

Analytical Solutions of Chemical Reaction Kinetic Models Through Integral Transform Techniques

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ABSTRACT

Experts in mathematical modeling are currently using integral transforms to model many scientific phenomena. In this sense, the current work evaluates the success rate of the HK transform relative to the well-known Laplace transform by examining how it can be used to solve differential equations describing chemical processes. A first-order differential equation representing chemical reaction and diffusion models was used to demonstrate the HK transform's ability to simplify calculations and yield exact analytical solutions. The same method was then applied to a model that generated component diffusion in a reactive medium with a time-dependent coefficient, demonstrating the transform's ability in handling various coefficients. Lastly, the study examined a single step reversible chemical process represented by a second-order differential equation, and the outcomes of the Laplace and HK transforms were contrasted. The comparison established the HK transform as a trustworthy substitute mathematical tool for modeling and studying a variety of chemical systems by confirming that both transformations provide com-parable accuracy and efficacy.

1. Introduction

In a variety of scientific, technological, economic, and artificial intelligence domains, mathematics is essential for simplifying complex problems and deriving significant findings. Because differential equations model dynamic changes across a wide range of systems, they constitute a significant portion of the mathematical tools taught in physics, chemistry, biology, and economics courses.[1], [2]

Chemical science heavily relies on mathematics, especially when modelling chemical reactions, transport phenomena, mixing processes, and concentration dynamics. Many models in physical chemistry, analytical chemistry, chemical engineering, and environmental chemistry are based on differential equations, which are frequently used to explain how chemical quantities vary over time and space. Since these equations often involve complex time-dependent behaviour, the development of precise and efficient analytical solution techniques is essential. Integral transforms have become useful tools in this discipline, offering accurate answers without requiring extensive computation and

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a systematic method for converting differential equations into simpler algebraic forms. One of them that is now becoming better known is the HK transform due to its use in chemical applications. Chemical processes that give rise to differential equations difficult or complex to solve using standard techniques include transfer processes, mixing systems, and reaction kinetics. It may be difficult, or even impossible, to find closed-form solutions using standard analytical or numerical techniques. Therefore, a simpler mathematical method that can handle changing chemical equations while maintaining analytical quality is required [3]–[6].

In recent years, integral transforms have proven to be a practical and efficient way to solve the complex problems in science, technology, engineering, and economics. One of the greatest advantages of integral transforms is their capacity to produce exact outcomes without requiring hard calculation [7]–[11] also many integral transform have been used to investigate differential equations and integral equations and integro differential equation, and fractional differential equations [12]–[14], Similarly, integral transforms are employed to represent more complex processes such as population dynamics, including growth and decay. has numerous real-world applications in differential equation modelling, particularly in advanced mathematical domains such as fractional calculus, physics, chemistry, and mechanics [15]–[17].

Researchers have found that the HK transformation is a helpful method for solving differential equations, particularly initial- and boundary-value problems. This technique, named after the mathematician HK, breaks down differential equations into simpler algebraic equations [18].

For example, a differential equation may be used to numerically represent the temporal change of a material in a mixture while taking into account the rates of input and outflow: [1]

$$\frac{dy}{dt} = \text{Rate in} - \text{Rate out}, \quad y(0) = y_0$$

By using the HK transformation on this differential equation, we can turn the time-domain issue into an algebraic equation in the HK transform domain. This reduction helps us compute the improved mixing function. After the algebraic problem has been solved, the mixing function in the original time domain may be obtained using the inverse HK transformation. [18], [19].

The current work aims to examine the application of the HK transformation to solve differential equations arising in mixing systems and similar dynamic systems, and to propose a reliable and safe computing approach.

The goal of this study is to investigate the analytical applications of the HK transform in chemical research by focusing on how the transform simplifies and solves differential equations that arise in chemical systems.

This study aims to investigate the mathematical properties of the HK transform and its application in solving differential equations for chemical mixing processes. By converting dynamic chemical models from the time domain to algebraic form, the HK transform, along with its inverse, provides a direct method for obtaining exact analytical solutions. The research further explores the utility of this transform in complex systems, such as catalytic processes, anomalous diffusion, and fractional-order kinetics. Following an introduction to the theoretical and chemical foundations of the method, the paper reviews current literature on integral transforms in the chemical sciences. The results section demonstrates the practical application of the HK transform to specific differential equations, and the study concludes by summarizing the findings and suggesting directions for future research in chemical modeling.

2. Preliminaries

The HK transform and its characteristics have been described in this section. We will have an overview of the new transition through several more investigations.

