APPLICATION OF LAPLACE-CARSON TRANSFORM FOR DETERMINING THE CONCENTRATIONS OF THE REACTANTS OF FIRST ORDER CONSECUTIVE CHEMICAL REACTION

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ABSTRACT: Chemical reactions play the important role for understanding the problems of Science and Engineering such as radioactive decay; photosynthesis; nuclear reactor; heat mass transfer and photon emission. The main objective of this chapter is to make use of Laplace-Carson transform in order to determine the concentrations of the reactants of first order consecutive chemical reaction. This chapter has a great practical importance due to achieve maximum production by eliminating waste or useless products in the transitional phase of chemical reaction. Results indicate that Laplace-Carson transform is an efficient analytical tool for obtaining the concentrations of the reactants of first order consecutive chemical reaction. Results of the chapter also demonstrate that Laplace-Carson transform provide exact results without doing intricate computational work.

KEYWORDS: Laplace-Carson Transform; Inverse Laplace-Carson Transform; Cramer Rule; Chemical Reaction; Concentration; Reactant.

MATHEMATICS SUBJECT CLASSIFICATION: 35A22; 44A05; 34A30; 65L05; 80A30

1.INTRODUCTION: In the recant years, integral transform methods are the first preference of the scholars for handling the problem of Science and Engineering such as growth of the species [1-12]; decay problem of radioactive substance [1-10]; Abel's problem of mechanics [13-20]; heat transfer problem [21]; circuit problems of electronics communication [22]; problem of infected cells during infection of HIV-1 [23]; concentration problem of drug during intravenous injection of drug [24-25] and vibration problem of string [21-22] because integral transform methods provide the exact solutions of these problems. Scholars are also very interested for developing new integral transform methods [26-27] nowadays due to their high-yielding characteristic of providing results of the problems with good accuracy.

Recently scholars [28-35] developed the duality relation among the various integral transforms and successfully utilized these relations for developing new properties and theories of integral transforms. Higazy and Aggarwal [36] applied Sawi transform on the mathematical model of the chemical reaction in series and estimated the concentration of chemical substances. Murphy [37] analyzed the consecutive chemical reactions of first and second orders. Lin [38] analyzed the consecutive reactions (homogeneous) performed in an annular reactor with non Newtonian flow.

Chrastil [39] obtained the value of rate constants of consecutive chemical reaction of first order by the aid of final product. The mathematical models of the consecutive reactions were suggested by Westman and DeLury [40]. Erdogdn and Sahmurat [41] obtained the kinetic constants of first-order consecutive chemical reactions.

The main interest of this chapter is to determine the concentrations of the reactants of first order consecutive chemical reaction by using Laplace-Carson transform.

2. NOMENCLATURE OF SYMBOLS

$\mathcal{F}$, family of piecewise continuous and exponential order function;

$\mathcal{L}$, Laplace-Carson transform operator;

$\mathcal{L}^{-1}$, inverse Laplace-Carson transform operator;

$\in$, belongs to;

!, the usual factorial notation;

Γ, the classical Gamma function;

N, the set of natural numbers;

R, the set of reals;

$\theta_1(t)$, concentration of a chemical reactant X at any time t;

$\theta_2(t)$, concentration of a chemical reactant Y at any time t;

$\theta_3(t)$, concentration of a chemical reactant Z at any time t;

$\theta_1(0) = \omega$, initial concentration of a chemical reactant X;

$\theta_2(0)$, initial concentration of a chemical reactant Y;

$\theta_3(0)$, initial concentration of a chemical reactant Z;

$\beta_1, \beta_2 > 0$, rate constants

3. DEFINITION OF LAPLACE-CARSON TRANSFORM:

If $H(t) \in \mathcal{F}, t \geq 0$ then the Laplace-Carson transform of $H(t)$ is defined as [20]

$$\mathcal{L}\{H(t)\} = r\int_0^\infty H(t)e^{-rt}\,dt = h(r),\ r > 0 \quad (1)$$

4. INVERSE LAPLACE-CARSON TRANSFORM:

The inverse Laplace-Carson transform of $h(r)$, denoted by $\mathcal{L}^{-1}\{h(r)\}$, is another function $H(t)$ having the characteristic that $\mathcal{L}\{H(t)\} = h(r)$.

5. PROPERTIES OF LAPLACE-CARSON TRANSFORM: In this part, we will describe the properties of Laplace-Carson transform that will be used in later section of this chapter.

5.1 Linearity [20]: If $H_j(t) \in \mathcal{F},\ t \geq 0, j = 1, 2, 3, \ldots\ldots, n$ with $\mathcal{L}\{H_j(t)\} = h_j(r), j = 1, 2, 3, \ldots\ldots n$ then $\mathcal{L}\{\sum_{j=1}^n \ell_j H_j(t)\} = \sum_{j=1}^n \ell_j\, \mathcal{L}\{H_j(t)\} = \sum_{j=1}^n \ell_j\, h_j(r)$, where ℓ_j are arbitrary constants.

