Analysis of Dynamical Systems for Synthesis of Phenobarbital

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Objectives

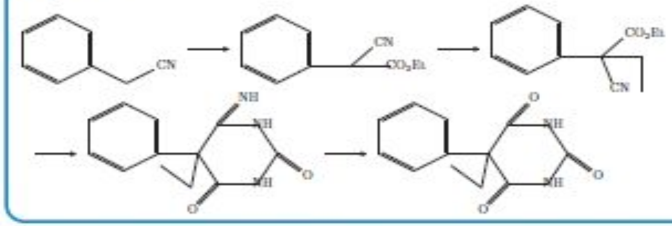
1. Understanding sequential chemical reactions.
2. Understanding basic mathematical theories in the Linear Algebra and Differential Equations.
3. Investigating the synthesis of industrial aromatic compounds and experiencing their visualization using computational programs such as Python and Mathematica.
4. Enhancing the ability to analyze the phenomena in the chemical reactions using the data coming from the mathematical works.

Introduction

The use of mathematical methods for the analysis of chemical reaction systems is one of the useful tools. Phenobarbital (a barbiturate tyype medication also called phenobarb) is a prescription drug used to control seizures, relieve anxiety, treat epilepsy (in some countries), and prevent withdrawal symptoms in people dependent on other barbiture drugs. We followed the strategy employed in the paper [1] but approaches it with different mathematical approaches: matrix analysis [2] and ODE system [3] which will help us understand the chemical stoichiometry of these synthesis reactions.

Chemical Model

We consider the following sequential chemical reactions showing the synthesis of Phenobarbital as the final product:



Mathematical Model

Also, the following system of ordinary differential equation (ODE System) led to the deduction:

$$\frac{dA_0}{dt} = -k[A_0]$$
$$\frac{dA_1}{dt} = k[A_0] - k[A_1]$$
$$\frac{dA_2}{dt} = k[A_1] - k[A_2]$$
$$\frac{dA_3}{dt} = k[A_2] - k[A_3]$$
$$\frac{dA_4}{dt} = -k[A_4]$$

Mathematical Methods

The main idea to solve the ODE System is to consider the following matrix:

$$\frac{d\vec{x}}{dt}(t) = A\vec{x}(t)$$

where

$$\vec{x}(t) = \begin{pmatrix} A_0(t) \\ A_1(t) \\ A_2(t) \\ A_3(t) \\ A_4(t) \end{pmatrix},$$

$$A = \begin{pmatrix} -k & 0 & 0 & 0 & 0 \\ k & -k & 0 & 0 & 0 \\ 0 & k & -k & 0 & 0 \\ 0 & 0 & k & -k & 0 \\ 0 & 0 & 0 & k & 0 \end{pmatrix}.$$

Mathematical and Numerical Result

Using principles and techniques from Linear Algebra we are able to find the eigenvalues and its corresponding eigenvectors for the matrix which are key elements to finding the general solution.

$$\lambda_1 = 0,\ \lambda_2 = -k,\ \text{(algebraic multiplicity} = 4), \tag{1}$$

$$\vec{x}_1 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \vec{x}_2 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ -1 \end{pmatrix}, \vec{x}_3 = \begin{pmatrix} 0 \\ 0 \\ 1/k \\ -1/2k \\ -1/2k \end{pmatrix},$$

$$\vec{x}_4 = \begin{pmatrix} 0 \\ 1/k^2 \\ -1/2k^2 \\ -1/4k^2 \\ -1/4k^2 \end{pmatrix}, \vec{x}_5 = \begin{pmatrix} 1/k^3 \\ -1/2k^3 \\ -1/4k^3 \\ -1/8k^3 \\ -1/8k^3 \end{pmatrix}$$

Finally, the eigenvalues and eigenvectors give us the general solution of the ODE system:

$$\begin{aligned}
A_0(t) &= c_1[1/k^3]e^{-kt} \\
A_1(t) &= c_1[-1/2k^3]e^{-kt} + c_1[-1/k^2]te^{-kt} \\
A_2(t) &= c_1[-1/4k^3]e^{-kt} + c_1[-1/2k^2]te^{-kt} \\
&\quad + c_1[-1/k][t^2e^{-kt/2}] \\
A_3(t) &= c_1[-1/8k^3]e^{-kt} + c_1[-1/4k^2]te^{-kt} \\
&\quad + c_1[-1/2k][t^2e^{-kt/2}] + c_1[t^3e^{-kt}]/6 \\
A_4(t) &= c_1[-1/8k^3]e^{-kt} + c_1[-1/4k^2]te^{-kt} \\
&\quad + c_1[-1/2k][t^2e^{-kt/2}] + c_1[t^3e^{-kt}]/6.
\end{aligned}$$

References

[1] Jack McGeachy. The progression of sequential reactions. *Undergraduate Journal of Mathematical Modeling: One + Two*, 2:Iss 2, Article 5, 2010.

[2] Ilijas Farah and Ken Kuttler. *A First Course in Linear Algebra*. Lyryx Learning, free edition edition, 2017.

[3] William F. Trench. *Elementary Differential Equations with Boundary Value Problem*. Brooks/Cole Thomson Learning, free edition edition, 2013.

Numerical Simulation and Conclusion

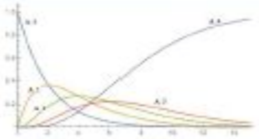


Figure 1: The Shape of Solution Graphs as $k = 0.5$

- The mathematical works and numerical visualization allow us find a **Maximum Points** for each solution function and intermediate involved in the reaction.
- Our analysis shows that chemical **stoichiometry of Phenobarbital** can be approximated from these results.

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