Definition 1 [HK transforms,]. [18] The exponentially ordered piecewise continuous function with the HK transform $y(t)$ defined in the interval $[0, \infty)$, is given by:

$$HK\{y(t)\} = \frac{1}{\sqrt{\rho}} \int_0^{\infty} e^{-t\rho} y(t) dt = Y(\rho), \quad t > 0, \quad (1)$$

Property 1: [18] Some basic functions and their *HK* transform

$y(t)$	$HK\{y(t)\} = Y(\rho)$	$y(t)$	$HK\{y(t)\} = Y(\rho)$
1	$\frac{1}{\rho^{\frac{3}{2}}}$	$\sin(kt)$	$\frac{a}{\sqrt{\rho(\rho^2 + k^2)}}$
e^{kt}	$\frac{1}{\sqrt{\rho(\rho - k)}}$	$\cos(kt)$	$\frac{\sqrt{\rho}}{\rho^2 + k^2}$
$t^n, n \in N$	$\frac{n!}{\rho^{n+\frac{3}{2}}}$	$\sinh(kt)$	$\frac{a}{\sqrt{\rho(\rho^2 - k^2)}}$
$t^\beta, \beta > -1$	$\frac{\Gamma(\beta + 1)}{\rho^{\beta+3/2}}$	$\cosh(kt)$	$\frac{\sqrt{\rho}}{\rho^2 - k^2}$

Property 2: [18] Some basic functions and their inverse *HK* transform

$Y(\rho)$	$HK^{-1}\{Y(\rho)\} = y(t)$	$Y(\rho)$	$HK^{-1}\{Y(\rho)\} = y(t)$
$\frac{1}{\rho^{\frac{3}{2}}}$	1	$\frac{a}{\sqrt{\rho(\rho^2 + k^2)}}$	$\sin(kt)$
$\frac{1}{\sqrt{\rho(\rho - k)}}$	e^{kt}	$\frac{\sqrt{\rho}}{\rho^2 + k^2}$	$\cos(kt)$
$\frac{1}{\rho^{n+\frac{3}{2}}}$	$\frac{t^n}{n!}, n \in N$	$\frac{a}{\sqrt{\rho(\rho^2 - k^2)}}$	$\sinh(kt)$
$\frac{1}{\rho^{\beta+3/2}}$	$\frac{t^\beta}{\Gamma(\beta + 1)}, \beta > -1$	$\frac{\sqrt{\rho}}{\rho^2 - k^2}$	$\cosh(kt)$

Property 3: (see[18]). The *HK* transformation for integer order derivative of $y(t)$ is:

1. $HK(y'(t)) = \rho Y(\rho) - \rho^{-\frac{1}{2}} y(0),$
2. $HK\{y''(t)\} = \rho^2 Y(\rho) - \rho^{\frac{1}{2}} y(0) - \rho^{-\frac{1}{2}} y'(0),$
3. $HK\{y^n(t)\} = \rho^n Y(\rho) - \sum_{k=0}^{n-1} \rho^{k-\frac{1}{2}} y^{n-1-k}(0).$

Remark 1: The *HK* transform has a duality relation with the famous and mostly used integral transform "Laplace transform", if $L(f(t)) = \int_0^{\infty} f(t)e^{-st} dt = F(s)$, where L is the Laplace transform, and $HK(u(t)) = U(\rho)$, then $U(\rho) = \frac{F(\rho)}{\sqrt{\rho}}$.

3. HK TRANSFORM OF VARIABLE COEFFICIENTS

The *HK* transform formulae for ordinary differential equations with variable coefficients should be derived in this section. This is the main aim and focus of our research, since the creation of these formulas provides a systematic approach to using the *HK* transform effectively.

Theorem 1:[18] If $HK\{y(t)\} = Y(\rho)$, then

a) $HK\{ty(t)\} = -\frac{d}{d\rho}(Y(\rho)) - \frac{1}{2\rho}Y(\rho).$

$$b) \quad HK\{ty'(t)\} = -\rho \frac{d}{d\rho}(Y(\rho)) - \frac{3}{2}Y(\rho).$$

Proof:

$$a) \quad HK\{y(t)\} = \frac{1}{\sqrt{\rho}} \int_0^\infty y(t) e^{-t\rho} dt = Y(\rho)$$

$$\text{now } \frac{d}{d\rho}(Y(\rho)) = \frac{1}{\sqrt{\rho}} \int_0^\infty -ty(t) e^{-t\rho} dt - \frac{1}{2\rho\sqrt{\rho}} \int_0^\infty y(t) e^{-t\rho} dt$$

$$\frac{d}{d\rho}(Y(\rho)) = -HK\{ty(t)\} - \frac{1}{2\rho}Y(\rho)$$

$$HK\{ty(t)\} = -\frac{d}{d\rho}(Y(\rho)) - \frac{1}{2\rho}Y(\rho). \quad \blacksquare$$

