0001
0.150	0.8607	0.1390	0.0003
0.200	0.8187	0.1806	0.0007
0.250	0.7788	0.2200	0.0012
0.300	0.7408	0.2572	0.0020
0.350	0.7047	0.2923	0.0030
0.400	0.6703	0.3254	0.0043
0.450	0.6376	0.3566	0.0058
0.500	0.6065	0.3860	0.0075
0.550	0.5769	0.4136	0.0095
0.600	0.5488	0.4395	0.0117
0.650	0.5220	0.4639	0.0141
0.700	0.4966	0.4867	0.0167
0.750	0.4724	0.5081	0.0195
0.800	0.4493	0.5282	0.0225
0.850	0.4274	0.5469	0.0256
0.900	0.4066	0.5645	0.0289
0.950	0.3867	0.5810	0.0323
1.193	0.3034	0.6466	0.0500
1.873	0.1538	0.7462	0.1000
2.831	0.0591	0.7909	0.1500
4.116	0.0163	0.8033	0.1804
6.705	0.0012	0.8054	0.1934

Table A-III, continued. Composition vs. Time for Two Consecutive Reaction Steps with Second Step Reversible ($A \rightarrow B$, $2B \rightleftharpoons C$).

K1 = 0.30 AND K2 = 3.00

τ	α	β	γ
0.050	0.9512	0.0488	0.0000
0.100	0.9048	0.0951	0.0001
0.150	0.8607	0.1390	0.0003
0.200	0.8187	0.1807	0.0006
0.250	0.7788	0.2201	0.0011
0.300	0.7408	0.2575	0.0017
0.350	0.7047	0.2928	0.0025
0.400	0.6703	0.3261	0.0035
0.450	0.6376	0.3577	0.0047
0.500	0.6065	0.3875	0.0060
0.550	0.5769	0.4157	0.0074
0.600	0.5488	0.4423	0.0089
0.650	0.5220	0.4674	0.0106
0.700	0.4966	0.4911	0.0123
0.750	0.4724	0.5135	0.0141
0.800	0.4493	0.5347	0.0160
0.850	0.4274	0.5547	0.0179
0.900	0.4066	0.5736	0.0198
0.950	0.3867	0.5915	0.0218
1.551	0.2120	0.7437	0.0443
2.527	0.0799	0.8526	0.0675
4.116	0.0163	0.9033	0.0804

K1 = 0.30 AND K2 = 10.00

0.050	0.9512	0.0488	0.0000
0.100	0.9048	0.0951	0.0001
0.150	0.8607	0.1391	0.0002
0.200	0.8187	0.1808	0.0004
0.250	0.7788	0.2204	0.0008
0.300	0.7408	0.2580	0.0011
0.350	0.7047	0.2937	0.0016
0.400	0.6703	0.3276	0.0021
0.450	0.6376	0.3597	0.0027
0.500	0.6065	0.3902	0.0033
0.550	0.5769	0.4191	0.0040
0.600	0.5488	0.4466	0.0046
0.650	0.5220	0.4726	0.0053
0.700	0.4966	0.4974	0.0060
0.750	0.4724	0.5209	0.0067
0.800	0.4493	0.5432	0.0074
0.850	0.4274	0.5644	0.0081
0.900	0.4066	0.5846	0.0088
0.950	0.3867	0.6037	0.0095
1.551	0.2120	0.7712	0.0168
2.527	0.0799	0.8964	0.0237

K1 = 1.00 AND K2 = 0.10

τ	α	β	γ
0.050	0.9512	0.0487	0.0000
0.100	0.9048	0.0949	0.0003
0.150	0.8607	0.1383	0.0010
0.200	0.8187	0.1790	0.0023
0.250	0.7788	0.2170	0.0042
0.300	0.7408	0.2522	0.0069
0.350	0.7047	0.2848	0.0105
0.400	0.6703	0.3147	0.0150
0.450	0.6376	0.3421	0.0203
0.500	0.6065	0.3670	0.0265
0.651	0.5216	0.4284	0.0500
0.892	0.4098	0.4902	0.1000
1.098	0.3334	0.5166	0.1500
1.294	0.2742	0.5258	0.2000
1.491	0.2252	0.5248	0.2500
1.696	0.1835	0.5165	0.3000
1.916	0.1473	0.5027	0.3500
2.158	0.1156	0.4844	0.4000
2.434	0.0878	0.4622	0.4500
2.758	0.0635	0.4365	0.5000
3.158	0.0426	0.4074	0.5500
3.685	0.0252	0.3748	0.6000
4.469	0.0115	0.3385	0.6500
6.051	0.0024	0.2976	0.7000
6.705	0.0012	0.2888	0.7100
10.921	0.0000	0.2715	0.7285
17.790	0.0000	0.2702	0.7298

K1 = 1.00 AND K2 = 0.30

0.050	0.9512	0.0487	0.0000
0.100	0.9048	0.0949	0.0003
0.150	0.8607	0.1383	0.0010
0.200	0.8187	0.1790	0.0022
0.250	0.7788	0.2170	0.0042
0.300	0.7408	0.2523	0.0068
0.350	0.7047	0.2850	0.0103
0.400	0.6703	0.3150	0.0147
0.450	0.6376	0.3426	0.0198
0.500	0.6065	0.3677	0.0258
0.660	0.5169	0.4331	0.0500
0.912	0.4017	0.4983	0.1000
1.132	0.3225	0.5275	0.1500
1.346	0.2603	0.5397	0.2000
1.568	0.2085	0.5415	0.2500
1.808	0.1640	0.5360	0.3000
2.080	0.1250	0.5250	0.3500
2.403	0.0905	0.5095	0.4000
2.814	0.0600	0.4900	0.4500
3.400	0.0334	0.4666	0.5000
4.512	0.0110	0.4390	0.5500
6.705	0.0012	0.4212	0.5776
10.921	0.0000	0.4180	0.5820
17.790	0.0000	0.4179	0.5821

Table A-III, continued. Composition vs. Time for Two Consecutive Reaction Steps with Second Step Reversible ($A \rightarrow B$, $2B \rightleftarrows C$).

K1 = 1.00 AND K2 = 1.00

τ	α	β	γ
0.050	0.9512	0.0487	0.0000
0.100	0.9048	0.0949	0.0003
0.150	0.8607	0.1383	0.0010
0.200	0.8187	0.1791	0.0022
0.250	0.7788	0.2172	0.0040
0.300	0.7408	0.2527	0.0065
0.350	0.7047	0.2856	0.0097
0.400	0.6703	0.3160	0.0137
0.450	0.6376	0.3440	0.0183
0.500	0.6065	0.3698	0.0237
0.695	0.4990	0.4510	0.0500
0.990	0.3717	0.5283	0.1000
1.270	0.2808	0.5692	0.1500
1.576	0.2069	0.5931	0.2000
1.946	0.1430	0.6070	0.2500
2.461	0.0855	0.6145	0.3000
3.433	0.0324	0.6176	0.3500
4.116	0.0163	0.6179	0.3657
6.705	0.0012	0.6180	0.3807
10.921	0.0000	0.6180	0.3819

K1 = 1.00 AND K2 = 10.00

τ	α	β	γ
0.050	0.9512	0.0487	0.0000
0.100	0.9048	0.0949	0.0002
0.150	0.8607	0.1386	0.0007
0.200	0.8167	0.1798	0.0015
0.250	0.7788	0.2187	0.0025
0.300	0.7408	0.2554	0.0038
0.350	0.7047	0.2901	0.0052
0.400	0.6703	0.3228	0.0069
0.450	0.6376	0.3536	0.0087
0.500	0.6065	0.3828	0.0107
0.550	0.5769	0.4103	0.0127
0.600	0.5488	0.4364	0.0148
0.650	0.5220	0.4610	0.0169
0.700	0.4966	0.4843	0.0191
0.750	0.4724	0.5063	0.0213
0.800	0.4493	0.5272	0.0235
0.850	0.4274	0.5470	0.0256
0.900	0.4066	0.5657	0.0278
0.950	0.3867	0.5834	0.0299
1.551	0.2120	0.7367	0.0514
2.527	0.0799	0.8492	0.0709
4.116	0.0163	0.9025	0.0812

K1 = 1.00 AND K2 = 3.00

0.050	0.9512	0.0487	0.0000
0.100	0.9048	0.0949	0.0003
0.150	0.8607	0.1384	0.0009
0.200	0.8187	0.1793	0.0020
0.250	0.7788	0.2177	0.0035
0.300	0.7408	0.2535	0.0056
0.350	0.7047	0.2870	0.0083
0.400	0.6703	0.3183	0.0114
0.450	0.6376	0.3474	0.0150
0.500	0.6065	0.3745	0.0189
0.550	0.5769	0.3998	0.0233
0.600	0.5488	0.4233	0.0279
0.650	0.5220	0.4451	0.0328
0.700	0.4966	0.4655	0.0379
0.750	0.4724	0.4845	0.0431
0.800	0.4493	0.5023	0.0484
0.850	0.4274	0.5188	0.0538
0.900	0.4066	0.5342	0.0592
0.950	0.3867	0.5487	0.0646
1.299	0.2728	0.6272	0.1000
1.974	0.1389	0.7111	0.1500
2.527	0.0799	0.7459	0.1742
4.116	0.0163	0.7822	0.2015
6.705	0.0012	0.7906	0.2082
10.921	0.0000	0.7913	0.2087

K1 = 3.00 AND K2 = 0.10

0.050	0.9512	0.0487	0.0001
0.100	0.9048	0.0942	0.0009
0.150	0.8607	0.1364	0.0029
0.200	0.8187	0.1747	0.0066
0.250	0.7788	0.2091	0.0121
0.300	0.7408	0.2396	0.0196
0.350	0.7047	0.2662	0.0291
0.400	0.6703	0.2892	0.0405
0.450	0.6376	0.3087	0.0537
0.500	0.6065	0.3250	0.0685
0.594	0.5520	0.3480	0.1000
0.728	0.4830	0.3670	0.1500
0.854	0.4256	0.3744	0.2000
0.980	0.3756	0.3744	0.2500
1.108	0.3302	0.3698	0.3000
1.244	0.2884	0.3616	0.3500
1.389	0.2493	0.3507	0.4000
1.549	0.2125	0.3375	0.4500
1.729	0.1776	0.3224	0.5000
1.935	0.1446	0.3054	0.5500
2.178	0.1133	0.2867	0.6000
2.480	0.0839	0.2661	0.6500
2.875	0.0566	0.2434	0.7000
3.455	0.0317	0.2183	0.7500
4.565	0.0104	0.1896	0.8000
6.705	0.0012	0.1708	0.8280
10.921	0.0000	0.1668	0.8332
17.790	0.0000	0.1667	0.8333

Table A-III, continued. Composition vs. Time for Two Consecutive Reaction Steps with Second Step Reversible (A → B, 2B $\rightleftharpoons$ C).