5.2 Change of Scale [20]: If $H(t) \in \mathcal{F}, t \geq 0$ with $\mathcal{L}\{H(t)\} = h(r)$ then $\mathcal{L}\{H(\ell t)\} = h\left(\frac{r}{\ell}\right)$, where ℓ is arbitrary constant.

5.3 Translation [20]: If $H(t) \in \mathcal{F}, t \geq 0$ with $\mathcal{L}\{H(t)\} = h(r)$ then

$\mathcal{L}\{e^{\ell t}H(t)\} = \left(\frac{r}{r-\ell}\right)h(r-\ell)$, where ℓ is arbitrary constant.

6. LAPLACE-CARSON (MAHGOUB) TRANSFORMS OF THE DERIVATIVES OF A FUNCTION [3]: If $H(t) \in \mathcal{F}, t \geq 0$ with $\mathcal{L}\{H(t)\} = h(r)$ then

a) $\mathcal{L}\{H'(t)\} = rh(r) - rH(0)$.

b) $\mathcal{L}\{H''(t)\} = r^2h(r) - r^2H(0) - rH'(0)$.

c) $\mathcal{L}\{H'''(t)\} = r^3h(r) - r^3H(0) - r^2H'(0) - rH''(0)$.

Remark 1: Tables 1-2 visualized the Laplace-Carson transforms and inverse Laplace-Carson transforms of fundamental functions respectively.

Table-1: Laplace-Carson transforms of fundamental functions [20]

S.N.	$H(t) \in \mathcal{F}, t > 0$	$\mathcal{L}\{H(t)\} = h(r)$
1	1	1
2	$e^{\ell t}$	$\left(\frac{r}{r-\ell}\right)$
3	$t^{\lambda}, \lambda \in N$	$\frac{\lambda!}{r^{\lambda}}$
4	$t^{\lambda}, \lambda > -1, \lambda \in R$	$\frac{\Gamma(\lambda+1)}{r^{\lambda}}$
5	$sin(\ell t)$	$\left(\frac{\ell r}{r^2+\ell^2}\right)$
6	$cos(\ell t)$	$\left(\frac{r^2}{r^2+\ell^2}\right)$
7	$sinh(\ell t)$	$\left(\frac{\ell r}{r^2-\ell^2}\right)$
8	$cosh(\ell t)$	$\left(\frac{r^2}{r^2-\ell^2}\right)$

Table-2: Inverse Laplace-Carson transforms of fundamental functions [20]

S.N.	$h(r)$	$H(t) = \mathcal{L}^{-1}\{h(r)\}$
1	1	1
2	$\left(\frac{r}{r-\ell}\right)$	$e^{\ell t}$
3	$\frac{1}{r^{\lambda}}, \lambda \in N$	$\frac{t^{\lambda}}{\lambda!}$
4	$\frac{1}{r^{\lambda}}, \lambda > -1, \lambda \in R$	$\frac{t^{\lambda}}{\Gamma(\lambda+1)}$
5	$\left(\frac{r}{r^2+\ell^2}\right)$	$\frac{sin(\ell t)}{\ell}$
6	$\left(\frac{r^2}{r^2+\ell^2}\right)$	$cos(\ell t)$
7	$\left(\frac{r}{r^2-\ell^2}\right)$	$\frac{sinh(\ell t)}{\ell}$
8	$\left(\frac{r^2}{r^2-\ell^2}\right)$	$cosh(\ell t)$

7. APPLICATION OF LAPLACE-CARSON TRANSFORM FOR DETERMINING THE CONCENTRATIONS OF THE REACTANTS OF FIRST ORDER CONSECUTIVE CHEMICAL REACTION:

The concentrations $\theta_1(t), \theta_2(t)$ and $\theta_3(t)$ of three chemical reactants X, Y and Z of first order consecutive chemical reaction

$$Chemical\ reactant\ \ X ---\rightarrow Chemical\ reactant\ \ Y ---\rightarrow Chemical\ reactant\ \ Z \qquad (2)$$

at any time t is determined by the following system of linear ordinary differential equations as [36]

$$\left.\begin{aligned} \frac{d\theta_1}{dt} &= -\beta_1\theta_1 \\ \frac{d\theta_2}{dt} &= \beta_1\theta_1 - \beta_2\theta_2 \\ \frac{d\theta_3}{dt} &= \beta_2\theta_2 \end{aligned}\right\} \qquad (3)$$

with $\theta_1(0) = \omega,\ \theta_2(0) = 0$ and $\theta_3(0) = 0$ (4)