$$b) \quad \text{From part (a), we have } HK\{ty(t)\} = -\frac{d}{d\rho}(Y(\rho)) - \frac{1}{2\rho}Y(\rho).$$

$$\text{That means } HK\{ty(t)\} = -\frac{d}{d\rho}(HK\{y(t)\}) - \frac{1}{2\rho}HK\{y(t)\}$$

$$\text{Now } HK\{ty'(t)\} = -\frac{d}{d\rho}(HK\{y'(t)\}) - \frac{1}{2\rho}HK\{y'(t)\}.$$

$$\text{And from property 3 part (a), we have } HK(y'(t)) = \rho Y(\rho) - \rho^{-\frac{1}{2}}y(0)$$

$$\text{So } HK\{ty'(t)\} = -\frac{d}{d\rho}(\rho Y(\rho) - \rho^{-\frac{1}{2}}y(0)) - \frac{1}{2\rho}(\rho Y(\rho) - \rho^{-\frac{1}{2}}y(0)),$$

$$HK\{ty'(t)\} = -\frac{d}{d\rho}(\rho Y(\rho)) + \frac{d}{d\rho}(\rho^{-\frac{1}{2}}y(0)) - \frac{1}{2}Y(\rho) + \frac{1}{2}\rho^{-\frac{3}{2}}y(0),$$

$$HK\{ty'(t)\} = -\rho \frac{d}{d\rho}(Y(\rho)) - Y(\rho) - \frac{1}{2}\rho^{-\frac{3}{2}}y(0) - \frac{1}{2}Y(\rho) + \frac{1}{2}\rho^{-\frac{3}{2}}y(0),$$

$$HK\{ty'(t)\} = -\rho \frac{d}{d\rho}(Y(\rho)) - \frac{3}{2}Y(\rho). \quad \blacksquare$$

4. Applications in Chemistry

This section examines the use of the HK transform for various chemical science issues. The HK transform is an effective technique for solving mathematical problems in this field. In the chemical sciences, mixing difficulties are very significant. A fixed-capacity tank holding a well-mixed fluid, like salt in water, is a typical example. After full mixing, a solution of a certain concentration enters the tank at a set rate, and the resulting mixture leaves the tank at a possibly different fixed rate.

Let the amount of material in the tank at time t be represented by $y(t)$. The rate at which material enters the tank and the rate at which it exits are equal to the rate of change of this quantity, $y'(t)$. A first-order differential equation can frequently be used to model such systems, offering a straightforward mathematical framework for examining mixing phenomena. The model is

$$\frac{dy}{dt} = \text{Rate of amount, or } \frac{dy}{dt} = \text{Rate in} - \text{Rate out},$$

with initial conditions, we explain the model

$$\frac{dy}{dt} = (r_{\text{in}} \cdot C_{\text{in}}) - \left(r_{\text{out}} \cdot \frac{A(t)}{V}\right),$$

such that $y(t)$ Represents the total amount of salt present in the tank at any time t .

$\frac{dy}{dt}$: The time rate of change of the salt mass.

r_{in} : The volumetric flow rate of the incoming brine solution.

C_{in} : The concentration of salt in the incoming stream.

r_{out} : The volumetric flow rate of the mixture leaving the tank.

$V(t)$: The total volume of liquid in the tank. If $r_{\text{in}} = r_{\text{out}}$, the volume V remains constant.

Problem 1: In a tank with 6000 L of water containing 30 kg of dissolved salt. A brine solution, with a constant salt concentration of 0.04 kg/L, is introduced into the reservoir at a flow rate of

25 L/min. To maintain a constant volume, the tank's well-mixed fluid flows out at the same rate of 25 L/min. Determine the total mass of salt present in the reservoir after 1 hour.

Solution: At time $t = 0$, $y(t)$ Describe the salt content. Thus, 30 kg of salt are in the tank. i.e. $y(0) = 30$ and the quantity of salt left after 60 minutes, i.e., $y(60)$

$\frac{dy}{dt} = \text{Rate of amount of salt}$, or $\frac{dy}{dt} = \text{Rate in} - \text{Rate out}$

$$\frac{dy}{dt} = (r_{in} \cdot C_{in}) - \left(r_{out} \cdot \frac{y(t)}{V}\right),$$

$$\text{Rate in} = 0.04 \left(\frac{kg}{L}\right) \times 25 \left(\frac{L}{min}\right) = 1 \left(\frac{kg}{min}\right),$$

$$\text{Rate out} = \left(\frac{y(t)}{6000}\right) \left(\frac{kg}{L}\right) \times 25 \left(\frac{L}{min}\right) = \frac{y(t)}{240} \left(\frac{kg}{min}\right),$$

$$\text{From the modelling we have } \frac{dy}{dt} = \text{Rate in} - \text{Rate out} \Rightarrow \frac{dy}{dt} = 1 \left(\frac{kg}{min}\right) - \frac{y(t)}{240} \left(\frac{kg}{min}\right)$$

$y'(t) + \frac{y(t)}{240} = 1$ The first-order differential equation may be solved using the HK transform.

