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Mathematical Modeling of Alcohol-Drug Concentration in the Bloodstream

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ABSTRACT

This research involved the formulation of a system of mathematical models mimicking alcohol concentration in the human body and in the bloodstream, which are subjected to some initial conditions. The formulation starts with the an ideal presentation of the compartment diagram in Figure 1, the figure clearly indicates the two compartment in focus and the diffusion of alcohol from one compartment to the other with different rates including the elimination rate through urination and sweating that were not considered in this research. The aim of the research is to investigate the importance of the various rate constants on the alcohol concentration in the bloodstream, as well as investigating the drug dosage and volume of alcohol concentration impact in the bloodstream. The Laplace method (LM) was adopted to solve the model which represents, firstly, the alcohol concentration in the body where an exact solution was obtained, secondly, the exact solution was also obtained for the model depicting the alcohol concentration in the bloodstream with all pertinent parameters clearly spelt out. Lastly, numerical simulation was carried out using Wolfram Mathematica, version 12, where the pertinent parameters values were varied and the results presented graphically. The graphical results indicate that the various rate constants, dosage increase and the volumetric increase have impact and showed a corresponding effect on the drug concentration in the bloodstream. The novelty of this research is the fact that we've been able to mimic a real-life scenario, an alcohol concentration in the bloodstream, mathematically, and solved the system using Laplace methods and performed numerical simulation to show the importance of the pertinent parameters. This system can be recommended for scientists and engineers alike who could be interested in pharmacokinetics and Pharmacodynamics research.

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Introduction

Blood is a body fluid in the circulatory system of humans and other vertebrates that transports metabolic waste products away from cells while delivering necessary substances such as nutrients and oxygen to them [1]. They stated that the blood in the circulatory system is also known as peripheral blood, and the blood cells it carries are peripheral blood cells. Plasma, which constitutes 55% of blood fluid, is mostly water (92% by volume) and contains proteins, glucose, mineral ions, hormones, carbon dioxide (plasma being the main medium for excretory product transportation), and blood cells themselves [2]. The percentage of alcohol (ethyl alcohol or ethanol) in a person's blood is referred to as the blood alcohol concentration (BAC). Some of the authors who have studied drug use and blood level who explored the drug delivery system due to its distinguished potential for modulating the pharmacokinetics, pharmacodynamics, and biological activities of carrying payloads [3]. Investigated fractional differential equations with Caputo fractional derivatives of real-order dependence [4]. Their goal is to show some concrete examples and experimental data from investigations, that fractional differential equations can model certain problems more effectively than ordinary differential equations used a set of differential equations describing blood alcohol content as a function of time and integrated the equations to obtain a general solution [5]. Used a class of fractional-order differential models to investigate biological systems with memory [6]. Developed a deterministic mathematical model of social media addiction (SMA) with an optimal control strategy [7]. The sensitivity of model parameters is determined using the normalized forward sensitivity index definition. Analyzed an alcoholism model through the Liouville-Caputo and Atangana-Baleanu-Caputo fractional derivatives with constant and variable order [8]. The stability and convergence of the numerical solutions were presented in detail. The investigation established a complete and realistic indicator of the alcoholism model and its effect on the spread of drinking [9]. Formulated binge drinking models incorporating demographics on different weighted networks [10]. Investigated dynamic alcohol consumption using a model with awareness programs and time delays. An awareness program by the media was introduced in the model as a separate class, with the growth rate of the cumulative density of them being proportional to the number of mortalities induced by heavy drinking [11]. Illustrated the dynamics of the drinking epidemic using mathematical models, where the existence and stability of the drinking-free and endemic equilibria were discussed. Numerical simulations were conducted to confirm the analytic results, and the findings revealed that reducing the contact rate between non-drinkers and heavy drinkers, increasing the number of drinkers that go into treatment, and educating drinkers to refrain from drinking can be useful in combating the drinking epidemic [12]. Proposed and analyzed a fuzzy model for the health risk challenges associated with alcoholism. The model reveals that fuzziness gets into the system by assuming uncertainty in the measure of the influence of the risky individual and the additional death rate. The analysis reveals that the health risks associated with alcoholism can be effectively controlled by raising the resistance of susceptible individuals and consequently reducing their chances of initiating drinking behavior [13]. Research found that total deaths are related to alcohol consumption worldwide, and concluded that mathematical models are important tools to estimate disease burden and assess the cost-effectiveness of interventions to address this burden. However, in his research, we shall formulate mathematical models to investigate the alcohol-drug concentration in the bloodstream. The models also entail numerical simulation of the exact solution using Wolfram Mathematica, version 12, and conclude based on research evidence.