K1 = 3.00 AND K2 = 0.30

τ	α	β	γ
0.050	0.9512	0.0487	0.0001
0.100	0.9048	0.0943	0.0009
0.150	0.8607	0.1364	0.0029
0.200	0.8187	0.1748	0.0065
0.250	0.7788	0.2093	0.0119
0.300	0.7408	0.2399	0.0193
0.350	0.7047	0.2667	0.0286
0.400	0.6703	0.2899	0.0397
0.450	0.6376	0.3098	0.0526
0.500	0.6065	0.3266	0.0669
0.602	0.5475	0.3525	0.1000
0.741	0.4767	0.3733	0.1500
0.874	0.4176	0.3824	0.2000
1.007	0.3654	0.3846	0.2500
1.146	0.3179	0.3821	0.3000
1.296	0.2737	0.3763	0.3500
1.461	0.2321	0.3679	0.4000
1.648	0.1925	0.3575	0.4500
1.868	0.1546	0.3454	0.5000
2.137	0.1181	0.3319	0.5500
2.489	0.0831	0.3169	0.6000
3.006	0.0496	0.3004	0.6500
4.034	0.0178	0.2822	0.7000
4.116	0.0163	0.2813	0.7024
6.705	0.0012	0.2711	0.7277
10.921	0.0000	0.2702	0.7298

K1 = 3.00 AND K2 = 1.00

0.050	0.9512	0.0487	0.0001
0.100	0.9048	0.0943	0.0009
0.150	0.8607	0.1365	0.0028
0.200	0.8187	0.1750	0.0063
0.250	0.7788	0.2098	0.0114
0.300	0.7408	0.2408	0.0183
0.350	0.7047	0.2683	0.0270
0.400	0.6703	0.2925	0.0372
0.450	0.6376	0.3135	0.0489
0.500	0.6065	0.3317	0.0617
0.632	0.5318	0.3682	0.1000
0.790	0.4540	0.3960	0.1500
0.948	0.3877	0.4123	0.2000
1.115	0.3278	0.4222	0.2500
1.303	0.2720	0.4280	0.3000
1.521	0.2186	0.4314	0.3500
1.791	0.1668	0.4332	0.4000
2.155	0.1160	0.4340	0.4500
2.724	0.0658	0.4342	0.5000
4.155	0.0157	0.4343	0.5500
6.705	0.0012	0.4343	0.5645
10.921	0.0000	0.4343	0.5657

K1 = 3.00 AND K2 = 3.00

τ	α	β	γ
0.050	0.9512	0.0487	0.0001
0.100	0.9048	0.0943	0.0009
0.150	0.8607	0.1367	0.0026
0.200	0.8187	0.1756	0.0057
0.250	0.7788	0.2110	0.0102
0.300	0.7408	0.2432	0.0160
0.350	0.7047	0.2722	0.0231
0.400	0.6703	0.2984	0.0313
0.450	0.6376	0.3220	0.0404
0.500	0.6065	0.3433	0.0502
0.729	0.4826	0.4174	0.1000
0.961	0.3828	0.4672	0.1500
1.227	0.2934	0.5066	0.2000
1.565	0.2093	0.5407	0.2500
2.054	0.1283	0.5717	0.3000
3.008	0.0495	0.6005	0.3500
4.116	0.0163	0.6123	0.3714
6.705	0.0012	0.6176	0.3812
10.921	0.0000	0.6180	0.3820

K1 = 3.00 AND K2 = 10.00

0.050	0.9512	0.0487	0.0001
0.100	0.9048	0.0944	0.0007
0.150	0.8607	0.1372	0.0021
0.200	0.8187	0.1770	0.0043
0.250	0.7788	0.2140	0.0072
0.300	0.7408	0.2484	0.0108
0.350	0.7047	0.2804	0.0149
0.400	0.6703	0.3102	0.0194
0.450	0.6376	0.3381	0.0243
0.500	0.6065	0.3641	0.0294
0.693	0.5001	0.4499	0.0500
1.207	0.2990	0.6010	0.1000
2.019	0.1329	0.7171	0.1500
2.527	0.0799	0.7528	0.1673
4.116	0.0163	0.7948	0.1889
5.711	0.0033	0.7967	0.2000

K1 = 10.00 AND K2 = 0.10

0.050	0.9512	0.0484	0.0004
0.100	0.9048	0.0922	0.0030
0.150	0.8607	0.1301	0.0092
0.200	0.8187	0.1614	0.0199
0.250	0.7788	0.1862	0.0350
0.300	0.7408	0.2052	0.0540
0.350	0.7047	0.2190	0.0763
0.400	0.6703	0.2287	0.1010
0.450	0.6376	0.2350	0.1273
0.500	0.6065	0.2387	0.1547
0.581	0.5595	0.2000	0.2405
0.671	0.5111	0.2500	0.2389
0.765	0.4654	0.3000	0.2346
0.864	0.4215	0.3500	0.2285
0.971	0.3788	0.4000	0.2212
1.088	0.3371	0.4500	0.2129
1.217	0.2962	0.5000	0.2038
1.363	0.2560	0.5500	0.1940
1.531	0.2165	0.6000	0.1835
1.728	0.1778	0.6500	0.1722
1.968	0.1398	0.7000	0.1602
2.275	0.1029	0.7500	0.1471
2.702	0.0672	0.8000	0.1328
3.402	0.0334	0.8500	0.1166

Table A-III, continued. Composition vs. Time for Two Consecutive Reaction Steps with Second Step Reversible ($A \rightarrow B$, $2B \rightleftharpoons C$).

K1 = 10.00 AND K2 = 0.30

TAU	A	B	C
0.050	0.9512	0.0484	0.0004
0.100	0.9048	0.0922	0.0030
0.150	0.8607	0.1301	0.0092
0.200	0.8187	0.1616	0.0197
0.250	0.7788	0.1866	0.0346
0.300	0.7408	0.2059	0.0533
0.350	0.7047	0.2202	0.0751
0.400	0.6703	0.2304	0.0993
0.450	0.6376	0.2374	0.1250
0.500	0.6065	0.2418	0.1517
0.589	0.5549	0.2451	0.2000
0.683	0.5053	0.2447	0.2500
0.781	0.4581	0.2419	0.3000
0.886	0.4125	0.2375	0.3500
1.000	0.3681	0.2319	0.4000
1.126	0.3244	0.2256	0.4500
1.269	0.2813	0.2187	0.5000
1.433	0.2387	0.2113	0.5500
1.627	0.1965	0.2035	0.6000
1.867	0.1548	0.1952	0.6500
2.177	0.1134	0.1866	0.7000
2.624	0.0726	0.1774	0.7500
3.431	0.0324	0.1676	0.8000
4.116	0.0163	0.1633	0.8204
6.705	0.0012	0.1592	0.8396
10.921	0.0000	0.1589	0.8411
17.790	0.0000	0.1589	0.8411

K1 = 10.00 AND K2 = 1.00

0.050	0.9512	0.0484	0.0004
0.100	0.9048	0.0923	0.0029
0.150	0.8607	0.1304	0.0089
0.200	0.8187	0.1622	0.0191
0.250	0.7788	0.1880	0.0332
0.300	0.7408	0.2083	0.0509
0.350	0.7047	0.2240	0.0713
0.400	0.6703	0.2360	0.0937
0.450	0.6376	0.2450	0.1174
0.500	0.6065	0.2517	0.1418
0.517	0.5967	0.2533	0.1500
0.619	0.5387	0.2613	0.2000
0.725	0.4844	0.2656	0.2500
0.839	0.4320	0.2680	0.3000
0.966	0.3808	0.2692	0.3500
1.108	0.3302	0.2698	0.4000
1.273	0.2800	0.2700	0.4500
1.470	0.2299	0.2701	0.5000
1.716	0.1799	0.2701	0.5500
2.043	0.1298	0.2702	0.6000
2.528	0.0798	0.2702	0.6500
3.514	0.0298	0.2702	0.7000
4.116	0.0163	0.2702	0.7135
6.705	0.0012	0.2702	0.7286
10.921	0.0000	0.2702	0.7298

K1 = 10.00 AND K2 = 3.00

TAU	A	B	C
0.050	0.9512	0.0484	0.0004
0.100	0.9048	0.0924	0.0028
0.150	0.8607	0.1310	0.0083
0.200	0.8187	0.1638	0.0174
0.250	0.7788	0.1914	0.0298
0.300	0.7408	0.2143	0.0449
0.350	0.7047	0.2333	0.0620
0.400	0.6703	0.2492	0.0805
0.450	0.6376	0.2626	0.0998
0.500	0.6065	0.2741	0.1194
0.578	0.5609	0.2891	0.1500
0.712	0.4905	0.3095	0.2000
0.860	0.4231	0.3269	0.2500
1.029	0.3574	0.3426	0.3000
1.229	0.2926	0.3574	0.3500
1.476	0.2286	0.3714	0.4000
1.801	0.1652	0.3848	0.4500
2.280	0.1023	0.3977	0.5000
3.222	0.0399	0.4101	0.5500
4.116	0.0163	0.4147	0.5690
6.705	0.0012	0.4176	0.5811

K1 = 10.00 AND K2 = 10.00

0.050	0.9512	0.0484	0.0004
0.100	0.9048	0.0928	0.0024
0.150	0.8607	0.1326	0.0067
0.200	0.8187	0.1681	0.0132
0.250	0.7788	0.1996	0.0216
0.300	0.7408	0.2278	0.0313
0.350	0.7047	0.2533	0.0420
0.400	0.6703	0.2763	0.0534
0.450	0.6376	0.2974	0.0650
0.500	0.6065	0.3167	0.0768
0.599	0.5492	0.3508	0.1000
0.828	0.4371	0.4129	0.1500
1.096	0.3344	0.4656	0.2000
1.438	0.2376	0.5124	0.2500
1.932	0.1451	0.5549	0.3000
2.888	0.0558	0.5942	0.3500

Table A-IV. Composition vs. Time for Two Consecutive Reaction Steps with Second Step Reversible ($2A \rightarrow B$, $B \rightleftharpoons C$).