The HK transform $HK\{y(t)\}$ of a function $y(t)$ is defined as:

$$HK\{y(t)\} = \frac{1}{\sqrt{\rho}} \int_0^{\infty} e^{-t\rho} y(t) dt = Y(\rho), \quad \rho > 0$$

Using both sides of the equation with the HK transform: $HK\left\{y'(t) + \frac{y(t)}{240}\right\} = HK\{1\}$

From the properties that we have $HK\{y^{(m)}(t)\} = \rho Y(\rho) - \rho^{\frac{1}{2}} y(0)$

Using the HK transform's characteristics: $\rho Y(\rho) - \rho^{\frac{1}{2}} y(0) + \frac{Y(\rho)}{240} = \frac{1}{\rho^{\frac{3}{2}}}$

We have to solve for $Y(\rho)$: $\rho Y(\rho) + \frac{Y(\rho)}{240} = \frac{1}{\rho^{\frac{3}{2}}} + \frac{30}{\rho^{\frac{3}{2}}}$

$$\left(\rho + \frac{1}{240}\right) Y(\rho) = \frac{1}{\rho^{\frac{3}{2}}} + \frac{30}{\rho^{\frac{3}{2}}} \Rightarrow \left(\rho + \frac{1}{240}\right) Y(\rho) = \frac{1+30\rho}{\rho^{\frac{3}{2}}} \Rightarrow Y(\rho) = \frac{1+30\rho}{\rho^{\frac{3}{2}}\left(\rho + \frac{1}{240}\right)},$$

By Partial fraction $Y(\rho) = \frac{A}{\rho^{\frac{3}{2}}} + \frac{B}{\rho^{\frac{1}{2}}\left(\rho + \frac{1}{240}\right)}$ therefore $A = 240$, $B = -210$ so

$$Y(\rho) = \frac{240}{\rho^{\frac{3}{2}}} - \frac{210}{\rho^{\frac{1}{2}}\left(\rho + \frac{1}{240}\right)}.$$

Inverse HK transform: To find $y(t)$, we take the inverse HK transform:

$$y(t) = HK^{-1}\left\{\frac{240}{\rho^{\frac{3}{2}}} - \frac{210}{\rho^{\frac{1}{2}}\left(\rho + \frac{1}{240}\right)}\right\} \text{ We get } y(t) = 240 - 210e^{\frac{-t}{240}}.$$

One hour later, we can see $y(60) = 240 - 210e^{\frac{-60}{240}} = 240 - 210e^{-0.25} = 76.45 \text{ kg}$ of salt.

In conclusion, the tank's salt content asymptotically reaches 240 kg, with about 76.45 kg of salt still in the tank after 60 minutes.

From the starting value of 30 kg to the steady-state value of 240 kg, the quantity of salt in the tank grows exponentially, as shown in Figure 1. The salt content at $t = 60$ minutes is around 76.45 kg. As time goes on, the salt content approaches equilibrium, indicating that the rates of input and outflow are balanced. This is shown in Figure 1.

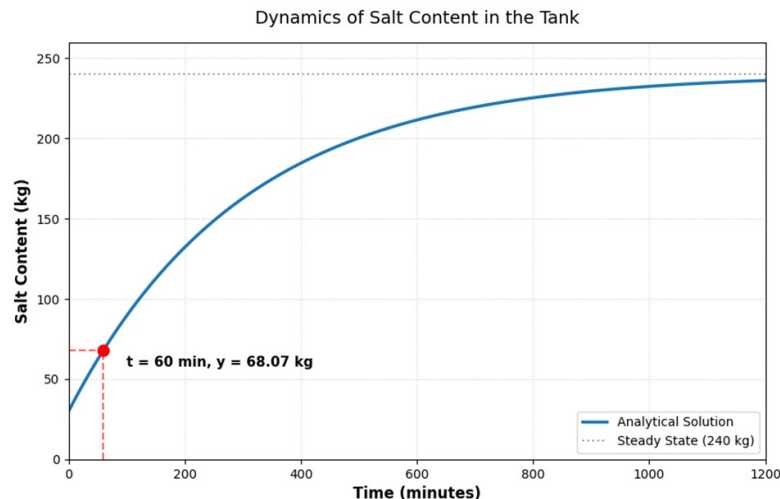


Fig. 1. Changes in the tank's salt content over time

Problem 2: In a localized industrial setting, a 15-liter waste tank is utilized to manage the discharge of sodium chloride from a homemade soap operation, where the tank is initially filled with 15 Liters of water containing 750 grams of dissolved salt. To maintain a constant volume and comply with local environmental regulations, the system operates under dynamic conditions in which brine enters the tank as Process Waste (Stream A) at a rate of 1.5 L/min and a concentration of 25 g/L. In comparison, pure Fresh Water (Stream B) is simultaneously pumped into the system at 2.0 L/min to dilute the mixture. To keep the liquid level constant at 15 Liters, the well-mixed solution is discharged into the environment C is the discharge stream at a total rate of 3.5 L/min. According to the principle of mass balance, the rate of change of salt in the tank is defined by the relation: accumulation equals the input rate minus the output rate.