Materials and Methods

This research is a theoretical study that involves the representation of alcohol concentration in the body and bloodstream compartments using mathematical models. Proffering exact analytical solutions to the models using Laplace method and performing numerical simulation using Wolfram Mathematica software, where the pertinent parameters are varied for the purpose of studying their importance to alcohol concentration in a particular compartment.

Assumptions

Before we go ahead and formulate mathematical models to investigate the alcohol-drug concentration in the bloodstream, let's consider the following assumptions:

- The alcohol-drug diffused from the body compartment to the bloodstream compartment and vice versa.
- There could be an influence of the inter-compartmental distribution rate constants on alcohol-drug diffusion in the bloodstream compartment.
- There could be an influence of the excretion of alcohol-drug on its presence in the bloodstream.
- The change in volumetric and dosage could influence the alcohol-drug concentration in the bloodstream.

Nomenclature

c_1 : Concentration of Alcohol-drug in the human body compartment
c_2 : Concentration of Alcohol-drug in bloodstream compartment
k_{12}, k_{21}: Inter-compartmental distribution rate constant
k_e : Excretion rate constant
k_a : First order rate constant
V : Volume of Alcohol-drug in both compartments
D : Alcohol-drug dosage in both compartments

Mathematical Formulation

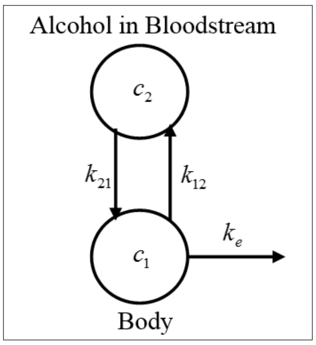

Figure 1: Diagram Showing Concentration of Alcohol in Bloodstream and Body Compartments

Following [14, 15] and Figure 1 above, we presented the formulated mathematical models as follows:

$$\frac{dc_1}{dt} = k_{21}c_2 - k_{12}c_1 - k_e c_1 \qquad (1)$$

$$\frac{dc_2}{dt} = k_{12}c_1 - k_{21}c_2 \qquad (2)$$

The equations (1) and (2) are subjected o the initial conditions, such as:

$$\left. \begin{aligned} c_1(0) &= \frac{D}{V} \\ c_2(0) &= 0 \end{aligned} \right\} \qquad (3)$$

Laplace Method (LM)

The Laplace Method can be defined as:

$$\left. \begin{aligned} L\{c_1(t)\} &= c_1(s) = \int_0^\infty e^{-st} c_1(t)dt \\ L\{c_2(t)\} &= c_2(s) = \int_0^\infty e^{-st} c_2(t)dt \end{aligned} \right\} \qquad (4)$$

where L denotes the Laplace.

Taking the Laplace of equation (2), we have:

$$L\left\{\frac{dc_2}{dt}\right\} = L\{k_{12}c_1\} - L\{k_{21}c_2\} \qquad (5)$$

Simplifying equation (5), we have:

$$L\left\{\frac{dc_2}{dt}\right\} = k_{12}L\{c_1\} - k_{21}L\{c_2\} \qquad (6)$$

Equation (6) can be simplified as:

$$sc_2(s) - c_2(0) = k_{12}c_1(s) - k_{21}c_2(s) \qquad (7)$$

Simplifying equation (7), we have the following:

$$sc_2(s) + k_{21}c_2(s) = k_{12}c_1(s) - c_2(0) \qquad (8)$$

Substituting the initial value in equation (3) into equation (8), and upon simplification, we have:

$$(s + k_{21})c_2(s) = k_{12}c_1(s) \qquad (9)$$

Simplifying equation (9), we have:

$$c_2(s) = k_{12}\frac{c_1(s)}{(s + k_{21})} \qquad (10)$$

In order to study the impact of the concentration of in concentration, we shall first take the In a similar vein, applying the Laplace method on equation (1), which is:

$$L\left\{\frac{dc_1}{dt}\right\} = k_{21}L\{c_2\} - k_{12}L\{c_1\} - k_e L\{c_1\} \qquad (11)$$

