Learnings from the Relation between the Number of Forward and Reverse Reactions (Transfer Cycles) Required to Converge to Equilibrium and the Ratio of the Forward to the Reverse Rate Constants in Simple Chemical Reactions

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ABSTRACT: In simple, reversible, chemical reactions of the type \( A \rightleftharpoons B \), chemical equilibrium is related to chemical kinetics via the equality between the equilibrium constant and the ratio of the forward to the reverse rate-constant, i.e., \( K_{eq} = k_f/k_r \), where \( K_{eq} \) is the equilibrium constant and \( k_f \) and \( k_r \) denote the rate constants for the forward \( (A \rightarrow B) \) and reverse \( (B \rightarrow A) \) reactions, respectively. We review and examine the relation between the number of forward and reverse reactions required to take place for the aforementioned system to reach equilibrium and the ratio of the forward to the reverse rate constant. Each cycle of reactants becoming products and the products becoming reactants is defined as a transfer cycle (TC). Therefore, we underscore the relation between the number of TCs required for the system to equilibrate and \( k_f/k_r \). We also vary the initial concentrations of the reactants and products to examine their dependency of the relation between the number of TCs required to reach equilibrium and \( k_f/k_r \). The data reveal a logarithmic growth-type relation between the number of TCs required for the system to achieve equilibrium and \( k_f/k_r \). The results of this relation are discussed in the context of several scenarios that populate the trajectory. We conclude by introducing students and researchers in the area of chemistry and biochemistry to physical phenomena that relate the initial concentrations of the reactants and products and \( k_f/k_r \) to the number of TCs necessary for the system to equilibrate.

INTRODUCTION

Chemical equilibrium is important in most chemical reactions. Furthermore, equilibration of a chemical system has significance in all branches of chemistry, biochemistry, biology, geology, and environmental sciences and disciplines in engineering such as chemical engineering and metallurgical and materials engineering.\(^1\)\(^ -\)\(^5\)

For a number of reasons, chemical equilibrium remains a difficult concept for some to master. The predecessor to chemical equilibrium is chemical kinetics wherein reactions proceed to completion;\(^2\)\(^ -\)\(^5\) i.e., the reactant is completely consumed to form product. However, if one of the reactants in a multireactant reaction is limiting in concentration, then the reaction goes to completion only with respect to that limiting reagent.\(^6\) Furthermore, in the study of chemical kinetics, the emphasis is on unidirectionality. A one-way arrow denotes the direction of reaction progress (from reactants to products) in the forward direction. For example, a typical generic reaction used as an example in chemical kinetics is

\[ A \rightarrow B \]

Here, \( A \) is consumed, and \( B \) is generated. The rate of this reaction, when first-order in \( A \), is given by

\[ \text{Rate} = k[A] \]

where \( k \) is the rate constant and \([A]\) is the concentration of the reactant expressed in molarity (M). Students of chemical kinetics are taught that the reactant is consumed completely in a finite amount of time, and no more product is produced once the reactant is completely exhausted. This is an outcome of the law of conservation of matter.

CHEMICAL EQUILIBRIUM

In the succeeding topic involving equilibrium, they are introduced to the concept of reversibility and reversible reactions. Here, the conversion of \( A \) to \( B \) is not unidirectional. The here-tofore “product”, \( B \), acts as a “reactant” and forms \( A \), the “product”, with respect to “reactant” \( B \). As a result, \( A \) is never completely consumed. The “undoing” of the complete consumption of \( A \) in the preceding kinetics chapter, via the reversibility of \( B \), is a
necessary and first step toward understanding what chemical equilibrium is all about. The reaction \( A \rightarrow B \) is now transformed into

\[ A \rightleftharpoons B \]

Simultaneously, a new rate constant is introduced, and the unidirectional arrow is replaced by half-headed arrows, indicating the direction of each reaction. The back-conversion of B to A is governed by the reverse rate constant \( k_r \). The forward rate constant, reserved for the process \( A \rightarrow B \), is henceforth referred to as \( k_f \).