Solution: Since there isn't a chemical reaction occurring in the storage tank, the equation above may be written as

$$\frac{dy}{dt} = (r_{in} \cdot C_{in}) - \left(r_{out} \cdot \frac{y(t)}{V}\right)$$

$$\frac{dy}{dt} = \left(25 \frac{g}{L}\right) \left(1.5 \frac{L}{min}\right) + \left(0 \frac{g}{L}\right) \cdot \left(2 \frac{L}{min}\right) - \left(\frac{y(t)}{15 L}\right) \cdot \left(3.5 \frac{L}{min}\right) + 0 = 37.5 \frac{g}{min} + 0 - 3.5y(t) \frac{g}{min}, \text{ Therefore, } \frac{dy}{dt} + \frac{7}{30}y = 37.5$$

for the ordinary diff's starting condition. equation for the salt concentration at $t = 0$. in the tank was provided as $y(0) = 750$, that means 50 g/L

The first-order differential equation can be solved using the HK transform.

The HK transforms $HK\{y(t)\}$ of a function $y(t)$ is defined as:

$$HK\{y(t)\} = \frac{1}{\sqrt{\rho}} \int_0^\infty e^{-t\rho} y(t) dt = Y(\rho), \quad \rho > 0$$

Applying the HK transform on both sides of the differential equation will transform it:

$$HK\left\{\frac{dy}{dt} + \frac{7}{30}y\right\} = HK\{37.5\}$$

From the properties that we have $HK\{y'(t)\} = HK(y'(t)) = \rho Y(\rho) - \rho^{-\frac{1}{2}}y(0)$

Using the HK transform's characteristics: $\rho Y(\rho) - \rho^{-\frac{1}{2}}y(0) + 3.5Y(\rho) = \frac{37.5}{\rho^{\frac{3}{2}}}$

We have to solve $Y(\rho) : \rho Y(\rho) + \frac{7}{30}Y(\rho) = \frac{37.5}{\rho^{\frac{3}{2}}} + \frac{750}{\rho^{\frac{1}{2}}}$

$$\left(\rho + \frac{7}{30}\right)Y(\rho) = \frac{37.5}{\rho^{\frac{3}{2}}} + \frac{750}{\rho^{\frac{1}{2}}} \Rightarrow \left(\rho + \frac{7}{30}\right)Y(\rho) = \frac{750\rho + 37.5}{\rho^{\frac{3}{2}}}, Y(\rho) = \frac{750\rho + 37.5}{\rho^{\frac{3}{2}}\left(\rho + \frac{7}{30}\right)}$$

By Partial fraction $Y(v) = \frac{A}{\frac{3}{\rho^2}} + \frac{B}{\frac{1}{\rho^2}(\rho + \frac{7}{30})}$ therefore $A = \frac{1125}{7}$, $B = \frac{4125}{7}$ so

$Y(v) = \frac{\frac{1125}{7}}{\frac{3}{\rho^2}} + \frac{\frac{4125}{7}}{\frac{1}{\rho^2}(\rho + \frac{7}{30})}$. To find $y(t)$, we take the inverse HK transform:

$$y(t) = HK^{-1} \left\{ \frac{1125}{7\rho^2} + \frac{4125}{7\rho^2(\rho + 3.5)} \right\} \text{ We get } y(t) = \frac{1125}{7} + \frac{4125}{7} e^{-\frac{7}{30}t}.$$

The time evolution of the 15-liter waste tank's sodium chloride concentration is shown in Figure 2. The concentration starts at 50 grams per Liter and drops dramatically when fresh water is added, and saltwater is released. The system gets closer to its steady-state condition as time goes on because the exponential term $e^{(-\frac{7}{30}t)}$ decreases, and the transient component of the solution disappears. The blue curve illustrates how the concentration changes over time, while the red dashed line represents the concentration's near-stabilization at a constant value of $y_{\infty} = \frac{1125}{7}$ and for volume 15 it is near 10.7143g/L at about 1.5 minutes.