K1 = 0.10 AND K2 = 0.10

τ	α	β	γ
0.050	0.9524	0.0475	0.0001
0.100	0.9091	0.0904	0.0005
0.150	0.8696	0.1294	0.0010
0.200	0.8333	0.1649	0.0017
0.250	0.8000	0.1974	0.0026
0.300	0.7692	0.2271	0.0037
0.350	0.7407	0.2544	0.0049
0.400	0.7143	0.2795	0.0062
0.450	0.6897	0.3027	0.0076
0.500	0.6667	0.3242	0.0091
0.950	0.5128	0.4608	0.0263
1.455	0.4073	0.5427	0.0500
2.440	0.2908	0.6092	0.1000
3.451	0.2247	0.6253	0.1500
4.566	0.1797	0.6203	0.2000
5.859	0.1458	0.6042	0.2500
7.437	0.1185	0.5815	0.3000
9.510	0.0952	0.5548	0.3500
12.587	0.0736	0.5264	0.4000
18.722	0.0507	0.4993	0.4500

K1 = 0.10 AND K2 = 0.30

0.050	0.9524	0.0475	0.0001
0.100	0.9091	0.0904	0.0005
0.150	0.8696	0.1294	0.0010
0.200	0.8333	0.1649	0.0017
0.250	0.8000	0.1974	0.0026
0.300	0.7692	0.2272	0.0036
0.350	0.7407	0.2545	0.0048
0.400	0.7143	0.2797	0.0060
0.450	0.6897	0.3030	0.0074
0.500	0.6667	0.3245	0.0088
0.950	0.5128	0.4626	0.0246
1.551	0.3920	0.5590	0.0490
2.527	0.2835	0.6290	0.0874
4.116	0.1955	0.6676	0.1369
6.705	0.1298	0.6850	0.1852
8.073	0.1102	0.6898	0.2000
10.921	0.0839	0.6980	0.2181

K1 = 0.10 AND K2 = 1.00

τ	α	β	γ
0.050	0.9524	0.0475	0.0001
0.100	0.9091	0.0905	0.0005
0.150	0.8696	0.1295	0.0010
0.200	0.8333	0.1650	0.0016
0.250	0.8000	0.1976	0.0024
0.300	0.7692	0.2274	0.0034
0.350	0.7407	0.2549	0.0044
0.400	0.7143	0.2802	0.0055
0.450	0.6897	0.3037	0.0066
0.500	0.6667	0.3255	0.0078
0.950	0.5128	0.4674	0.0198
1.551	0.3920	0.5732	0.0348
2.527	0.2835	0.6640	0.0524
4.116	0.1955	0.7370	0.0675
6.705	0.1298	0.7931	0.0771

K1 = 0.10 AND K2 = 3.00

0.050	0.9524	0.0475	0.0001
0.100	0.9091	0.0905	0.0004
0.150	0.8696	0.1296	0.0009
0.200	0.8333	0.1652	0.0014
0.250	0.8000	0.1979	0.0021
0.300	0.7692	0.2280	0.0028
0.350	0.7407	0.2557	0.0035
0.400	0.7143	0.2814	0.0043
0.450	0.6897	0.3053	0.0051
0.500	0.6667	0.3275	0.0058
0.950	0.5128	0.4752	0.0120
1.551	0.3920	0.5906	0.0174
2.527	0.2835	0.6944	0.0221
4.116	0.1955	0.7790	0.0255
6.705	0.1298	0.8423	0.0279

K1 = 0.10 AND K2 = 10.00

0.050	0.9524	0.0475	0.0001
0.100	0.9091	0.0906	0.0003
0.150	0.8696	0.1298	0.0006
0.200	0.8333	0.1657	0.0010
0.250	0.8000	0.1987	0.0013
0.300	0.7692	0.2291	0.0016
0.350	0.7407	0.2573	0.0020
0.400	0.7143	0.2835	0.0023
0.450	0.6897	0.3078	0.0025
0.500	0.6667	0.3305	0.0028
0.950	0.5128	0.4826	0.0045
1.551	0.3920	0.6022	0.0059
2.527	0.2835	0.7095	0.0070
4.116	0.1955	0.7966	0.0079
6.705	0.1298	0.8616	0.0086
9.720	0.0933	0.8988	0.0079
12.064	0.0765	0.9188	0.0046

Table A-IV, continued. Composition vs. Time for Two Consecutive Reaction Steps with Second Step Reversible (2A → B, B $\rightleftharpoons$ C).

K1 = 0.30 AND K2 = 0.10

τ	α	β	γ
0.050	0.9524	0.0473	0.0004
0.100	0.9091	0.0895	0.0014
0.150	0.8696	0.1274	0.0030
0.200	0.8333	0.1615	0.0052
0.250	0.8000	0.1922	0.0078
0.300	0.7692	0.2199	0.0108
0.350	0.7407	0.2450	0.0143
0.400	0.7143	0.2677	0.0180
0.450	0.6897	0.2882	0.0221
0.500	0.6667	0.3069	0.0264
0.737	0.5757	0.3743	0.0500
1.169	0.4612	0.4388	0.1000
1.574	0.3885	0.4615	0.1500
1.985	0.3350	0.4650	0.2000
2.416	0.2928	0.4572	0.2500
2.881	0.2577	0.4423	0.3000
3.395	0.2275	0.4225	0.3500
3.980	0.2009	0.3991	0.4000
4.663	0.1767	0.3733	0.4500
5.493	0.1540	0.3460	0.5000
6.565	0.1322	0.3178	0.5500
8.073	0.1102	0.2898	0.6000
10.608	0.0862	0.2638	0.6500

K1 = 0.30 AND K2 = 0.30

0.050	0.9524	0.0473	0.0004
0.100	0.9091	0.0895	0.0014
0.150	0.8696	0.1275	0.0030
0.200	0.8333	0.1616	0.0051
0.250	0.8000	0.1923	0.0077
0.300	0.7692	0.2202	0.0106
0.350	0.7407	0.2453	0.0139
0.400	0.7143	0.2682	0.0175
0.450	0.6897	0.2889	0.0214
0.500	0.6667	0.3078	0.0256
0.762	0.5676	0.3824	0.0500
1.241	0.4464	0.4536	0.1000
1.723	0.3672	0.4828	0.1500
2.255	0.3073	0.4927	0.2000
2.879	0.2579	0.4921	0.2500
3.662	0.2146	0.4854	0.3000
4.745	0.1741	0.4759	0.3500
6.536	0.1327	0.4673	0.4000
11.200	0.0820	0.4680	0.4500

K1 = 0.30 AND K2 = 1.00

τ	α	β	γ
0.050	0.9524	0.0473	0.0004
0.100	0.9091	0.0896	0.0013
0.150	0.8696	0.1276	0.0029
0.200	0.8333	0.1618	0.0049
0.250	0.8000	0.1928	0.0072
0.300	0.7692	0.2209	0.0099
0.350	0.7407	0.2464	0.0128
0.400	0.7143	0.2697	0.0160
0.450	0.6897	0.2910	0.0193
0.500	0.6667	0.3106	0.0228
0.950	0.5128	0.4311	0.0561
1.551	0.3920	0.5122	0.0958
2.527	0.2835	0.5769	0.1396
4.116	0.1955	0.6297	0.1748
6.705	0.1298	0.6733	0.1969

K1 = 0.30 AND K2 = 3.00

0.050	0.9524	0.0473	0.0003
0.100	0.9091	0.0896	0.0013
0.150	0.8696	0.1278	0.0026
0.200	0.8333	0.1624	0.0043
0.250	0.8000	0.1938	0.0062
0.300	0.7692	0.2225	0.0082
0.350	0.7407	0.2489	0.0104
0.400	0.7143	0.2731	0.0126
0.450	0.6897	0.2956	0.0148
0.500	0.6667	0.3163	0.0170
0.950	0.5128	0.4527	0.0344
1.551	0.3920	0.5585	0.0495
2.527	0.2835	0.6541	0.0624
4.116	0.1955	0.7326	0.0719
6.705	0.1298	0.7916	0.0786

K1 = 0.30 AND K2 = 10.00

0.050	0.9524	0.0473	0.0003
0.100	0.9091	0.0899	0.0010
0.150	0.8696	0.1285	0.0019
0.200	0.8333	0.1637	0.0029
0.250	0.8000	0.1961	0.0039
0.300	0.7692	0.2259	0.0049
0.350	0.7407	0.2535	0.0058
0.400	0.7143	0.2790	0.0067
0.450	0.6897	0.3028	0.0075
0.500	0.6667	0.3251	0.0083
0.950	0.5128	0.4738	0.0134
1.551	0.3920	0.5908	0.0172
2.527	0.2835	0.6958	0.0206
4.116	0.1955	0.7812	0.0233
6.705	0.1298	0.8449	0.0253
9.720	0.0933	0.8886	0.0181
11.604	0.0793	0.8944	0.0263

Table A-IV, continued. Composition vs. Time for Two Consecutive Reaction Steps with Second Step Reversible (2A → B, B $\rightleftharpoons$ C).