**RELATION BETWEEN** \( K_{eq}, K_{fwd}, \) **AND** \( K_{rev} \)**

The equilibrium constant \( K_{eq} \) for the aforementioned reaction of the type \( A \rightleftharpoons B \) is given by \( K_{eq} = [B]/[A] \), where the subscripts denote the concentrations of the reactants and products when the system has reached equilibrium.

A popular exercise for students involves arriving at the equality

\[ k_f[A]_i = k_r[B]_i \quad \text{(A)} \]

from the initial reaction conditions, i.e., initial concentrations of the reactants and the products at the start of the reaction and their respective associated rate constants, viz., \( k_f \) for \( A \rightarrow B \) and \( k_r \) for \( B \rightarrow A \). For convenience, we introduce a term, \( Q \), defined as \([B]/[A]_i\); i.e., \( Q \) is the ratio of the initial concentrations of reactant to the product when \( t = 0 \). The exercise then involves the transformation of the system from its initial conditions, i.e., at \( Q \) to that at equilibrium (\( K_{eq} \)).

This transformation from \( Q \) to \( K_{eq} \) takes place because the initial reactant and product concentrations are more often than not different from their concentrations when the system reaches equilibrium. The students are encouraged in the exercise to “manually convert” reactants to products and vice versa until \( Q = K_{eq} \), i.e., until the system attains equilibrium and the concentrations of the reactants and products are transformed from their initial concentrations, to the concentrations found at equilibrium.

\[ Q \rightarrow K_{eq}, \ [A] \rightarrow [A]_e \text{ and } [B] \rightarrow [B]_e \]

By conducting the manual transformation (discussed below) of reactants into products and vice versa, the students derive an understanding of how the equality, \( k_f[A]_e = k_r[B]_e \), is achieved. This process is iterative. That is, the reactants are consumed to form products and vice versa until \( Q \) tends to \( K_{eq} \) (or \([B]/[A]_i \rightarrow [B]_t/[A]_t\)). The expert will recognize that the equality follows from the principle that at equilibrium the forward reaction rate equals the reverse reaction rate.

To reiterate, a typical exercise provided to students and researchers involves understanding how the system, \( A \rightleftharpoons B \), proceeds to equilibrium by sequential transferring of units of \( A \) to \( B \) and vice versa. Each cycle in which reactants become products and the products become reactants is defined as the transfer cycle (TC). Repetitive TCs permit the reaction, from its arbitrary starting conditions such as \([A]_i = 100 \text{ M}, [B]_i = 0 \text{ M}, k_f = 0.01 \text{ s}^{-1} \), and \( k_r = 0.005 \text{ s}^{-1} \), to reach equilibrium.

Frequently, objects such as uncooked beans, tokens, or cardboard cut-outs are employed in a laboratory setting for students to “feel” the process of chemical transfer in a safe manner. The stress on units is less important at this stage. For example, one “uncooked bean” may represent 1 M without taking into consideration the “volume” that the bean resides in. In practice, it is convenient to use, say, 100 beans to represent \([A]_i\) and “0 beans” to represent \([B]_i\). The process by which \( A \) chemically converts to \( B \) is also not important. Lastly, the uncooked bean represents both \( A \) and \( B \). Therefore, the chemical conversion of \( A \) to \( B \), and vice versa, is achieved by physically moving (transferring) the bean from position “A” on a desk or a lab bench to another position, viz., “B.” The number of beans moved in the forward direction, every transfer cycle, is given by \( \text{Rate} = k_f[A]_i \) or, in this case, 0.01×[100] = 10 beans in the first TC. The number of beans back-transferred (in the direction \( B \rightarrow A \)) in the first TC is given by \( k_r[B]_i = 0.005[0] = 0 \).