Performing Laplace-Carson transform on equation (3), we have

$$\left.\begin{aligned} \mathcal{L}\left\{\frac{d\theta_1}{dt}\right\} &= -\mathcal{L}\{\beta_1\theta_1\} \\ \mathcal{L}\left\{\frac{d\theta_2}{dt}\right\} &= \mathcal{L}\{\beta_1\theta_1 - \beta_2\theta_2\} \\ \mathcal{L}\left\{\frac{d\theta_3}{dt}\right\} &= \mathcal{L}\{\beta_2\theta_2\} \end{aligned}\right\} \qquad (5)$$

Use of 5.1 in equation (5) gives

$$\left.\begin{aligned} \mathcal{L}\left\{\frac{d\theta_1}{dt}\right\} &= -\beta_1\mathcal{L}\{\theta_1\} \\ \mathcal{L}\left\{\frac{d\theta_2}{dt}\right\} &= \beta_1\mathcal{L}\{\theta_1\} - \beta_2\mathcal{L}\{\theta_2\} \\ \mathcal{L}\left\{\frac{d\theta_3}{dt}\right\} &= \beta_2\mathcal{L}\{\theta_2\} \end{aligned}\right\} \qquad (6)$$

Use of 6(a) in equation (6) gives

$$\left.\begin{aligned} r\mathcal{L}\{\theta_1\} - r\theta_1(0) &= -\beta_1\mathcal{L}\{\theta_1\} \\ r\mathcal{L}\{\theta_2\} - r\theta_2(0) &= \beta_1\mathcal{L}\{\theta_1\} - \beta_2\mathcal{L}\{\theta_2\} \\ r\mathcal{L}\{\theta_3\} - r\theta_3(0) &= \beta_2\mathcal{L}\{\theta_2\} \end{aligned}\right\}$$

$$\Rightarrow \left.\begin{aligned} (r+\beta_1)\mathcal{L}\{\theta_1\} - r\theta_1(0) &= 0 \\ -\beta_1\mathcal{L}\{\theta_1\} + (r+\beta_2)\mathcal{L}\{\theta_2\} - r\theta_2(0) &= 0 \\ \beta_2\mathcal{L}\{\theta_2\} + r\mathcal{L}\{\theta_3\} - r\theta_3(0) &= 0 \end{aligned}\right\} \qquad (7)$$

Use of equation (4) in equation (7) provides

$$\left.\begin{aligned} (r+\beta_1)\mathcal{L}\{\theta_1\} - r\omega &= 0 \\ -\beta_1\mathcal{L}\{\theta_1\} + (r+\beta_2)\mathcal{L}\{\theta_2\} &= 0 \\ \beta_2\mathcal{L}\{\theta_2\} + r\mathcal{L}\{\theta_3\} &= 0 \end{aligned}\right\}$$

$$\Rightarrow \left.\begin{aligned} (r+\beta_1)\mathcal{L}\{\theta_1\} &= r\omega \\ -\beta_1\mathcal{L}\{\theta_1\} + (r+\beta_2)\mathcal{L}\{\theta_2\} &= 0 \\ \beta_2\mathcal{L}\{\theta_2\} + r\mathcal{L}\{\theta_3\} &= 0 \end{aligned}\right\} \qquad (8)$$

Equation (8) represents a system of three non-homogeneous linear equations in $\mathcal{L}\{\theta_1\}, \mathcal{L}\{\theta_2\}$ and $\mathcal{L}\{\theta_3\}$ unknowns. Now use of Cramer's rule in equation (8) gives the values of unknowns $\mathcal{L}\{\theta_1\}, \mathcal{L}\{\theta_2\}$ and $\mathcal{L}\{\theta_3\}$ as:

$$\mathcal{L}\{\theta_1\} = \frac{\begin{vmatrix} r\omega & 0 & 0 \\ 0 & (r+\beta_2) & 0 \\ 0 & \beta_2 & r \end{vmatrix}}{\begin{vmatrix} (r+\beta_1) & 0 & 0 \\ -\beta_1 & (r+\beta_2) & 0 \\ 0 & \beta_2 & r \end{vmatrix}}, \begin{vmatrix} (r+\beta_1) & 0 & 0 \\ -\beta_1 & (r+\beta_2) & 0 \\ 0 & \beta_2 & r \end{vmatrix} \neq 0$$

$$\Rightarrow \mathcal{L}\{\theta_1\} = \left(\frac{\omega r}{r+\beta_1}\right) \quad (9)$$