Simplifying equation (11), we have:

$$sc_1(s) - c_1(0) = k_{21}c_2(s) - k_{12}c_1(s) - k_e c_1(s) \quad (12)$$

Simplifying equation (12), we have:

$$sc_1(s) + k_{12}c_1(s) + k_e c_1(s) = k_{21}c_2(s) + c_1(0) \quad (13)$$

Simplifying equation (13), we have:

$$(s + k_{12} + k_e)c_1(s) = k_{21}c_2(s) + c_1(0) \quad (14)$$

Substitute equations (3) and (10) into equation (14), we have:

$$(s + k_{12} + k_e)c_1(s) = \frac{k_{21}k_{12}c_1(s)}{(s + k_{21})} + \frac{D}{V} \quad (15)$$

Simplifying equation (15), we have:

$$\left((s + k_\alpha) + \frac{k_{21}k_{12}}{(s + k_{21})}\right)c_1(s) = \frac{D}{V} \quad (16)$$

where $k_\alpha = [k_{12} + k_e]$

We can simplify equation (16) as:

$$\left(\frac{(s + k_\alpha)(s + k_{21}) + k_{21}k_{12}}{(s + k_{21})}\right)c_1(s) = \frac{D}{V} \quad (17)$$

Simplify equation (17) as follows:

$$c_1(s) = \frac{D}{V}\left(\frac{(s + k_{21})}{(s + k_\alpha)(s + k_{21}) + k_{21}k_{12}}\right) \quad (18)$$

The inverse Laplace transform can be stated as:

$$c_1(t) = L^{-1}\{c_1(s)\} \quad (19)$$

Substituting equation (18) into equation (19), we have:

$$c_1(t) = L^{-1}\left\{\frac{D}{V}\left(\frac{(s + k_{21})}{(s + k_\alpha)(s + k_{21}) + k_{21}k_{12}}\right)\right\} \quad (20)$$

We can simplify the expression in equation (20) into partial fraction as:

$$\frac{(s + k_{21})}{(s + k_\alpha)(s + k_{21}) + k_{21}k_{12}} = \frac{(s + k_{21})}{s^2 + (k_\alpha + k_{21})s + k_\beta} \quad (21)$$

where $k_\beta = k_\alpha + k_{21} + k_{21}k_{12}$

Substitute equation (21) into equation (20), we have:

$$c_1(t) = L^{-1}\left\{\frac{D}{V}\left(\frac{(s + k_{21})}{s^2 + (k_\alpha + k_{21})s + k_\beta}\right)\right\} \quad (22)$$

Simplifying equation (22), we have:

$$c_1(t) = \frac{D}{V}\left\{\frac{k_{21} - \lambda_1}{\lambda_2 - \lambda_1}\right\}L^{-1}\left\{\frac{1}{(s + \lambda_1)}\right\} + \frac{D}{V}\left\{\frac{\lambda_2 - k_{21}}{\lambda_2 - \lambda_1}\right\}L^{-1}\left\{\frac{1}{(s + \lambda_2)}\right\} \quad (23)$$

Equation (23) can be solved as:

$$c_1(t) = \frac{D}{V}\left\{\frac{k_{21} - \lambda_1}{\lambda_2 - \lambda_1}\right\}e^{-\lambda_1 t} + \frac{D}{V}\left\{\frac{\lambda_2 - k_{21}}{\lambda_2 - \lambda_1}\right\}e^{-\lambda_2 t} \quad (24)$$

where $\lambda_1 = \dfrac{-(k_\alpha + k_{21}) + \sqrt{(k_\alpha + k_{21})^2 - 4k_\beta}}{2}$,

$$\lambda_2 = \frac{-(k_\alpha + k_{21}) - \sqrt{(k_\alpha + k_{21})^2 - 4k_\beta}}{2}$$

For the solution to be real $k_{21} > k_\alpha + 2\sqrt{k_\beta}$

We substitute equation (18) into (10) in order to get the impact of alcohol concentration in the body on that in the bloodstream, which is:

$$c_2(s) = \frac{Dk_{12}}{V}\left(\frac{1}{(s + k_\alpha)(s + k_{21}) + k_{21}k_{12}}\right) \quad (25)$$