K1 = 1.00 AND K2 = 0.10

τ	α	β	γ
0.050	0.9524	0.0464	0.0012
0.100	0.9091	0.0864	0.0045
0.150	0.8696	0.1207	0.0097
0.200	0.8333	0.1503	0.0164
0.250	0.8000	0.1755	0.0245
0.300	0.7692	0.1971	0.0337
0.350	0.7407	0.2155	0.0438
0.400	0.7143	0.2310	0.0547
0.450	0.6897	0.2440	0.0663
0.500	0.6667	0.2549	0.0784
0.585	0.6311	0.2689	0.1000
0.773	0.5642	0.2858	0.1500
0.957	0.5109	0.2891	0.2000
1.146	0.4660	0.2840	0.2500
1.345	0.4264	0.2736	0.3000
1.559	0.3908	0.2592	0.3500
1.793	0.3580	0.2420	0.4000
2.057	0.3272	0.2228	0.4500
2.361	0.2976	0.2024	0.5000
2.721	0.2688	0.1812	0.5500
3.166	0.2401	0.1599	0.6000
3.744	0.2108	0.1392	0.6500
4.562	0.1798	0.1202	0.7000
5.864	0.1457	0.1043	0.7500
6.705	0.1298	0.0989	0.7713
8.389	0.1066	0.0934	0.8000

K1 = 1.00 AND K2 = 0.30

0.050	0.9524	0.0464	0.0012
0.100	0.9091	0.0864	0.0045
0.150	0.8696	0.1208	0.0096
0.200	0.8333	0.1505	0.0162
0.250	0.8000	0.1759	0.0241
0.300	0.7692	0.1978	0.0330
0.350	0.7407	0.2165	0.0428
0.400	0.7143	0.2324	0.0533
0.450	0.6897	0.2459	0.0644
0.500	0.6667	0.2574	0.0759
0.600	0.6250	0.2750	0.1000
0.801	0.5553	0.2947	0.1500
1.004	0.4990	0.3010	0.2000
1.219	0.4507	0.2993	0.2500
1.453	0.4077	0.2923	0.3000
1.717	0.3681	0.2819	0.3500
2.024	0.3307	0.2693	0.4000
2.396	0.2945	0.2555	0.4500
2.872	0.2584	0.2416	0.5000
3.523	0.2211	0.2289	0.5500
4.522	0.1811	0.2189	0.6000
6.357	0.1359	0.2141	0.6500

K1 = 1.00 AND K2 = 1.00

τ	α	β	γ
0.050	0.9524	0.0464	0.0012
0.100	0.9091	0.0865	0.0044
0.150	0.8696	0.1212	0.0093
0.200	0.8333	0.1512	0.0155
0.250	0.8000	0.1772	0.0228
0.300	0.7692	0.1999	0.0309
0.350	0.7407	0.2197	0.0396
0.400	0.7143	0.2369	0.0488
0.450	0.6897	0.2520	0.0584
0.500	0.6667	0.2652	0.0681
0.661	0.6023	0.2977	0.1000
0.924	0.5200	0.3300	0.1500
1.226	0.4494	0.3506	0.2000
1.603	0.3843	0.3657	0.2500
2.122	0.3204	0.3796	0.3000
2.941	0.2538	0.3962	0.3500
4.568	0.1796	0.4204	0.4000
6.705	0.1298	0.4400	0.4302
9.532	0.0950	0.4550	0.4500

K1 = 1.00 AND K2 = 3.00

0.050	0.9524	0.0465	0.0011
0.100	0.9091	0.0868	0.0041
0.150	0.8696	0.1220	0.0084
0.200	0.8333	0.1530	0.0137
0.250	0.8000	0.1805	0.0195
0.300	0.7692	0.2050	0.0258
0.350	0.7407	0.2270	0.0322
0.400	0.7143	0.2469	0.0388
0.450	0.6897	0.2651	0.0453
0.500	0.6667	0.2817	0.0517
0.950	0.5128	0.3872	0.1000
1.551	0.3920	0.4683	0.1397
2.527	0.2835	0.5433	0.1732
4.116	0.1955	0.6061	0.1985
6.705	0.1298	0.6538	0.2164

K1 = 1.00 AND K2 = 10.00

0.050	0.9524	0.0466	0.0010
0.100	0.9091	0.0876	0.0033
0.150	0.8696	0.1242	0.0063
0.200	0.8333	0.1573	0.0094
0.250	0.8000	0.1875	0.0125
0.300	0.7692	0.2152	0.0156
0.350	0.7407	0.2408	0.0185
0.400	0.7143	0.2645	0.0212
0.450	0.6897	0.2866	0.0237
0.500	0.6667	0.3072	0.0261
0.950	0.5128	0.4453	0.0419
1.551	0.3920	0.5541	0.0539
2.527	0.2835	0.6520	0.0644
4.116	0.1955	0.7317	0.0728
6.705	0.1298	0.7913	0.0789
9.350	0.0966	0.8468	0.0565
11.162	0.0822	0.8362	0.0816

Table A-IV, continued. Composition vs. Time for Two Consecutive Reaction Steps with Second Step Reversible ($2A \rightarrow B$, $B \rightleftharpoons C$).

K1 = 3.00 AND K2 = 0.10

τ	α	β	γ
0.050	0.9524	0.0442	0.0034
0.100	0.9091	0.0782	0.0127
0.150	0.8696	0.1041	0.0264
0.200	0.8333	0.1233	0.0433
0.250	0.8000	0.1373	0.0627
0.300	0.7692	0.1471	0.0837
0.350	0.7407	0.1535	0.1058
0.400	0.7143	0.1572	0.1285
0.450	0.6897	0.1588	0.1516
0.500	0.6667	0.1588	0.1746
0.556	0.6428	0.1572	0.2000
0.669	0.5991	0.1509	0.2500
0.791	0.5585	0.1415	0.3000
0.924	0.5198	0.1302	0.3500
1.074	0.4823	0.1177	0.4000
1.246	0.4453	0.1047	0.4500
1.449	0.4084	0.0916	0.5000
1.696	0.3710	0.0790	0.5500
2.007	0.3326	0.0674	0.6000
2.414	0.2930	0.0570	0.6500
2.975	0.2516	0.0484	0.7000
3.797	0.2085	0.0415	0.7500
5.115	0.1636	0.0364	0.8000
7.560	0.1169	0.0331	0.8500

K1 = 3.00 AND K2 = 0.30

0.050	0.9524	0.0442	0.0034
0.100	0.9091	0.0783	0.0126
0.150	0.8696	0.1043	0.0261
0.200	0.8333	0.1239	0.0428
0.250	0.8000	0.1383	0.0617
0.300	0.7692	0.1486	0.0822
0.350	0.7407	0.1556	0.1037
0.400	0.7143	0.1601	0.1256
0.450	0.6897	0.1625	0.1478
0.500	0.6667	0.1634	0.1699
0.569	0.6373	0.1627	0.2000
0.690	0.5918	0.1582	0.2500
0.821	0.5492	0.1508	0.3000
0.968	0.5083	0.1417	0.3500
1.136	0.4682	0.1318	0.4000
1.334	0.4284	0.1216	0.4500
1.577	0.3882	0.1118	0.5000
1.882	0.3470	0.1030	0.5500
2.285	0.3044	0.0956	0.6000
2.846	0.2601	0.0899	0.6500
3.678	0.2138	0.0862	0.7000
5.037	0.1657	0.0843	0.7500
7.652	0.1156	0.0844	0.8000

K1 = 3.00 AND K2 = 1.00

τ	α	β	γ
0.050	0.9524	0.0442	0.0034
0.100	0.9091	0.0786	0.0123
0.150	0.8696	0.1052	0.0253
0.200	0.8333	0.1257	0.0410
0.250	0.8000	0.1414	0.0586
0.300	0.7692	0.1534	0.0774
0.350	0.7407	0.1625	0.0967
0.400	0.7143	0.1694	0.1163
0.450	0.6897	0.1745	0.1358
0.500	0.6667	0.1783	0.1550
0.623	0.6163	0.1837	0.2000
0.774	0.5637	0.1863	0.2500
0.950	0.5129	0.1871	0.3000
1.162	0.4626	0.1874	0.3500
1.429	0.4117	0.1883	0.4000
1.782	0.3595	0.1905	0.4500
2.276	0.3053	0.1947	0.5000
3.021	0.2488	0.2012	0.5500
4.266	0.1900	0.2100	0.6000
6.761	0.1289	0.2211	0.6500

K1 = 3.00 AND K2 = 3.00

0.050	0.9524	0.0443	0.0033
0.100	0.9091	0.0793	0.0116
0.150	0.8696	0.1073	0.0231
0.200	0.8333	0.1301	0.0365
0.250	0.8000	0.1491	0.0509
0.300	0.7692	0.1650	0.0658
0.350	0.7407	0.1787	0.0806
0.400	0.7143	0.1906	0.0951
0.450	0.6897	0.2012	0.1092
0.500	0.6667	0.2106	0.1227
0.950	0.5128	0.2704	0.2168
1.551	0.3920	0.3190	0.2891
2.527	0.2835	0.3657	0.3508
4.116	0.1955	0.4057	0.3989
6.705	0.1298	0.4366	0.4336
9.175	0.0983	0.4517	0.4500

K1 = 3.00 AND K2 = 10.00

0.050	0.9524	0.0446	0.0030
0.100	0.9091	0.0814	0.0095
0.150	0.8696	0.1130	0.0174
0.200	0.8333	0.1409	0.0257
0.250	0.8000	0.1661	0.0339
0.300	0.7692	0.1891	0.0416
0.350	0.7407	0.2103	0.0490
0.400	0.7143	0.2299	0.0558
0.450	0.6897	0.2482	0.0622
0.500	0.6667	0.2652	0.0681
0.950	0.5128	0.3798	0.1073
1.551	0.3920	0.4706	0.1374
2.527	0.2835	0.5526	0.1638
4.116	0.1955	0.6196	0.1850
6.705	0.1298	0.6787	0.1915
8.321	0.1073	0.6975	0.1952
10.328	0.0883	0.7786	0.1331

Table A-IV, continued. Composition vs. Time for Two Consecutive Reaction Steps with Second Step Reversible (2A → B, B ⇄ C).