By repeating the TCs, the students recognize that the flux of beans from one direction eventually equals that in the other direction. This is because, even though the magnitude of the rate constants \( (k_f \text{ and } k_r) \) does not change, the concentrations of the reactants and the products do. Thus, with each TC, the forward rate decreases because the initial concentration of \( A \) depletes rapidly because \( k_f[A]_i \) is large given that there is 100% \( A \) in the beginning of the reaction. Conversely, with each TC, the concentration of \( B \) increases, and the reverse rate, \( k_r[B] \), increases. The system reaches equilibrium when the forward rate \( (k_f[A]) \) equals the reverse rate \( (k_r[B]) \), and there is no more change in the concentration of the reactant or the product.

Thus, the equality in (A) is eventually used to derive the relationship between the rate constants and the equilibrium constant \( (K_{eq}) \). Through the “transfer” exercise, students learn that at equilibrium, given that \( k_f[A]_e = k_r[B]_e \),

\[ k_f/k_r = [B]_i/[A]_i = K_{eq} \quad \text{(B)} \]

The students can then proceed toward analyzing more complex chemical reactions such as

\[ 2A \rightleftharpoons B \text{ or } aA + bB \rightleftharpoons cC + dD \]

**TRANSFER CYCLES (TCs) AND THE RATIO OF THE RATE CONSTANTS** (\( K_f/K_r \))

Here, we examine and review the number of TCs \((\#TCs)\) required for a simple system, \( A \rightleftharpoons B \), to reach equilibrium as a function of the ratio of forward to reverse rate constants \( (k_f/k_r) \). We also explore the said relation, viz., \#TC vs \( k_f/k_r \), as a function of the initial concentrations chosen for the reactants and products \([A]_i\) and \([B]_i\), respectively.

By permitting both students and instructors to choose appropriate values of the rate constants and starting concentrations of the reactants and products (various \( Q \)’s), this study facilitates an understanding of the relation between \( k_f, k_r, [A]_i, \) and \([B]_i\). In more general terms, we advance an understanding of the relation between \( k_f, k_r, [A]_i, \) and \([B]_i\), where the subscript “0” denotes the concentration of the reactant and product at any point during the reaction progress. For example, \([A]_i = [A], [B]_i = [B], [A]_t = [A]_t, \) and \([B]_t = [B]_t, \) when \( t = 0, \) and \([A]_t \rightarrow [A]_t, [B]_t \rightarrow [B]_t, \) as \( t \rightarrow \infty \).

Our analysis reveals a logarithmic growth-type relationship between the \#TCs and \( k_f/k_r \). The work underscores several special scenarios that are encountered in the relation between these variables which further enable students to understand the physics behind the conclusions drawn.

We also provide an online link that permits students to explore this relation by allowing the parameters \(([A]_i, [B]_i, k_f, \) and \( k_r) \) to float.

**PRACTICAL DETAILS AND REQUIREMENTS**

Paper, pencil, calculator, and graph paper can be used. A computer with a plotting program could be used in lieu of graph
paper as it provides a more rapid mechanism to plot #TCs vs $k_f/k_r$. Access to the Internet is required to use the online program that allows users to input variables ($[A]_i$, $[B]_i$, $k_f$, and $k_r$). The program is available freely at https://repl.it/@jaehayi/K-and-Cycles. The "run" command executes the program. The initial reactant and product concentration and the rate constants can be input in the windows provided. They can be varied, and the program can be executed once more as follows: input values of $[A]_i$, $[B]_i$, $k_f$, and $k_r$ into the program and execute it; record the number of transfer cycles required to achieve equilibrium and the ratio of $k_f$ to $k_r$; and repeat the procedure choosing a larger ratio. For example, keeping $[A]_i$ and $[B]_i$ fixed at 100 and 0, respectively, use the program to compute the number of transfer cycles to reach equilibrium for $k_f$ to $k_r$ varying from, say, 2 to 10 in increments of 1 ratio unit. Record the number of transfer cycles required to achieve equilibrium for every $k_f$ to $k_r$ selected. Either using graph paper or a graphing program, plot the number of transfer cycles required to achieve equilibrium ($y$-axis) vs the $k_f$ to $k_r$ ratio ($x$-axis).