$$\mathcal{L}\{\theta_2\} = \frac{\begin{vmatrix} (r+\beta_1) & r\omega & 0 \\ -\beta_1 & 0 & 0 \\ 0 & 0 & r \end{vmatrix}}{\begin{vmatrix} (r+\beta_1) & 0 & 0 \\ -\beta_1 & (r+\beta_2) & 0 \\ 0 & \beta_2 & r \end{vmatrix}}, \begin{vmatrix} (r+\beta_1) & 0 & 0 \\ -\beta_1 & (r+\beta_2) & 0 \\ 0 & \beta_2 & r \end{vmatrix} \neq 0$$

$$\Rightarrow \mathcal{L}\{\theta_2\} = \left(\frac{\omega\beta_1}{\beta_2-\beta_1}\right)\left[\frac{r}{r+\beta_1} - \frac{r}{r+\beta_2}\right] \quad (10)$$

$$\mathcal{L}\{\theta_3\} = \frac{\begin{vmatrix} (r+\beta_1) & 0 & r\omega \\ -\beta_1 & (r+\beta_2) & 0 \\ 0 & \beta_2 & 0 \end{vmatrix}}{\begin{vmatrix} (r+\beta_1) & 0 & 0 \\ -\beta_1 & (r+\beta_2) & 0 \\ 0 & \beta_2 & r \end{vmatrix}}, \begin{vmatrix} (r+\beta_1) & 0 & 0 \\ -\beta_1 & (r+\beta_2) & 0 \\ 0 & \beta_2 & r \end{vmatrix} \neq 0$$

$$\Rightarrow \mathcal{L}\{\theta_3\} = \omega\left[r^3 - \left(\frac{\beta_2}{\beta_2-\beta_1}\right)\left(\frac{r}{r+\beta_1}\right) + \left(\frac{\beta_1}{\beta_2-\beta_1}\right)\left(\frac{r}{r+\beta_2}\right)\right] \quad (11)$$

Performing inverse Laplace-Carson transform on equations (9), (10) and (11) gives the required concentrations $\theta_1(t), \theta_2(t)$ and $\theta_3(t)$ as:

$$\theta_1 = \mathcal{L}^{-1}\left\{\frac{\omega r}{r+\beta_1}\right\}$$

$$\Rightarrow \theta_1 = \omega\mathcal{L}^{-1}\left\{\frac{r}{r+\beta_1}\right\} = \omega e^{-\beta_1 t} \quad (12)$$

$$\theta_2 = \mathcal{L}^{-1}\left\{\left(\frac{\omega\beta_1}{\beta_2-\beta_1}\right)\left[\frac{r}{r+\beta_1} - \frac{r}{r+\beta_2}\right]\right\}$$

$$\Rightarrow \theta_2 = \left(\frac{\omega\beta_1}{\beta_2-\beta_1}\right)\left[\mathcal{L}^{-1}\left\{\frac{r}{r+\beta_1}\right\} - \mathcal{L}^{-1}\left\{\frac{r}{r+\beta_2}\right\}\right]$$

$$\Rightarrow \theta_2 = \left(\frac{\omega\beta_1}{\beta_2-\beta_1}\right)\left[e^{-\beta_1 t} - e^{-\beta_2 t}\right] \quad (13)$$

$$\theta_3 = \mathcal{L}^{-1}\left\{\omega\left[r^3 - \left(\frac{\beta_2}{\beta_2-\beta_1}\right)\left(\frac{r}{r+\beta_1}\right) + \left(\frac{\beta_1}{\beta_2-\beta_1}\right)\left(\frac{r}{r+\beta_2}\right)\right]\right\}$$

$$\Rightarrow \theta_3 = \omega\left[\mathcal{L}^{-1}\{r^3\} - \left(\frac{\beta_2}{\beta_2-\beta_1}\right)\mathcal{L}^{-1}\left\{\frac{r}{r+\beta_1}\right\} + \left(\frac{\beta_1}{\beta_2-\beta_1}\right)\mathcal{L}^{-1}\left\{\frac{r}{r+\beta_2}\right\}\right]$$

$$\Rightarrow \theta_3 = \omega\left[1 - \left(\frac{\beta_2}{\beta_2-\beta_1}\right)e^{-\beta_1 t} + \left(\frac{\beta_1}{\beta_2-\beta_1}\right)e^{-\beta_2 t}\right] \quad (14)$$

Remark 2: Results given by equations (12), (13) and (14) have perfect agreement with [36].

8. CONCLUSIONS: In this chapter, we have profitably determined the concentrations of the reactants of first order consecutive chemical reaction by using Laplace-Carson transform. It is observed that Laplace-Carson transform provide the exact analytical primitive of this problem with good accuracy. We can use Laplace-Carson transform to study the problems of chemical engineering in future that involve different order reversible and parallel chemical reactions.

DATA AVAILABILITY: Not applicable.

CONFLICTS OF INTEREST: There are no conflicts of interest between the authors.

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