Simplifying equation (25), we have:

$$c_2(s) = \frac{Dk_{12}}{V}\left(\frac{1}{(s + k_\alpha)(s + k_{21}) + k_{21}k_{12}}\right) =$$

$$\frac{Dk_{12}}{V}\left(\frac{1 - r_1 r_2}{r_2 - r_1}\right)\frac{1}{(s + r_1)} + \frac{Dk_{12}}{V}\left(\frac{r_1 r_2 - 1}{r_2 - r_1}\right)\frac{1}{(s + r_2)} \quad (26)$$

Taking the inverse Laplace of equation (26), we have:

$$c_2(t) = \frac{Dk_{12}}{V}\left(\frac{1 - r_1 r_2}{r_2 - r_1}\right)e^{-r_1 t} + \frac{Dk_{12}}{V}\left(\frac{r_1 r_2 - 1}{r_2 - r_1}\right)e^{-r_2 t} \quad (27)$$

where $r_1 = \dfrac{-(k_\alpha + k_{21}) + \sqrt{(k_\alpha + k_{21})^2 - 4k_\beta}}{2}$,

$$r_2 = \frac{-(k_\alpha + k_{21}) - \sqrt{(k_\alpha + k_{21})^2 - 4k_\beta}}{2}$$

Results

In this section, we shall present the numerically simulated results graphically; they are labeled as Figure 2 to Figure 6 accordingly, and as follows:

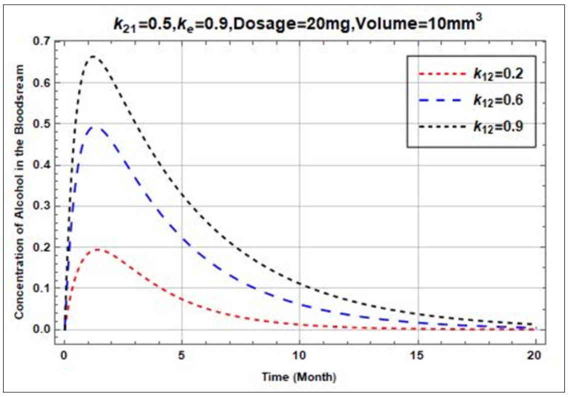

Figure 2: The Impact of Body Inter-Compartmental Rate Constant on Alcohol Concentration in the Bloodstream

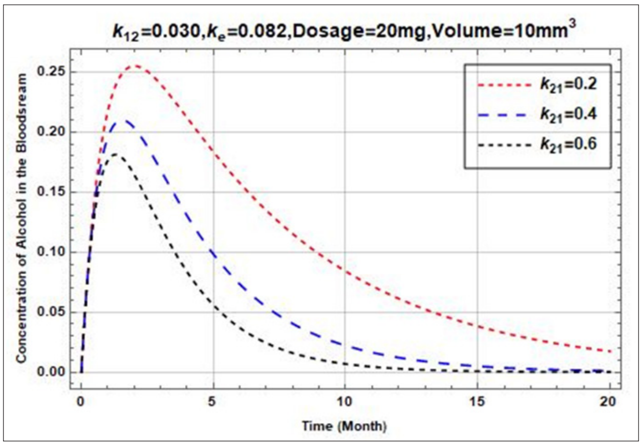

Figure 3: The Impact of Bloodstream Inter-Compartmental Rate Constant on Alcohol Concentration in the Bloodstream

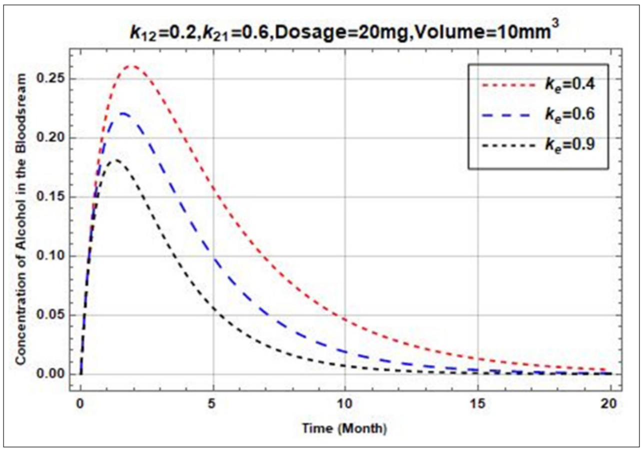

Figure 4: The Impact of the Elimination Rate on Alcohol Concentration in the Bloodstream