### DISCUSSION

#### Relation between #TCs and $k_f/k_r$

All discussions pertain to the simple reaction type $A \rightleftharpoons B$ for which the following equality applies:

$$k_f/k_r = [B]_i/[A]_i = K$$

Units (M and s$^{-1}$) have been omitted for simplicity and to better focus on understanding the physics behind the processes involved.

Figure 1 shows the number of transfer cycles required to reach equilibrium when only reactant is present ($[A]_i = 100$, $[B]_i = 0$, $k_f = 0.1$, and $k_r = 0.01$ to 0.9).

| $k_f/k_r$ | #TC |
|-----------|-----|
| 10        | 55  |
| 5         | 45  |
| 3.33      | 39  |
| 2.5       | 35  |
| 2         | 31  |
| 1.7       | 29  |
| 1.4       | 26  |
| 1.25      | 24  |
| 1.11      | 23  |
| 1         | 21  |
| 0.5       | 13  |
| 0.33      | 9   |
| 0.25      | 6   |
| 0.2       | 5   |
| 0.16      | 4   |
| 0.14      | 3   |
| 0.12      | 2   |
| 0.11      | 1   |

#### Table 1. $k_f/k_r$ vs #TC When $[A]_i = 100$, $[B]_i = 0$, $k_f = 0.1$, and $k_r = 0.01$ → 0.9

To converge decreases (55 → 23). This is because the product $k_f[A]$ is much larger than the product $k_f[B]$ when the difference between $k_f$ and $k_r$ is the largest ($k_f/k_r = 10$) compared to when the ratio between them is the smallest (1.111). Thus, the #TCs required to converge to equilibrium are correspondingly large since $k_f[A]$ has to "catch up" to $k_f[B]$ and requires the largest

![Figure 2. #TCs vs $k_f/k_r$ when $[A]_i = 100$, $[B]_i = 0$, $k_f = 0.1$, and $k_r = 0.01$ → 0.9.](https://dx.doi.org/10.1021/acsomega.0c05130)
number of cycles to do so when the ratio between \( k_f \) and \( k_r \) is the largest (for a fixed value of initial reactant and product concentrations). Lastly, the plot reveals a logarithmic growth-type relation between \( k_f/k_r \) versus the number of transfer cycles; i.e., as the ratio increases, the #TCs required for the system to converge to equilibrium increase. These results suggest that the number of transfer cycles required to reach the equilibrium ratio of reactant and product concentrations, viz., \([B]/[A]_o\) in a simple reaction of the type \( A \rightleftharpoons B \) is dependent on the magnitude of the forward to reverse rate constant ratio \( (k_f/k_r) \).

Figure 2 shows the same system as before with the ratio now further reduced from a previous minimum of 1.1 (in Figure 1) to 0.11 (Table 2). A further smooth decrease in the number of transfer cycles required to achieve equilibrium is observed as \( k_f/k_r \) recedes from 1.1 to 0.11. Overall, the #TC vs \( k_f/k_r \) plot mimics that in Figure 1. An interesting observation can be made while comparing the data in Tables 1 and 2. An ~9-fold increase in \( k_f/k_r \) from 1.1 to 10 results in an ~2.4-fold increase in the #TCs required for the system to equilibrate (Table 1). However, the same increase (from 0.11 to 1) results in a 21-fold increase (from 1 to 21) in the #TCs required to reach equilibrium (Table 2). This is consistent with the logarithmic growth nature of the relation between the #TCs required to reach equilibrium vs \( k_f/k_r \), which initially rapidly rises before starting to flatten. Furthermore, the #TC required for equilibration of the system when \( k_f/k_r \) is reduced from 1.11 to 0.11 also decreases, a finding consistent with the previous conclusions (pertaining to Figure 1) where the #TC increased as the \( k_f/k_r \) ratio increased.