K1 = 10.00 AND K2 = 0.10

τ	α	β	γ
0.050	0.9524	0.0373	0.0103
0.100	0.9091	0.0566	0.0343
0.150	0.8696	0.0655	0.0649
0.200	0.8333	0.0685	0.0982
0.250	0.8000	0.0681	0.1319
0.300	0.7692	0.0660	0.1647
0.350	0.7407	0.0631	0.1961
0.400	0.7143	0.0599	0.2258
0.450	0.6897	0.0566	0.2538
0.500	0.6667	0.0534	0.2799
0.653	0.6050	0.0450	0.3500
0.784	0.5607	0.0393	0.4000
0.938	0.5159	0.0341	0.4500
1.125	0.4707	0.0293	0.5000
1.354	0.4249	0.0251	0.5500
1.642	0.3786	0.0214	0.6000
2.015	0.3318	0.0182	0.6500
2.515	0.2845	0.0155	0.7000
3.225	0.2367	0.0133	0.7500
4.310	0.1883	0.0117	0.8000
6.171	0.1395	0.0105	0.8500

K1 = 10.00 AND K2 = 0.30

0.050	0.9524	0.0373	0.0103
0.100	0.9091	0.0568	0.0341
0.150	0.8696	0.0660	0.0644
0.200	0.8333	0.0694	0.0972
0.250	0.8000	0.0696	0.1304
0.300	0.7692	0.0681	0.1627
0.350	0.7407	0.0658	0.1935
0.400	0.7143	0.0631	0.2226
0.450	0.6897	0.0604	0.2499
0.500	0.6667	0.0578	0.2755
0.551	0.6447	0.0553	0.3000
0.668	0.5997	0.0503	0.3500
0.804	0.5543	0.0457	0.4000
0.967	0.5085	0.0415	0.4500
1.164	0.4621	0.0379	0.5000
1.408	0.4152	0.0348	0.5500
1.719	0.3678	0.0322	0.6000
2.127	0.3199	0.0301	0.6500
2.685	0.2714	0.0286	0.7000
3.496	0.2225	0.0275	0.7500
4.781	0.1730	0.0270	0.8000
7.149	0.1228	0.0272	0.8500

K1 = 10.00 AND K2 = 1.00

τ	α	β	γ
0.050	0.9524	0.0374	0.0102
0.100	0.9091	0.0575	0.0334
0.150	0.8696	0.0678	0.0627
0.200	0.8333	0.0726	0.0940
0.250	0.8000	0.0746	0.1254
0.300	0.7692	0.0749	0.1558
0.350	0.7407	0.0746	0.1847
0.400	0.7143	0.0738	0.2119
0.450	0.6897	0.0730	0.2374
0.500	0.6667	0.0722	0.2612
0.590	0.6291	0.0709	0.3000
0.723	0.5805	0.0695	0.3500
0.882	0.5314	0.0686	0.4000
1.076	0.4818	0.0682	0.4500
1.318	0.4315	0.0685	0.5000
1.626	0.3808	0.0692	0.5500
2.036	0.3295	0.0705	0.6000
2.603	0.2776	0.0724	0.6500
3.442	0.2252	0.0748	0.7000
4.808	0.1722	0.0778	0.7500
6.705	0.1298	0.0807	0.7895

K1 = 10.00 AND K2 = 3.00

0.050	0.9524	0.0377	0.0099
0.100	0.9091	0.0593	0.0316
0.150	0.8696	0.0723	0.0581
0.200	0.8333	0.0809	0.0858
0.250	0.8000	0.0871	0.1129
0.300	0.7692	0.0919	0.1388
0.350	0.7407	0.0961	0.1632
0.400	0.7143	0.0998	0.1860
0.450	0.6897	0.1032	0.2072
0.500	0.6667	0.1063	0.2270
0.563	0.6399	0.1101	0.2500
0.721	0.5813	0.1187	0.3000
0.916	0.5221	0.1279	0.3500
1.163	0.4622	0.1378	0.4000
1.490	0.4017	0.1483	0.4500
1.937	0.3406	0.1594	0.5000
2.589	0.2787	0.1713	0.5500
3.625	0.2163	0.1837	0.6000
5.536	0.1530	0.1970	0.6500
6.705	0.1298	0.2322	0.6380
8.321	0.1073	0.2424	0.6503

K1 = 10.00 AND K2 = 10.00

0.050	0.9524	0.0385	0.0091
0.100	0.9091	0.0644	0.0265
0.150	0.8696	0.0846	0.0459
0.200	0.8333	0.1018	0.0649
0.250	0.8000	0.1173	0.0827
0.300	0.7692	0.1314	0.0994
0.350	0.7407	0.1445	0.1148
0.400	0.7143	0.1566	0.1291
0.450	0.6897	0.1680	0.1424
0.500	0.6667	0.1786	0.1547
0.719	0.5820	0.2180	0.2000
1.051	0.4875	0.2625	0.2500
1.551	0.3920	0.3080	0.3000
2.385	0.2955	0.3545	0.3500
4.116	0.1955	0.4058	0.3987
5.311	0.1585	0.4599	0.3816
6.592	0.1317	0.7273	0.1410
7.869	0.1127	0.4942	0.3931
9.395	0.0962	0.4858	0.4180

Table A-V. Composition vs. Time for Two Consecutive Reaction Steps with Second Step Reversible (A → B, B $\rightleftharpoons$ 2C).

K1 = 0.10 AND K2 = 0.10

τ	α	β	γ
0.050	0.9512	0.0486	0.0001
0.100	0.9048	0.0947	0.0005
0.150	0.8607	0.1382	0.0011
0.200	0.8187	0.1794	0.0019
0.250	0.7788	0.2183	0.0029
0.300	0.7408	0.2551	0.0040
0.350	0.7047	0.2899	0.0054
0.400	0.6703	0.3227	0.0069
0.450	0.6376	0.3537	0.0086
0.500	0.6065	0.3830	0.0105
0.950	0.3867	0.5807	0.0325
1.232	0.2920	0.6580	0.0500
1.936	0.1445	0.7555	0.1000
2.599	0.0745	0.7755	0.1500
3.275	0.0379	0.7621	0.2000
3.993	0.0185	0.7315	0.2500
4.779	0.0084	0.6916	0.3000
5.669	0.0035	0.6465	0.3500
6.708	0.0012	0.5988	0.4000
7.988	0.0003	0.5497	0.4500

K1 = 0.10 AND K2 = 0.30

0.050	0.9512	0.0486	0.0001
0.100	0.9048	0.0947	0.0005
0.150	0.8607	0.1382	0.0011
0.200	0.8187	0.1794	0.0019
0.250	0.7788	0.2183	0.0029
0.300	0.7408	0.2551	0.0040
0.350	0.7047	0.2899	0.0054
0.400	0.6703	0.3227	0.0069
0.450	0.6376	0.3537	0.0086
0.500	0.6065	0.3830	0.0105
0.950	0.3867	0.5808	0.0325
1.551	0.2120	0.7165	0.0716
1.948	0.1427	0.7573	0.1000
2.638	0.0715	0.7785	0.1500
3.373	0.0343	0.7657	0.2000

K1 = 0.10 AND K2 = 1.00

τ	α	β	γ
0.050	0.9512	0.0486	0.0001
0.100	0.9048	0.0947	0.0005
0.150	0.8607	0.1382	0.0011
0.200	0.8187	0.1794	0.0019
0.250	0.7788	0.2183	0.0029
0.300	0.7408	0.2551	0.0040
0.350	0.7047	0.2899	0.0054
0.400	0.6703	0.3227	0.0069
0.450	0.6376	0.3538	0.0086
0.500	0.6065	0.3830	0.0105
0.550	0.5769	0.4106	0.0124
0.600	0.5488	0.4366	0.0145
0.650	0.5220	0.4612	0.0168
0.700	0.4966	0.4843	0.0191
0.750	0.4724	0.5060	0.0216
0.800	0.4493	0.5265	0.0241
0.850	0.4274	0.5458	0.0268
0.900	0.4066	0.5639	0.0295
0.950	0.3867	0.5809	0.0323
1.000	0.3679	0.5969	0.0352
1.050	0.3499	0.6119	0.0382
1.126	0.3243	0.6329	0.0428
1.308	0.2703	0.6754	0.0543
1.505	0.2221	0.7107	0.0672
1.724	0.1784	0.7397	0.0819

K1 = 0.10 AND K2 = 3.00

0.050	0.9512	0.0486	0.0001
0.100	0.9048	0.0947	0.0005
0.150	0.8607	0.1382	0.0011
0.200	0.8187	0.1794	0.0019
0.250	0.7788	0.2183	0.0029
0.300	0.7408	0.2551	0.0040
0.350	0.7047	0.2899	0.0054
0.400	0.6703	0.3228	0.0069
0.450	0.6376	0.3538	0.0086
0.500	0.6065	0.3830	0.0104
0.550	0.5769	0.4106	0.0124
0.600	0.5488	0.4367	0.0145
0.650	0.5220	0.4613	0.0167
0.700	0.4966	0.4844	0.0190
0.750	0.4724	0.5062	0.0214
0.800	0.4493	0.5267	0.0239
0.850	0.4274	0.5461	0.0265
0.900	0.4066	0.5642	0.0292
0.950	0.3867	0.5813	0.0319
1.000	0.3679	0.5974	0.0347

K1 = 0.10 AND K2 = 10.00

0.050	0.9512	0.0486	0.0001
0.100	0.9048	0.0947	0.0005
0.150	0.8607	0.1382	0.0011
0.200	0.8187	0.1794	0.0019
0.250	0.7788	0.2183	0.0029
0.300	0.7408	0.2552	0.0040
0.350	0.7047	0.2899	0.0054
0.400	0.6703	0.3228	0.0069
0.450	0.6376	0.3538	0.0086
0.500	0.6065	0.3831	0.0104

Table A-V, continued. Composition vs. Time for Two Consecutive Reaction Steps with Second Step Reversible (A → B, B $\rightleftarrows$ 2C).