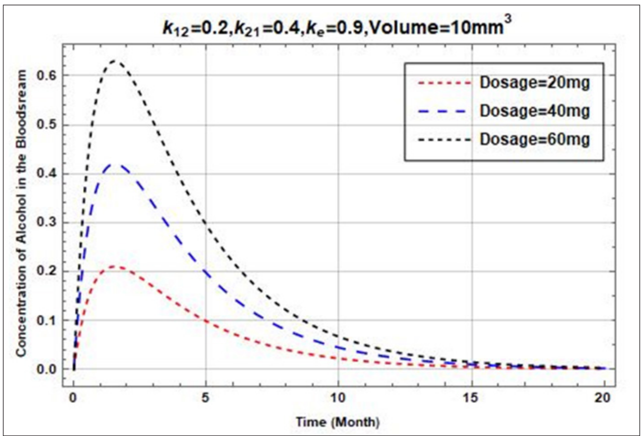

Figure 5: The Impact of Drug Dosage in the Body on Alcohol Concentration in the Bloodstream

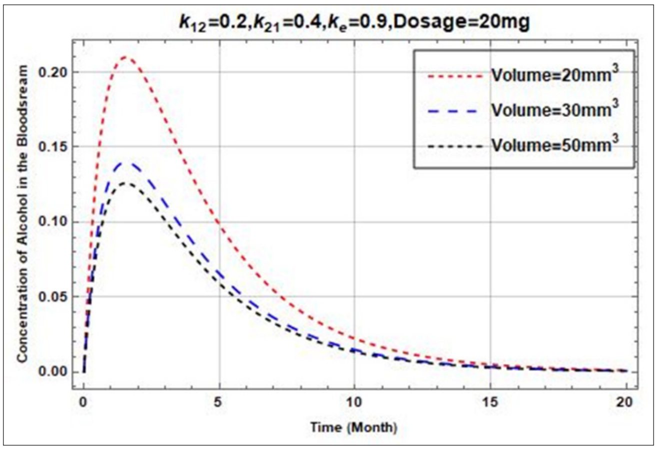

Figure 6: The Impact of Volume of Drug in the Body on Alcohol Concentration in the Bloodstream

Discussion

Figure 2 clearly indicated that increase in inter-compartmental rate constant from the body to the bloodstream also caused an increase in alcohol concentration in the bloodstream while other contributing pertinent parameter values are $k_e = 0.9$, $k_{21} = 0.6$, $V = 10\text{mm}^3$ and $D = 20\text{mg}$. The result showed that the alcohol concentration increased o the maximum before decelerating to zero from zero month of 20 months period. Figure 3 indicates that the increase in inter-compartmental rate constant from the bloodstream to the body also caused a decrease in alcohol concentration in the bloodstream while other contributing pertinent parameter values are $k_{12} = 0.2$, $k_e = 0.0832$, $V = 10mm^3$ and D = 20mg. The result showed that the alcohol concentration decreases from higher concentration to lower concentration before decelerating over the period of 20 months.

Figure 4 illustrates that the alcohol concentration decreases from higher concentration to lower concentration as the elimination rate of alcohol increases from 0.4, 0.6 and 0.9, while other contributing pertinent parameter values are k_{12} =0.2, k_{21}= 0.6, $V = 10\text{mm}^3$ and $D = 20mg$. This result is of the view that an increase in an elimination rate decreases an alcohol concentration in the bloodstream within the medication prescribed period of 20 months. Figure 5 illustrated the variation of dosages of drug from 20mg, 40mg and 60mg in the body and how it affects the alcohol concentration in the bloodstream while other contributing pertinent parameter values are $k_{12} = 0.2$, $k_{21} = 0.4$, $k_e = 0.9$ and V =$10mm^3$. It can be seen that increase in volume of drug in the body resulted to an increases in alcohol concentration in the bloodstream within an investigation period of 20 months.

Figure 6 illustrates the variation of volume of drug from 20mm3, 30mm3 and 50mm3 in the body and how it affected the alcohol concentration in the bloodstream while other contributing pertinent parameter values are k_{12}=0.2, $k_{12} = 0.4$, $k_e = 0.9$ and D= $20mg$. This is shown that the increase in volume of drug in the body caused the alcohol concentration in the bloodstream to decreases within the period of 20 months under the scope of this research.