Note: While it is easy to manually test scenarios where 1 or 2 transfer cycles alone suffice for equilibrium to be achieved, a true appreciation of how the system reaches equilibrium is realized when more transfer cycles are required. Such an approach helps a student examine how the concentration of the reactant progressively decreases and reactant increases (for \( k_f > k_r \)), while \( k_f \) and \( k_r \) remain constant throughout.

Figure 3 simulates a scenario where only the initial concentration of the reactant changes relative to the system in Figure 2. Here, the reactant concentration is 50 (Table 3) which is half the value of system 2. However, the \( k_f \) and \( k_r \) values (and hence the ratio \( k_f/k_r \)) are identical to the previous scenario. As can be predicted, the number of cycles required for the system to equilibrate as a function of \( k_f \) and \( k_r \) is the same. The student may infer that “smaller amounts” are being transferred since the initial concentration of the reactant is half that in the previous system.

The data (#TC) obtained are again self-consistent and consistent across scenarios in Figures 1 and 2. The initial value of \([A]_i\), as long as \([B]_i\) is 0, has no impact on the #TCs required for the system to equilibrate as the “flux” being transferred is proportional to the concentration of reactant (and product).

We now consider scenarios where product is initially present (values represented in Table 4).

Figure 4 depicts conditions wherein, for \([A]_i = 100\), \([B]_i\) varies as follows: 25, 50, 75, 100, 200, and 400. In each of these cases, since some \([B]_i\) is initially present, it requires fewer TCs to reach equilibrium as compared to when \([B]_i = 0\) (Figure 3), for every \(k_f/k_r\) ratio tested. Furthermore, even though the profiles of #TC vs \(k_f/k_r\) appear to follow logarithmic growths, closer inspection reveals there is a deviation from such behavior at each \([B]_i\) tested. For example, in 4(A), at \(k_f/k_r = 0.25\) for \([B]_i = 25\), the number of transfer cycles required is 0. This is because \(k_f[A]_i = 25\), which is the same as \([B]_i\), i.e., the system is already at equilibrium under the supplied conditions of \(k_f\), \(k_r\), \([A]_i\), and \([B]_i\). Similar “0” TCs are observed for \([B]_i = 50\) (4B), 100 (4D), and 200 (4E). This is because the initial conditions are such that the system is already at equilibrium. For \([B]_i\) values of 75 (4C) and 400 (4F), a downward curvature toward the abscissa is seen. Nevertheless, the “0” TC point is not realized, and the TC vs \(k_f/k_r\) profile inclines upward thereafter. This is simply because the “0” TC condition (i.e., \(K = Q\)) is not coincidentally met with any of the choices of \(k_f\), \(k_r\), \([A]_i\), and \([B]_i\). However, if we had selected a more closely spaced ratio of \(k_f/k_r\), a “0” point would have been realized.

Lastly, as the initial concentration of B appreciates from 0 to 400, the #TCs required to reach equilibrium deprecate as a function of the \(k_f/k_r\) ratio (Figure 5; Table 5 inset).

However, the “sensitivity” to the concentration appears to vanish as the \(k_f/k_r\) ratio subsides from 10 to 0.11. This is an outcome of the plot itself which arises from the nature of the demarcations used in the graph vis-à-vis the number of data points obtained per interval. A large number of y-values within the same excursion on the x-axis provide a skewed view of the data.

![Figure 3](https://dx.doi.org/10.1021/acsomega.0c05130)

Figure 3. #TCs vs \(k_f/k_r\) when \([A]_i = 50\), \([B]_i = 0\), \(k_f = 0.1\), and \(k_r = 0.01 \rightarrow 0.9\).