K1 = 0.30 AND K2 = 0.10

τ	α	β	γ
0.050	0.9512	0.0484	0.0004
0.100	0.9048	0.0937	0.0014
0.150	0.8607	0.1361	0.0032
0.200	0.8187	0.1758	0.0055
0.250	0.7788	0.2128	0.0084
0.300	0.7408	0.2473	0.0119
0.350	0.7047	0.2795	0.0158
0.400	0.6703	0.3094	0.0202
0.450	0.6376	0.3373	0.0251
0.500	0.6065	0.3631	0.0303
0.950	0.3867	0.5220	0.0913
1.551	0.2120	0.5955	0.1926
2.527	0.0799	0.5630	0.3571
4.116	0.0163	0.4258	0.5579
5.300	0.0050	0.3450	0.6500

K1 = 0.30 AND K2 = 0.30

0.050	0.9512	0.0484	0.0004
0.100	0.9048	0.0937	0.0014
0.150	0.8607	0.1361	0.0032
0.200	0.8187	0.1758	0.0055
0.250	0.7788	0.2128	0.0084
0.300	0.7408	0.2473	0.0119
0.350	0.7047	0.2795	0.0158
0.400	0.6703	0.3094	0.0202
0.450	0.6376	0.3373	0.0251
0.500	0.6065	0.3631	0.0303
0.950	0.3867	0.5223	0.0909
1.551	0.2120	0.5980	0.1900
2.581	0.0758	0.5742	0.3500
2.978	0.0510	0.5490	0.4000
3.452	0.0318	0.5182	0.4500

K1 = 0.30 AND K2 = 1.00

τ	α	β	γ
0.050	0.9512	0.0484	0.0004
0.100	0.9048	0.0937	0.0014
0.150	0.8607	0.1361	0.0032
0.200	0.8187	0.1758	0.0055
0.250	0.7788	0.2128	0.0084
0.300	0.7408	0.2473	0.0119
0.350	0.7047	0.2795	0.0158
0.400	0.6703	0.3095	0.0202
0.450	0.6376	0.3373	0.0250
0.500	0.6065	0.3632	0.0303
0.666	0.5139	0.4361	0.0500
1.018	0.3614	0.5386	0.1000
1.343	0.2612	0.5888	0.1500
1.676	0.1872	0.6128	0.2000

K1 = 0.30 AND K2 = 3.00

0.050	0.9512	0.0484	0.0004
0.100	0.9048	0.0937	0.0014
0.150	0.8607	0.1361	0.0032
0.200	0.8187	0.1758	0.0055
0.250	0.7788	0.2128	0.0084
0.300	0.7408	0.2473	0.0119
0.350	0.7047	0.2795	0.0158
0.400	0.6703	0.3095	0.0201
0.450	0.6376	0.3374	0.0249
0.500	0.6065	0.3634	0.0301
0.550	0.5769	0.3875	0.0355
0.600	0.5488	0.4099	0.0413
0.650	0.5220	0.4306	0.0473
0.700	0.4966	0.4499	0.0535
0.750	0.4724	0.4677	0.0599
0.800	0.4493	0.4842	0.0665
0.850	0.4274	0.4995	0.0731
0.900	0.4066	0.5136	0.0799
0.950	0.3867	0.5266	0.0866
1.000	0.3679	0.5387	0.0934

K1 = 0.30 AND K2 = 10.00

0.050	0.9512	0.0484	0.0004
0.100	0.9048	0.0937	0.0014
0.150	0.8607	0.1361	0.0032
0.200	0.8187	0.1758	0.0055
0.250	0.7786	0.2128	0.0084
0.300	0.7408	0.2474	0.0118
0.350	0.7047	0.2797	0.0157
0.400	0.6703	0.3098	0.0199
0.450	0.6376	0.3378	0.0245
0.500	0.6065	0.3640	0.0294

Table A-V, continued. Composition vs. Time for Two Consecutive Reaction Steps with Second Step Reversible (A → B, B ⇌ 2C).

K1 = 1.00 AND K2 = 0.10

τ	α	β	γ
0.050	0.9512	0.0476	0.0012
0.100	0.9048	0.0905	0.0047
0.150	0.8607	0.1291	0.0102
0.200	0.8187	0.1637	0.0175
0.250	0.7788	0.1947	0.0265
0.300	0.7408	0.2223	0.0369
0.350	0.7047	0.2467	0.0487
0.400	0.6703	0.2682	0.0615
0.450	0.6376	0.2870	0.0754
0.500	0.6065	0.3033	0.0901
0.684	0.5047	0.3453	0.1500
0.826	0.4378	0.3622	0.2000
0.965	0.3812	0.3688	0.2500
1.103	0.3319	0.3681	0.3000
1.244	0.2883	0.3617	0.3500
1.390	0.2492	0.3508	0.4000
1.544	0.2137	0.3363	0.4500
1.707	0.1814	0.3186	0.5000
1.885	0.1518	0.2982	0.5500
2.083	0.1246	0.2754	0.6000
2.307	0.0997	0.2503	0.6500
2.569	0.0767	0.2233	0.7000
2.890	0.0557	0.1943	0.7500
3.315	0.0364	0.1636	0.8000

K1 = 1.00 AND K2 = 0.30

0.050	0.9512	0.0476	0.0012
0.100	0.9048	0.0905	0.0047
0.150	0.8607	0.1291	0.0102
0.200	0.8187	0.1637	0.0175
0.250	0.7788	0.1947	0.0265
0.300	0.7408	0.2223	0.0369
0.350	0.7047	0.2467	0.0486
0.400	0.6703	0.2682	0.0615
0.450	0.6376	0.2871	0.0753
0.500	0.6065	0.3035	0.0900
0.686	0.5038	0.3462	0.1500
0.830	0.4361	0.3639	0.2000
0.972	0.3786	0.3714	0.2500
1.115	0.3281	0.3719	0.3000
1.263	0.2830	0.3670	0.3500
1.419	0.2421	0.3579	0.4000
1.587	0.2047	0.3453	0.4500
1.772	0.1700	0.3300	0.5000
1.982	0.1378	0.3122	0.5500
2.230	0.1077	0.2923	0.6000
2.535	0.0793	0.2707	0.6500

K1 = 1.00 AND K2 = 1.00

τ	α	β	γ
0.050	0.9512	0.0476	0.0012
0.100	0.9048	0.0905	0.0047
0.150	0.8607	0.1291	0.0102
0.200	0.8187	0.1638	0.0175
0.250	0.7788	0.1947	0.0265
0.300	0.7408	0.2223	0.0369
0.350	0.7047	0.2468	0.0485
0.400	0.6703	0.2684	0.0612
0.450	0.6376	0.2875	0.0749
0.500	0.6065	0.3041	0.0894
0.693	0.5003	0.3497	0.1500
0.844	0.4300	0.3700	0.2000
0.998	0.3687	0.3813	0.2500
1.160	0.3135	0.3865	0.3000
1.338	0.2624	0.3876	0.3500
1.542	0.2141	0.3859	0.4000
1.788	0.1673	0.3827	0.4500

K1 = 1.00 AND K2 = 3.00

0.050	0.9512	0.0476	0.0012
0.100	0.9048	0.0905	0.0047
0.150	0.8607	0.1291	0.0102
0.200	0.8187	0.1638	0.0175
0.250	0.7788	0.1948	0.0264
0.300	0.7408	0.2225	0.0367
0.350	0.7047	0.2471	0.0482
0.400	0.6703	0.2690	0.0606
0.450	0.6376	0.2885	0.0739
0.500	0.6065	0.3057	0.0878
0.550	0.5769	0.3209	0.1021
0.600	0.5488	0.3345	0.1167
0.650	0.5220	0.3465	0.1314
0.700	0.4966	0.3573	0.1461
0.750	0.4724	0.3669	0.1607
0.800	0.4493	0.3756	0.1750
0.850	0.4274	0.3835	0.1891
0.900	0.4066	0.3908	0.2027
0.950	0.3867	0.3975	0.2158
1.000	0.3679	0.4037	0.2284
1.050	0.3499	0.4096	0.2405
1.092	0.3356	0.4142	0.2502

K1 = 1.00 AND K2 = 10.00

0.050	0.9512	0.0476	0.0012
0.100	0.9048	0.0905	0.0047
0.150	0.8607	0.1291	0.0102
0.200	0.8187	0.1639	0.0174
0.250	0.7788	0.1950	0.0261
0.300	0.7408	0.2231	0.0361
0.350	0.7047	0.2483	0.0471
0.400	0.6703	0.2710	0.0586
0.450	0.6376	0.2917	0.0706
0.500	0.6065	0.3107	0.0828
0.550	0.5769	0.3283	0.0948

Table A-V, continued. Composition vs. Time for Two Consecutive Reaction Steps with Second Step Reversible (A → B, B $\rightleftharpoons$ 2C).