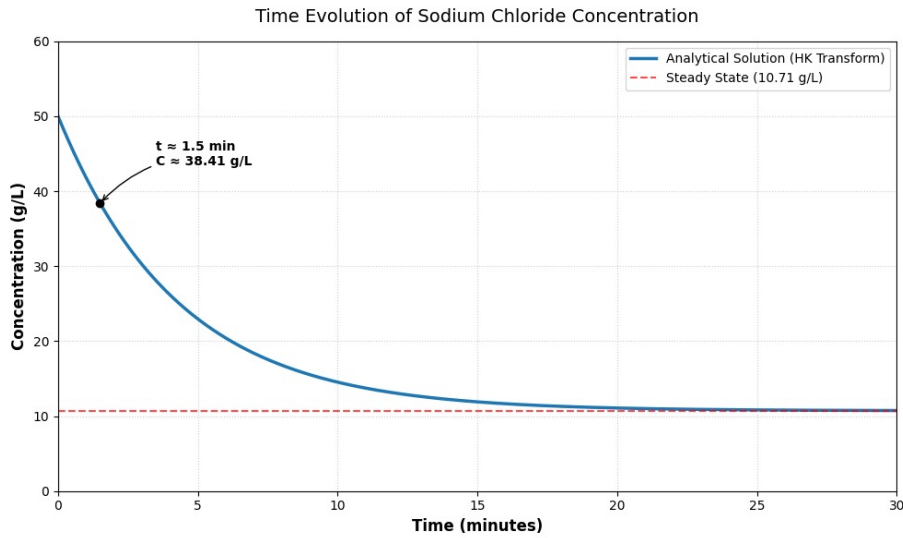


Fig. 2. The concentration of sodium chloride in a waste tank over time

Problem 3: This example shows a simple model of substance diffusion in a reactive medium with a time-dependent coefficient. The concentration $y(t)$ relies on both time t and its immediate value when a chemical is introduced into a porous medium, where the reaction or diffusion rate rises over time. The general relationship, assuming that the rate rises with coefficient k , is:[20]

$$\frac{d}{dt}(ty(t)) = k$$

where k is the reaction rate or diffusion coefficient.

If there is no material in the medium at $t = 0$, the system starts in an initial steady state, where $y(0) = 0$.

Using the HK transformation and the differential equation $HK \left\{ t \frac{dy}{dt} \right\} + HK\{y(t)\} = HK\{k\}$, we obtain.

$$HK\{ty'(t)\} = -\rho \frac{dY}{d\rho} - \frac{3}{2}Y(\rho) \text{ so } -\rho \frac{d}{d\rho}(Y(\rho)) - \frac{3}{2}Y(\rho) + Y(\rho) = \frac{k}{\rho^{\frac{3}{2}}}$$

$$\Rightarrow \rho \frac{d}{d\rho}(Y(\rho)) + \frac{1}{2}Y(\rho) = -\frac{k}{\rho^{\frac{3}{2}}} \Rightarrow \frac{d}{d\rho}(Y(\rho)) + \frac{1}{2\rho}Y(\rho) = -\frac{k}{\rho^{\frac{5}{2}}}$$

It is a differential equation with an integrating factor $I.F = \rho^{\frac{1}{2}}$, its solution takes the form:

$$\rho^{\frac{1}{2}}Y(\rho) = \frac{k}{\rho} + c \Rightarrow Y(\rho) = \frac{k}{\rho^{\frac{3}{2}}} + c\rho^{\frac{1}{2}}$$

From the initial condition $y(0) = 0$, we get $c = 0$, Consequently, the above equation may be written as: $Y(\rho) = \frac{k}{\rho^{\frac{3}{2}}}$

By applying the inverse HK transform, we find that $y(t) = k$

The reaction/diffusion coefficient $k = 2$ was assumed. Plotting the concentration $y(t)$ over time, the concentration stays constant at $y(t) = k$ because the reaction rate and time-dependent accumulation are balanced. Additionally, the beginning state $y(0) = 0$ is shown. Figure (3) illustrates the dynamics of the system with a constant reaction coefficient, showing how quickly the concentration reaches the steady-state value and then remains constant.