Conclusion

In view of this research, mathematical modelling of alcohol-drug concentration in the bloodstream and having performed the numerical simulation using numerical software, Wolfram Mathematica where results are present graphically and discussed comprehensively based on merits and novelty, we shall conclude as follows:

- To increase an alcohol concentration in the bloodstream, it is pertinent to consider an increase in the inter-compartmental rate constant in the body while maintaining other contributing parameter values.
- To decrease an alcohol concentration in the bloodstream, it is important to increase the inter-compartmental rate constant from the bloodstream while maintaining other contributing parameter values.
- To decrease an alcohol concentration from higher concentration to lower concentration, it is pertinent o increases the elimination rate of the drug from the body compartment.
- The variation of dosages of drug from 20mg, 40mg and 60mg in the body affects the alcohol concentration in the bloodstream to be increased.
- The variation of volume of drug in the body from 20mm3, 30mm3 and 50mm3 affects the alcohol concentration in the bloodstream to decrease within the research period of 20 months.

Appendix

$$\frac{(s+k_{21})}{s^2+(k_\alpha+k_{21})s+k_\beta} \equiv \frac{(s+k_{21})}{(s+\lambda_1)(s+\lambda_2)} = \frac{(s+k_{21})}{s^2+(\lambda_1+\lambda_2)s+\lambda_1\lambda_2}$$

where λ_1 and λ_2 are the roots

$$\frac{(s+k_{21})}{(s+\lambda_1)(s+\lambda_2)} \equiv \frac{A}{(s+\lambda_1)} + \frac{B}{(s+\lambda_2)}$$

$$\frac{(s+k_{21})}{(s+\lambda_1)(s+\lambda_2)} \equiv \frac{A(s+\lambda_2)+B(s+\lambda_1)}{(s+\lambda_1)(s+\lambda_2)}$$

$$A(s+\lambda_2)+B(s+\lambda_1) \equiv (s+k_{21})$$

$$(A+B)s + A\lambda_2 + B\lambda_1 \equiv s + k_{21}$$

$$A+B \equiv 1$$

$$A + B\frac{\lambda_1}{\lambda_2} \equiv \frac{k_{21}}{\lambda_2}$$

$$B\left(1-\frac{\lambda_1}{\lambda_2}\right) = 1 - \frac{k_{21}}{\lambda_2}$$

$$B = \frac{\lambda_2 - k_{21}}{\lambda_2 - \lambda_1}$$

$$A = 1 - \left(\frac{\lambda_2 - k_{21}}{\lambda_2 - \lambda_1}\right)$$

$$A = \frac{k_{21} - \lambda_1}{\lambda_2 - \lambda_1}$$

$$\frac{(s+k_{21})}{(s+\lambda_1)(s+\lambda_2)} \equiv \left\{\frac{k_{21}-\lambda_1}{\lambda_2-\lambda_1}\right\}\frac{1}{(s+\lambda_1)} + \left\{\frac{\lambda_2-k_{21}}{\lambda_2-\lambda_1}\right\}\frac{1}{(s+\lambda_2)}$$

$$c_1(t) = L^{-1}\left\{\left(\frac{D}{V}\left\{\frac{k_{21}-\lambda_1}{\lambda_2-\lambda_1}\right\}\frac{1}{(s+\lambda_1)} + \frac{D}{V}\left\{\frac{\lambda_2-k_{21}}{\lambda_2-\lambda_1}\right\}\frac{1}{(s+\lambda_2)}\right)\right\}$$

$$c_1(t) = \frac{D}{V}\left\{\frac{k_{21}-\lambda_1}{\lambda_2-\lambda_1}\right\}L^{-1}\left\{\frac{1}{(s+\lambda_1)}\right\} + \frac{D}{V}\left\{\frac{\lambda_2-k_{21}}{\lambda_2-\lambda_1}\right\}L^{-1}\left\{\frac{1}{(s+\lambda_2)}\right\}$$

$$c_1(t) = \frac{D}{V}\left\{\frac{k_{21}-\lambda_1}{\lambda_2-\lambda_1}\right\}e^{-\lambda_1 t} + \frac{D}{V}\left\{\frac{\lambda_2-k_{21}}{\lambda_2-\lambda_1}\right\}e^{-\lambda_2 t}$$

$$s^2+(k_\alpha+k_{21})s+k_\beta$$

$$s^2+(k_\alpha+k_{21})s+k_\beta = 0$$

$$a=1, b=(k_\alpha+k_{21}) \text{ and } c=k_\beta$$

$$\lambda_1 = \frac{-b+\sqrt{b^2-4ac}}{2a} \text{ and } \lambda_2 = \frac{-b-\sqrt{b^2-4ac}}{2a}$$