### Table 3. \(k_f/k_r\) vs #TC When \([A]_i = 50\), \([B]_i = 0\), \(k_f = 0.1\), and \(k_r = 0.01 \rightarrow 0.9\)

| \(k_f/k_r\) | #TC |
|-----------|-----|
| 10        | 55  |
| 5         | 45  |
| 3.33      | 39  |
| 2.5       | 35  |
| 2         | 31  |
| 1.67      | 29  |
| 1.42      | 26  |
| 1.25      | 24  |
| 1.11      | 23  |
| 1         | 21  |
| 0.5       | 13  |
| 0.33      | 9   |
| 0.25      | 6   |
| 0.2       | 5   |
| 0.16      | 4   |
| 0.14      | 3   |
| 0.12      | 2   |
| 0.11      | 1   |

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We also examined purely integral values of $k_f/k_r$ ratios where $k_i \geq k_r$. For this relation, we chose a fixed value of $[A]_i = 100$ and varied $[B]_i$ from 0 to 400 as before. For every $[B]_i$ selected, we varied $k_f/k_r$ from 1 to 20. The data (Figure 6) reveal that as the $k_f/k_r$ ratio increases from 1 to 20 the number of transfer cycles increases from 21 ($k_f/k_r = 1$) to 63 ($k_f/k_r = 20$) (Table 6). While the explanation for this has already been discussed, we reiterate that such a behavior is to be expected since a large ratio between the forward and reverse rate constants would require “many steps” for the process $B \rightarrow A$ to catch up with $A \rightarrow B$. Nevertheless, in conclusion, the trend seen in the plot is consistent with that observed in Figures 1–3 since it is the numerical value of $k_f/k_r$ that dictates the TCs required for the system to equilibrate.

As the concentration of $B$ is increased from 0 to 400 (Figure 7; Table 7), for a fixed value of $[A]_i = 100$, the number of cycles required to achieve equilibrium is attenuated (as previously seen for fractional values of the same ratio). In three selected conditions, the system is already at equilibrium as evidenced by the number (0) of cycles required for transfer.

It is to be noted that irrespective of the ratio of the rate constants being integral or fractional the function relating it to the number of transfer cycles remains similar in all cases (log growth) as long as the coincidental choice of $Q = K$ is not met within the series of ratios chosen. As the concentration of $[B]$ is increased (from 0 to 25 to 400), the number of cycles to reach $K_{eq}$ reduces as previously seen. Again, deviations from the logarithmic growth are encountered whenever $Q = K_{eq}$, but the lag in the deviations becomes smaller and approaches the origin as expected when $[B]_i$ increases from 0 to 400.

Table 4. $k_f/k_r$ vs #TC When $[A]_i = 100$, $[B]_i = 25–400$, $k_f = 0.1$, and $k_r = 0.01 \rightarrow 0.9$

| $[A]_i = 100$ | number of transfer cycles |
|--------------|----------------------------|
| $[B]_i = 25$ | $[B]_i = 50$ | $[B]_i = 75$ | $[B]_i = 100$ | $[B]_i = 200$ | $[B]_i = 400$ |
| $k_f/k_r$ | 53 | 51 | 49 | 48 | 43 | 36 |
| 10 | 53 | 51 | 49 | 48 | 43 | 36 |
| 5 | 45 | 43 | 39 | 38 | 33 | 20 |
| 3.33 | 37 | 35 | 33 | 32 | 25 | 16 |
| 2.5 | 33 | 31 | 29 | 27 | 17 | 21 |
| 2 | 29 | 27 | 25 | 23 | 0 | 21 |
| 1.67 | 26 | 24 | 22 | 19 | 13 | 21 |
| 1.42 | 24 | 22 | 19 | 16 | 15 | 21 |
| 1.25 | 22 | 20 | 17 | 13 | 16 | 20 |
| 1.11 | 20 | 18 | 15 | 18 | 16 | 19 |
| 1 | 19 | 16 | 12 | 0 | 16 | 19 |
| 0.5 | 10 | 10 | 9 | 11 | 13 | 14 |
| 0.33 | 6 | 7 | 8 | 9 | 10 | 10 |
| 0.25 | 0 | 6 | 7 | 7 | 8 | 8 |
| 0.2 | 3 | 5 | 5 | 6 | 6 | 6 |
| 0.16 | 3 | 4 | 4 | 5 | 5 | 5 |
| 0.14 | 3 | 3 | 3 | 4 | 4 | 4 |
| 0.12 | 2 | 3 | 3 | 3 | 3 | 3 |
| 0.11 | 1 | 1 | 1 | 1 | 1 | 1 |