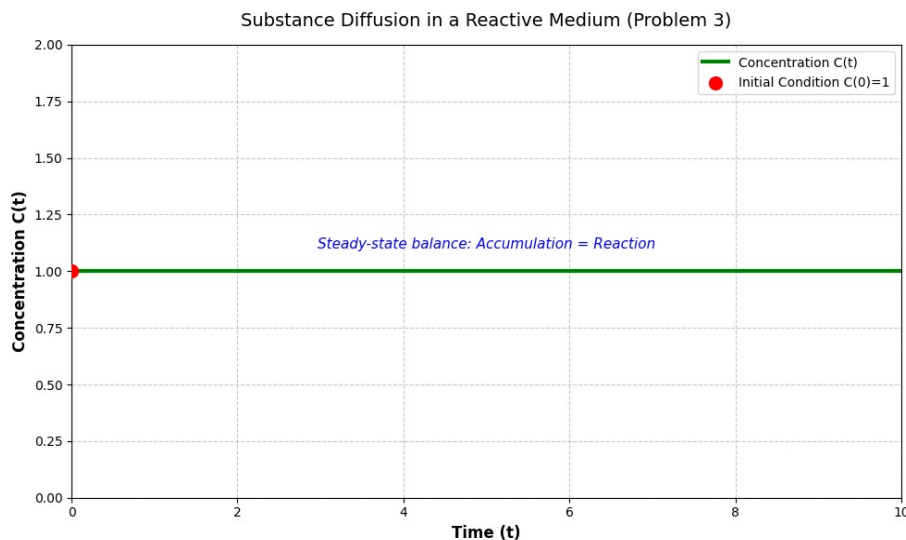


Fig. 3. A substance's concentration profile in a reactive porous medium

Problem 4: From the model of a first-order, single-step reversible reaction, the dynamics of the concentration of species y can be described by the following equation:[21]

$$\frac{d^2y}{dt^2} + (c_1 + c_{-1}) \frac{dy}{dt} = 0$$

Here, $\frac{dy}{dt}$ represents the instantaneous rate of change of y , while $\frac{d^2y}{dt^2}$ denotes the acceleration of this change. The constants c_1 and c_2 correspond to the forward and reverse reaction rate constants, respectively. This formulation captures the temporal evolution of y in a single-step reversible reaction and provides a foundation for further kinetic analysis.

Assuming that b_0 is the concentration of the substance at the initial time ($y(0) = b_0$) and that the initial rate of change of the concentration is b_1 , which represents the initial speed of formation (or consumption) of the substance at the start of the reaction ($y'(0) = b_1$).

We apply the HK transform to the given differential equation. By using property 4, parts 1 and 2

$$HK \left\{ \frac{d^2y}{dt^2} \right\} + (c_1 + c_{-1}) HK \left\{ \frac{dy}{dt} \right\} = 0,$$

$$\Rightarrow \rho^2 Y(\rho) - \rho^{\frac{1}{2}} y(0) - \rho^{-\frac{1}{2}} y'(0) + (c_1 + c_{-1}) \left(\rho Y(\rho) - \frac{1}{\rho^{\frac{1}{2}}} y(0) \right) = 0,$$

By substituting the initial conditions and rearranging the previous equation, we obtain:

$$(\rho^2 + (c_1 + c_{-1})\rho)Y(\rho) - \left(\rho^{\frac{1}{2}} + \frac{(c_1 + c_{-1})}{\rho^{\frac{1}{2}}} \right) b_0 - \rho^{-\frac{1}{2}} b_1 = 0, \text{ That is}$$

$$\rho(\rho + c_1 + c_{-1})Y(\rho) = \left(\frac{\rho + c_1 + c_{-1}}{\rho^{\frac{1}{2}}} \right) b_0 + \rho^{-\frac{1}{2}} b_1 \Rightarrow Y(\rho) = \frac{1}{\rho^{\frac{3}{2}}} b_0 + \frac{b_1}{\rho^{\frac{3}{2}}(\rho + c_1 + c_{-1})}$$

That is $Y(\rho) = \frac{1}{\rho^2} b_0 + \left(\frac{1}{(c_1+c_{-1})\rho^2} - \frac{1}{\rho^2(\rho+c_1+c_{-1})} \right) b_1$

So, applying the inverse HK transform yields the following result.

$$y(t) = b_0 + \frac{b_1}{c_1+c_{-1}} - \frac{b_1}{c_1+c_{-1}} e^{-(c_1+c_{-1})t}$$

From the solution, we deduce that as time ($t \rightarrow \infty$), the exponential term $e^{-(c_1+c_{-1})t}$, which represents the transient phase before reaching the steady state, vanishes, and the concentration of substance $y(t)$ gradually approaches the constant value at the steady state:

$$y_\infty = b_0 + \frac{b_1}{c_1+c_{-1}}.$$

In this example, it is assumed that the initial concentration of species B at time zero is $y(0) = 1 \text{ mol/L}$, and the initial rate of change of the concentration at the start is $y'(0) = 0.5 \text{ mol/L}$. Using these values and the reaction rate constants $c_1 = 0.3 \text{ s}^{-1}$ and $c_{-1} = 0.1 \text{ s}^{-1}$ The plot illustrates the temporal evolution of B in a first-order, single-step, reversible reaction. The curve shows that the concentration starts from the initial value and gradually increases toward equilibrium, with the red mark in Figure 4 representing the initial point $y(0) = 1 \text{ mol/L}$ at time zero.