K1 = 3.00 AND K2 = 0.10

τ	α	β	γ
0.050	0.9512	0.0453	0.0035
0.100	0.9048	0.0820	0.0132
0.150	0.8607	0.1115	0.0278
0.200	0.8187	0.1350	0.0463
0.250	0.7788	0.1532	0.0680
0.300	0.7408	0.1672	0.0920
0.350	0.7047	0.1775	0.1178
0.400	0.6703	0.1847	0.1450
0.450	0.6376	0.1895	0.1729
0.500	0.6065	0.1921	0.2014
0.673	0.5103	0.1897	0.3000
0.764	0.4660	0.1840	0.3500
0.950	0.3867	0.1677	0.4455
1.186	0.3056	0.1444	0.5500
1.551	0.2120	0.1120	0.6760
2.103	0.1222	0.0778	0.8000
2.527	0.0799	0.0615	0.8586

K1 = 3.00 AND K2 = 0.30

0.050	0.9512	0.0453	0.0035
0.100	0.9048	0.0820	0.0132
0.150	0.8607	0.1115	0.0277
0.200	0.8187	0.1350	0.0463
0.250	0.7788	0.1533	0.0679
0.300	0.7408	0.1673	0.0919
0.350	0.7047	0.1777	0.1177
0.400	0.6703	0.1850	0.1446
0.450	0.6376	0.1900	0.1724
0.500	0.6065	0.1928	0.2006
0.770	0.4630	0.1870	0.3500
0.950	0.3867	0.1741	0.4391
1.216	0.2964	0.1536	0.5500
1.551	0.2120	0.1320	0.6561
1.988	0.1370	0.1130	0.7500
2.527	0.0799	0.0998	0.8203

K1 = 3.00 AND K2 = 1.00

τ	α	β	γ
0.050	0.9512	0.0453	0.0035
0.100	0.9048	0.0820	0.0132
0.150	0.8607	0.1116	0.0277
0.200	0.8187	0.1350	0.0462
0.250	0.7788	0.1534	0.0678
0.300	0.7408	0.1676	0.0916
0.350	0.7047	0.1783	0.1170
0.400	0.6703	0.1862	0.1435
0.450	0.6376	0.1917	0.1707
0.500	0.6065	0.1955	0.1980
0.692	0.5008	0.1992	0.3000
0.950	0.3867	0.1945	0.4187
1.174	0.3094	0.1906	0.5000
1.551	0.2120	0.1891	0.5989
1.840	0.1590	0.1910	0.6500

K1 = 3.00 AND K2 = 3.00

0.050	0.9512	0.0453	0.0035
0.100	0.9048	0.0820	0.0131
0.150	0.8607	0.1116	0.0277
0.200	0.8187	0.1352	0.0461
0.250	0.7788	0.1539	0.0673
0.300	0.7408	0.1686	0.0906
0.350	0.7047	0.1801	0.1152
0.400	0.6703	0.1892	0.1405
0.450	0.6376	0.1965	0.1659
0.500	0.6065	0.2024	0.1910
0.950	0.3867	0.2400	0.3732
1.045	0.3518	0.2482	0.4000
1.265	0.2825	0.2675	0.4500

K1 = 3.00 AND K2 = 10.00

0.050	0.9512	0.0453	0.0035
0.100	0.9048	0.0820	0.0131
0.150	0.8607	0.1118	0.0275
0.200	0.8187	0.1358	0.0455
0.250	0.7788	0.1554	0.0658
0.300	0.7408	0.1717	0.0874
0.350	0.7047	0.1859	0.1094
0.400	0.6703	0.1987	0.1310
0.450	0.6376	0.2107	0.1517
0.500	0.6065	0.2224	0.1711
0.550	0.5769	0.2340	0.1891
0.600	0.5488	0.2456	0.2056
0.650	0.5220	0.2574	0.2205
0.700	0.4966	0.2692	0.2342

Table A-V, continued. Composition vs. Time for Two Consecutive Reaction Steps with Second Step Reversible ($A \rightarrow B$, $B \rightleftharpoons 2C$).

K1 = 10.00 AND K2 = 0.10

τ	α	β	γ
0.050	0.9512	0.0484	0.0004
0.100	0.9048	0.0922	0.0030
0.150	0.8607	0.1301	0.0092
0.200	0.8187	0.1614	0.0199
0.250	0.7788	0.1862	0.0350
0.300	0.7408	0.2052	0.0540
0.350	0.7047	0.2190	0.0763
0.400	0.6703	0.2287	0.1010
0.450	0.6376	0.2350	0.1273
0.500	0.6065	0.2387	0.1547
0.671	0.5111	0.2389	0.2500
0.765	0.4654	0.2346	0.3000
0.864	0.4215	0.2285	0.3500
0.971	0.3788	0.2212	0.4000
1.088	0.3371	0.2129	0.4500
1.217	0.2962	0.2038	0.5000
1.363	0.2560	0.1940	0.5500
1.531	0.2165	0.1835	0.6000
1.728	0.1778	0.1722	0.6500
1.968	0.1398	0.1602	0.7000
2.275	0.1029	0.1471	0.7500
2.702	0.0672	0.1328	0.8000
3.402	0.0334	0.1166	0.8500
4.116	0.0163	0.1069	0.8768

K1 = 10.00 AND K2 = 0.30

0.050	0.9512	0.0484	0.0004
0.100	0.9048	0.0922	0.0030
0.150	0.8607	0.1301	0.0092
0.200	0.8187	0.1616	0.0197
0.250	0.7788	0.1866	0.0346
0.300	0.7408	0.2059	0.0533
0.350	0.7047	0.2202	0.0751
0.400	0.6703	0.2304	0.0993
0.450	0.6376	0.2374	0.1250
0.500	0.6065	0.2418	0.1517
0.950	0.3867	0.2344	0.3789
1.551	0.2120	0.2064	0.5816
2.527	0.0799	0.1791	0.7410
4.116	0.0163	0.1633	0.8204
6.705	0.0012	0.1592	0.8396
10.921	0.0000	0.1589	0.8411

K1 = 10.00 AND K2 = 1.00

τ	α	β	γ
0.050	0.9512	0.0484	0.0004
0.100	0.9048	0.0923	0.0029
0.150	0.8607	0.1304	0.0089
0.200	0.8187	0.1622	0.0191
0.250	0.7788	0.1880	0.0332
0.300	0.7408	0.2083	0.0509
0.350	0.7047	0.2240	0.0713
0.400	0.6703	0.2360	0.0937
0.450	0.6376	0.2450	0.1174
0.500	0.6065	0.2517	0.1418
0.950	0.3867	0.2691	0.3442
1.551	0.2120	0.2701	0.5179
2.527	0.0799	0.2702	0.6499
4.116	0.0163	0.2702	0.7135
6.705	0.0012	0.2702	0.7286
10.921	0.0000	0.2702	0.7298

K1 = 10.00 AND K2 = 3.00

0.050	0.9512	0.0484	0.0004
0.100	0.9048	0.0924	0.0028
0.150	0.8607	0.1310	0.0083
0.200	0.8187	0.1638	0.0174
0.250	0.7788	0.1914	0.0298
0.300	0.7408	0.2143	0.0449
0.350	0.7047	0.2333	0.0620
0.400	0.6703	0.2492	0.0805
0.450	0.6376	0.2626	0.0998
0.500	0.6065	0.2741	0.1194
0.950	0.3867	0.3357	0.2775
1.551	0.2120	0.3750	0.4131
2.527	0.0799	0.4022	0.5179
4.116	0.0163	0.4147	0.5690
6.705	0.0012	0.4176	0.5811
8.280	0.0003	0.3497	0.6500

K1 = 10.00 AND K2 = 10.00

0.050	0.9512	0.0383	0.0105
0.100	0.9048	0.0599	0.0353
0.150	0.8607	0.0721	0.0672
0.200	0.8187	0.0796	0.1017
0.250	0.7788	0.0854	0.1358
0.300	0.7408	0.0909	0.1683
0.350	0.7047	0.0970	0.1983
0.400	0.6703	0.1038	0.2259
0.450	0.6376	0.1113	0.2511
0.500	0.6065	0.1193	0.2742
0.550	0.5769	0.1277	0.2953
0.600	0.5488	0.1364	0.3148
0.650	0.5220	0.1452	0.3327
0.700	0.4966	0.1541	0.3493
0.750	0.4724	0.1629	0.3648
0.800	0.4493	0.1715	0.3792
0.850	0.4274	0.1800	0.3926
0.900	0.4066	0.1883	0.4051
0.950	0.3867	0.1964	0.4168
1.000	0.3679	0.2043	0.4278
1.050	0.3499	0.2119	0.4381
1.104	0.3316	0.2199	0.4485
1.220	0.2953	0.2360	0.4688
1.439	0.2373	0.2627	0.5001