CONCLUSIONS

Using a simple chemical reaction, viz., $A \rightleftharpoons B$, as an example, we have examined the number of forward and reverse reactions (TC) between reactants and products that is required for the reaction to reach equilibrium from its initial condition as a function of the forward and reverse rate constant ratio ($k_f/k_r$). Our analyses reveal that a plot of TC vs $k_f/k_r$ follows a logarithmic growth curve, the reasons for which have been extensively discussed in this article. The exercise can be utilized by students of general chemistry to explore the nature of the components involved in the system, viz., the initial concentrations of reactant and product and the dependency of TC on these factors and the forward and reverse rate constant. Importantly, both the beginner student as well as researchers not familiar with the principles governing chemical equilibrium can potentially use this exercise to advance their understanding of the physics behind the chemistry or biology in any “real-world” scenarios. These include the role of chemical equilibria and their treatment in biological, environmental, chemical, and metallurgical engineering systems.20–24 The findings are also useful to design experiments in the laboratory for individual research applications and for teaching structured classes.

A user-friendly program that generates the number of TCs as a function of the rate constant ratio is made freely available for students and educators to peruse.

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Author Contributions

G.M.N., A.V., F.V., and J.Y. contributed equally. M.N. conceived the topic. G.M.N., A.V., F.V., and J.Y. performed the calculations, generated the data, and contributed to the
discussions. J.Y. compiled the program. All authors tested the program. M.N. wrote and reviewed the manuscript.

Notes
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Figure 4. #TCs vs $k_f/k_r$ when $[A]_i = 100$, $[B]_i = 25$ (A), 50 (B), 75 (C), 100 (D), 200 (E), and 400 (F); $k_f = 0.1$ and $k_r = 0.01 \rightarrow 0.9$. 

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Figure 5. #TCs vs \( k_f/k_r \).

Table 5. \( k_f/k_r \) vs #TC

| [B]_i | #TC |
|-------|-----|
| 0     | 55  |
| 25    | 53  |
| 50    | 51  |
| 75    | 49  |
| 100   | 48  |
| 200   | 43  |
| 400   | 36  |

Figure 6. \( k_f/k_r \) vs #TC, when \([A]_i = 100, [B]_i = 0 \rightarrow 400, \) and \( k_f/k_r = 1 \rightarrow 20 \).

Table 6. \( k_f/k_r \) vs #TC When \([A]_i = 100, [B]_i = 0 \rightarrow 400, \) and \( k_f/k_r = 1 \rightarrow 20 \)

| \( k_f/k_r \) | #TC |
|--------------|-----|
| 1            | 21  |
| 2            | 31  |
| 3            | 38  |
| 4            | 42  |
| 5            | 45  |
| 6            | 48  |
| 7            | 50  |
| 8            | 52  |
| 9            | 53  |
| 10           | 55  |
| 11           | 56  |
| 12           | 57  |
| 13           | 58  |
| 14           | 59  |
| 15           | 60  |
| 16           | 61  |
| 17           | 61  |
| 18           | 62  |
| 19           | 63  |
| 20           | 63  |

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Figure 7. #TCs vs $k_f/k_r$ when $[A] = 100$, $[B] = 0$–400, and $k_f/k_r = 1$ → 20. Bottom to top: $[B] = 0, 25, 50, 75, 100, 200, 400$.

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