$$\lambda_1 = \frac{-(k_\alpha+k_{21})+\sqrt{(k_\alpha+k_{21})^2-4k_\beta}}{2}$$

$$\lambda_2 = \frac{-(k_\alpha+k_{21})-\sqrt{(k_\alpha+k_{21})^2-4k_\beta}}{2}$$

$$k_{21} > k_\alpha + 2\sqrt{k_\beta}$$

$$c_2(s) = \frac{Dk_{12}}{V}\left(\frac{1}{(s+k_\alpha)(s+k_{21})+k_{21}k_{12}}\right)$$

$$c_2(s) = \frac{Dk_{12}}{V}\left(\frac{1}{(s+k_\alpha)(s+k_{21})+k_{21}k_{12}}\right)$$

$$c_2(s) = \frac{Dk_{12}}{V}\left(\frac{1}{(s+k_\alpha)(s+k_{21})+k_{21}k_{12}}\right)$$

$$s^2+(k_\alpha+k_{21})s+k_\beta$$

$$s^2+(k_\alpha+k_{21})s+k_\beta = 0$$

$$a=1, b=(k_\alpha+k_{21}) \text{ and } c=k_\beta$$

$$r_1 = \frac{-b+\sqrt{b^2-4ac}}{2a} \text{ and } r_2 = \frac{-b-\sqrt{b^2-4ac}}{2a}$$

$$r_1 = \frac{-(k_\alpha+k_{21})+\sqrt{(k_\alpha+k_{21})^2-4k_\beta}}{2}$$

$$r_2 = \frac{-(k_\alpha+k_{21})-\sqrt{(k_\alpha+k_{21})^2-4k_\beta}}{2}$$

$$k_{21} > k_\alpha + 2\sqrt{k_\beta}$$

$$c_2(s) = \frac{Dk_{12}}{V}\left(\frac{1}{(s+k_\alpha)(s+k_{21})+k_{21}k_{12}}\right) = \frac{Dk_{12}}{V}\left(\frac{1}{(s+r_1)(s+r_2)}\right)$$

$$\frac{1}{(s+r_1)(s+r_2)} \equiv \frac{A}{(s+r_1)} + \frac{A}{(s+r_2)}$$

$$\frac{1}{(s+r_1)(s+r_2)} \equiv \frac{A(s+r_2)+B(s+r_1)}{(s+r_1)(s+r_2)} = \frac{(A+B)s+Ar_2+Br_1+r_1r_2}{(s+r_1)(s+r_2)}$$

$$A+B=0$$

$$Ar_2+Br_1+r_1r_2 \equiv 1$$

$$B=-A$$

$$A=\frac{1-r_1r_2}{r_2-r_1}$$

$$B=\frac{r_1r_2-1}{r_2-r_1}$$

$$c_2(s)=\frac{Dk_{12}}{V}\left(\frac{1}{(s+k_\alpha)(s+k_{21})+k_{21}k_{12}}\right)=\frac{Dk_{12}}{V}\left(\frac{A}{(s+r_1)}+\frac{A}{(s+r_2)}\right)$$

$$c_2(s)=\frac{Dk_{12}}{V}\left(\frac{1}{(s+k_\alpha)(s+k_{21})+k_{21}k_{12}}\right)=\frac{Dk_{12}A}{V}\frac{1}{(s+r_1)}+\frac{Dk_{12}B}{V}\frac{1}{(s+r_2)}$$

$$c_2(s)=\frac{Dk_{12}}{V}\left(\frac{1}{(s+k_\alpha)(s+k_{21})+k_{21}k_{12}}\right)=\frac{Dk_{12}}{V}\left(\frac{1-r_1r_2}{r_2-r_1}\right)\frac{1}{(s+r_1)}+\frac{Dk_{12}}{V}\left(\frac{r_1r_2-1}{r_2-r_1}\right)\frac{1}{(s+r_2)}$$

$$c_2(t)=\frac{Dk_{12}}{V}\left(\frac{1-r_1r_2}{r_2-r_1}\right)e^{-r_1t}+\frac{Dk_{12}}{V}\left(\frac{r_1r_2-1}{r_2-r_1}\right)e^{-r_2t}$$

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