C. Fortran Program

```
C       DAUX  FIRST SET OF EQUATIONS
        SUBROUTINE DAUX
        DIMENSION T(27)
        COMMON T,N,B1,B2
        T(6)=1.0-T(4)-T(5)-B1*T(4)-B2*T(4)
        T(7)=B2*T(4)
        RETURN
C       DAUX  SECOND SET OF EQUATIONS
        SUBROUTINE DAUX
        DIMENSION T(27)
        COMMON T,N,B1,B2
        T(6)=1.0-T(4)-T(5)-B1*T(4)-B2*T(4)**2
        T(7)=B2*T(4)**2
        RETURN
        END
C       DAUX THIRD SET OF EQUATIONS
        SUBROUTINE DAUX
        DIMENSION T(27)
        COMMON T,N,B1,B2
        T(6)=(1.0-T(4)-T(5))**2-B1*T(4)-B2*T(4)
        T(7)=B2*T(4)
        RETURN
        END
C       DAUX  FOURTH SET OF EQUATIONS
        SUBROUTINE DAUX
        DIMENSION T(27)
        COMMON T,N,B1,B2
        T(6)=1.0-T(4)-T(5)-B1*T(4)-B2*T(4)
        T(7)=B2*T(4)
        RETURN
         END
C       DAUX  FIFTH SET OF EQUATIONS
        SUBROUTINE DAUX
        DIMENSION T(27)
        COMMON T,N,B1,B2
        T(6)=1.0-T(4)-T(5)-B1*T(4)**2+B2*T(5)
        T(7)=B1*T(4)**2-B2*T(5)
        RETURN
         END
C       DAUX  SIXTH SET OF EQUATIONS
        SUBROUTINE DAUX
        DIMENSION T(27)
        COMMON T,N,B1,B2
        T(6)=(1.0-T(4)-T(5))**2-B1*T(4)+B2*T(5)
        T(7)=B1*T(4)-B2*T(5)
        RETURN
         END
C       DAUX  SEVENTH SET OF EQUATIONS
        SUBROUTINE DAUX
        DIMENSION T(27)
        COMMON T,N,B1,B2
        T(6)=1.0-T(4)-T(5)-B1*T(4)+B2*T(5)**2
        T(7)=B1*T(4)-B2*T(5)**2
        RETURN
        END


C       DAUX  EIGHTH SET OF EQUATIONS
        SUBROUTINE DAUX
        DIMENSION T(27)
        COMMON T,N,B1,B2
        T(6)=1.0-T(4)-T(5)-B1*T(4)+B2*T(5)
        T(7)=B1*T(4)-B2*T(5)
        RETURN
         END



C       MAIN DAUX
C       THREE RECYCLES.
C       A2 GOVERNS THE SIZE OF THE INTERVAL.
C       A4 EXCEEDS ZERO IFF T(7) HAS TWO TERMS    EQUILIBRIUM LIMITED.
        FREQUENCY 60(1,2,2),1012(80,1,3),1000(100,100,1),1001(100,1,1),101
       13(3,1),51(1,1,3),61(1,1,4)
        DIMENSION T(27),AA(2000),BB(2000),CC(2000),TT(2000),TOPIC(36)
        COMMON T,N,B1,B2
        JJ=0
        J = 1
        CT=0.05
        L=1
        READ 12,(TOPIC(I),I=1,36)
        READ 1,N,A1,A2,A3,A4,A5,A6,A7,(T(I),I=2,7),TH,ER,BM,NX1,K
        SAVER = ER
 1010   READ2,B1,B2
        ASSIGN 1014 TO IR
        IF(A4)18,18,4001
4001    ER = SAVER*(B1/(B1+B2))
18      AA(1) = 1.0
        BB(1) = 0.0
        CC(1) = 0.0
        WA = 1.0
        WB = 0.0
        WC = 0.0
        WT = 0.0
        WDT = 0.05
        PRINT 121,(TOPIC(I),I=1,36)
        PRINT 4,B1,B2
 1002   CALL RKI
        Q1=1.0 - T(4) - T(5)
        IF(T(5))51,60,60
 60     IF(Q1)51,806,806
 806    IF(T(4))51,808,807
 807    IF(T(4)-1.)808,808,51
 808    IF(T(5)-0.91)52,52,51
52      T(3)=0.05
   50   J=J+1
        AA(J)=1.-T(4)-T(5)
        BB(J)=T(4)
        CC(J)=T(5)
        TT(J)=T(2)
        WA = AA(J)
        WB = T(4)
        WC = T(5)
        WT = T(2)
        WDT = T(3)
 1012   IF(T(5)-CT)1000,1005,1004
 1000   IF(T(2)-TH)1001,1001,1006
 1001   IF(T(5)-ER) 2000,1007,1007
2000    IF(J-NX1) 1002,1002,2001
 1003   PRINT3,T(2),AA(J),BB(J),CC(J),J
 1005   CT=CT+0.05
        GO TO 1000
 1004   FAC=(CT-CC(J-1))/(CC(J)-CC(J-1))
        SAVA=FAC*(AA(J)-AA(J-1))+AA(J-1)
        SAVB=FAC*(BB(J)-BB(J-1))+BB(J-1)
        SAVC=CT
        SAVT=FAC*(TT(J)-TT(J-1))+TT(J-1)
```

```
        IF(SAVC-ER)500,500,1007
500     PRINT3,SAVT,SAVA,SAVB,SAVC,J
        CT=CT+0.05
        GO TO 1012
1006    T(3)=A2*T(2)
        GO TO 1001
1007    PRINT 7,(TT(I),AA(I),BB(I),CC(I),I=2,21)
 55     PRINT8,(TT(I),AA(I),BB(I),CC(I),I=22,J,10)
        JJJ = J - XMODF(J,10) + 1
        PRINT 8,(TT(I),AA(I),BB(I),CC(I),I=JJJ,J)
 1013   GO TO IR, (1014,2003)
 1014   IF(L-K) 1008,1011,1011
 1008   L=L+1
        J = 1
        CT=0.05
        DO 1009 I=2,2000
        AA(I)=0.
        BB(I)=0.
        CC(I)=0.
 1009   TT(I)=0.
        T(2)=0.
        T(3)=.05
        T(4)=0.
        T(5)=0.
        GO TO 1010
1011    CALL EXIT
   51   T(2) = WT
        T(4) = WB
        T(5) = WC
        T(3) = BM*T(3)
        CALL RKI
        Q1 = 1.0 - T(4) - T(5)
        IF(T(5))800,801,801
 801    IF(Q1)800,809,809
 809    IF(T(4))800,811,810
 810    IF(T(4)-1.)811,811,800
 811    IF(T(5)-0.91)52,52,800
  800   T(2) = WT
        T(4) = WB
        T(5) = WC
        T(3) = BM*T(3)
        CALL RKI
        Q1 = 1.0 - T(4) - T(5)
        IF(T(5))62,805,805
805     IF(Q1)62,812,812
812     IF(T(4))62,814,813
813     IF(T(4)-1.)814,814,62
814     IF(T(5)-0.91)52,52,62
62      T(2)=WT
        T(4)=WB
        T(5)=WC
        T(3)=BM*T(3)
        CALL RKI
        Q1=1.0-T(4)-T(5)
        IF(T(5))61,901,901
901     IF(Q1)61,909,909
909     IF(T(4))61,911,910
910     IF(T(4)-1.)911,911,61
911     IF(T(5)-0.91)52,52,61


 61     IF(J-20)56,56,57
   57   PRINT 9,(TT(I),AA(I),BB(I),CC(I),I=2,21)
        ASSIGN 2003 TO IR
        GO TO 55
   56   PRINT 10,(TT(I),AA(I),BB(I),CC(I),I=2,J)
        ASSIGN 2003 TO IR
        GO TO 1013
2001    PRINT11,(TT(I),AA(I),BB(I),CC(I),I=2,11)
        ASSIGN 2003 TO IR
        GO TO 55
2003    PRINT 121,(TOPIC(I),I=1,36)
        PRINT 13,(B1,B2,WA,WB,WC,WT,WDT,AA(J),BB(J),CC(J),TT(J),DT,Q1,T(4)
       1,T(5),T(2),T(3),CT,TH,BM,ER)
        ASSIGN 1014 TO IR
        GO TO 1013
    1   FORMAT(2I2,6F10.2/6F10.2/3F6.4,2I5)
    2   FORMAT(2F10.2)
    3   FORMAT(1H F7.3,3F9.4,I7)
    4   FORMAT(20H0SOLUTIONS FOR K1 = ,F6.2,11H  AND K2 = ,F6.2//3X,3HTAU,
       17X,1HA,8X,1HB,8X,1HC,8X,1HN)
    7   FORMAT(41H0SOLUTION COMPLETED BY C GREATER THAN 0.9/33H THE FIRST
       1TEN DATA POINTS FOLLOW/(1H F7.3,3F9.4))
    8   FORMAT(48H                                              /(1H F7.
       13,3F9.4))
    9   FORMAT(32H0SOLUTION COMPLETED BY A MINUS B/33H THE FIRST TEN DATA
       1POINTS FOLLOW/(1H F7.3,3F9.4))
   10   FORMAT(32H0SOLUTION COMPLETED BY A MINUS B/23H ALL DATA POINTS FOL
       1LOW/(1H F7.3,3F9.4))
   11   FORMAT(14H0J EXCEEDS 100/33H THE FIRST TEN DATA POINTS FOLLOW/(1H
       1F7.3,3F9.4))
   12   FORMAT (12A6)
121     FORMAT(1H1,12A6/(1H ,12A6))
 122    FORMAT (1H+41X,5F10.4)
13      FORMAT(1H0,10X,3HK1=,F6.2,3HK2=F6.2/4H0WA=F10.7,3HWB=F10.7,3HWC=F1
       10.7,3HWT=F10.7,4HWDT=F10.7/4H AA=F10.7,3HBB=F10.7,3HCC=F10.7,3HTT=
       2F10.7,4H DT=F10.7/4H Q1=F10.7,3HT4=F10.7,3HT5=F10.7,3HT2=F10.7,4H
       3T3=F10.7/27X,3HCT=F10.7,3HTH=F10.7/4H BM=F10.7,13X,3HER=F10.7)
        END


C       RUNGE-KUTTA INTEGRATION SUBROUTINE    FOURTH ORDER
C       TWO SIMULTANEOUS EQUATIONS.
        SUBROUTINE RKI
        DIMENSION T(27)
        COMMON T
        Y1 = T(4)
        Y2 = T(5)
        TEE = T(3)
        CALL DAUX
        CK01 = TEE*T(6)
        CK02 = TEE*T(7)
        T(4) = Y1 + CK01/2.
        T(5) = Y2 + CK02/2.
        CALL DAUX
        CK11 = TEE*T(6)
        CK12 = TEE*T(7)
        T(4) = Y1 + CK11/2.
        T(5) = Y2 + CK12/2.
        CALL DAUX
        CK21 = TEE*T(6)
        CK22 = TEE*T(7)
        T(4) = Y1 + CK21
        T(5) = Y2 + CK22
        CALL DAUX
        CK31 = TEE*T(6)
        CK32 = TEE*T(7)
        T(2) = T(2) + T(3)
        T(4) = Y1 + (CK01 + 2.*CK11 + 2.*CK21 + CK31)/6.
        T(5) = Y2 + (CK02 + 2.*CK12 + 2.*CK22 + CK32)/6.
        RETURN
        END
```

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