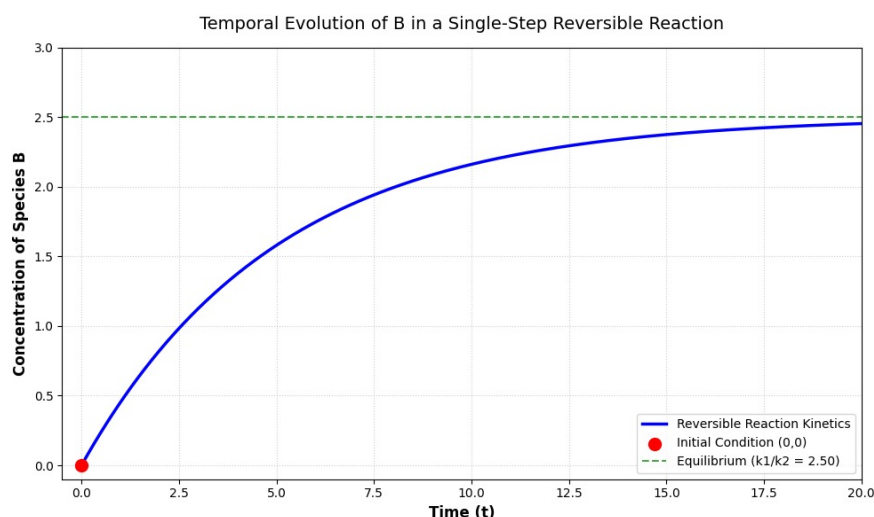


Fig. 4. Species B's time evolution in a first-order, single-step reversible reaction

5. Discussion

The study's findings show that the HK transform is a reliable and efficient method for deriving analytical solutions to kinetic models of chemical reactions. The HK transform offers high efficiency and a simple approach for solving first- and second-order differential equations, compared to the well-known Laplace transform. The accuracy of the HK transform in reducing complex mathematical structures to solvable algebraic forms in the time domain was confirmed by the identical exact solutions obtained by both approaches. However, this study found that the HK transform's current use with linear models is a primary limitation. The transform may need to be further modified or used in conjunction with numerical techniques for extremely nonlinear functions that often appear in more complex chemical dynamics. Despite this, it is a useful substitute for researchers in the field of mathematical chemistry, as it is reliable for solving standard chemical reaction models.

6. Conclusion

This study shows that the HK transform effectively solves mathematical problems in the chemical sciences. A comparison with the Laplace transform shows that both approaches preserve simplicity and avoid complicated calculations while yielding results of the same clarity. This demonstrates how the HK transform may provide accurate and effective solutions for chemical mixing issues. The findings also imply that the HK transform may be expanded in the future to apply mathematical modeling to a variety of difficult problems in science, technology, and medicine.

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8. Author contributions

Contribution was equal between authors.

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الحلول التحليلية لنماذج حركية التفاعلات الكيميائية باستخدام تقنيات التحويل التكاملي

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معلومات البحث	المخلص
الاستلام 16 كانون ثاني 2026	يستخدم الخبراء في النمذجة الرياضية حالياً التحويلات التكاملية لحل النماذج الرياضية للعديد من الظواهر العلمية. وفي هذا السياق، يقيم العمل الحالي معدل نجاح "تحويل HK" مقارنة بـ "تحويل لابلاس" الشهير، من خلال فحص كيفية استخدامه في المعادلات التفاضلية التي تصف العمليات الكيميائية. تم استخدام معادلة تفاضلية من الدرجة الأولى تمثل التفاعل الكيميائي وطرق الانتشار لإظهار قدرة "تحويل HK" على تبسيط الرياضيات وتقديم حلول تحليلية دقيقة. ثم طُبقت الطريقة نفسها على نموذج يولد انتشار المكونات في وسط تفاعلي مع معامل يعتمد على الوقت، مما أثبت قدرة التحويل على التعامل مع معاملات متنوعة. وأخيراً، فحصت الدراسة عملية كيميائية عكسية ذات خطوة واحدة تم تمثيلها بمعادلة تفاضلية من الدرجة الثانية، وتمت مقارنة نتائج تحويلي "لابلاس" و "HK". وقد أثبتت المقارنة أن "تحويل HK" يُعد أداة رياضية بديلة موثوقة لنمذجة ودراسة مجموعة متنوعة من الأنظمة الكيميائية، من خلال التأكيد على أن كلا التحويلين يقدمان دقة وكفاءة متماثلتين.
المراجعة 18 آذار 2026	
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الكلمات المفتاحية	
العلوم الكيميائية؛ تحويل HK؛ النمذجة الرياضية؛ حركية التفاعلات الكيميائية؛ الخليط الكيميائي.	
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