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Simulation of Hemoglobin and Oxyhemoglobin Dynamics Using a Robust Computational Technique

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Abstract:

In this study a robust computational technique is used for a better understand of the dynamics of hemoglobin and oxyhemoglobin in human blood.[1] Results obtained using this technique helps to calculate SpO_2 levels. The major goal of this research is to create a mathematical model that can explain how the concentrations of hemoglobin and oxyhemoglobin change over time. A graphical representation has been arrived with the solution of the proposed model using R-K method and MATLAB tool.

Keywords: hemoglobin, oxyhemoglobin, SpO_2, runge-Kutta method.

1. Introduction

Oxygen is transported from the lungs to tissues all over the human body via hemoglobin (Hb) and oxyhemoglobin (HbO_2). The efficient supply and release of oxygen, in response to shifting oxygen needs is made possible by the reversible binding of oxygen to hemoglobin. The study takes into account changes in oxygen and hemoglobin concentration over time as well as their association and dissociation. Popel[2] examined how microvascular networks in the brain transport oxygen and have created a mathematical model that explains how oxygen gets from blood arteries to brain tissue. Chandel[3] explained how cells react to low oxygen levels (hypoxia) and formulated a model to describe how hypoxia and oxidative stress cause cellular reactions and signalling pathways.

Hsu[4] studied a mathematical model that links temperature and the partial pressure of oxygen (pO_2) to the oxygen saturation of haemoglobin and created equations to explain how haemoglobin binds and releases oxygen under various oxygen concentration and temperature situations. Svetina[5] investigated how haemoglobin surface density affects oxygen binding which in turn affects oxygen transport and release that reveals a new information on the connection between surface density, oxygen binding, and transport.

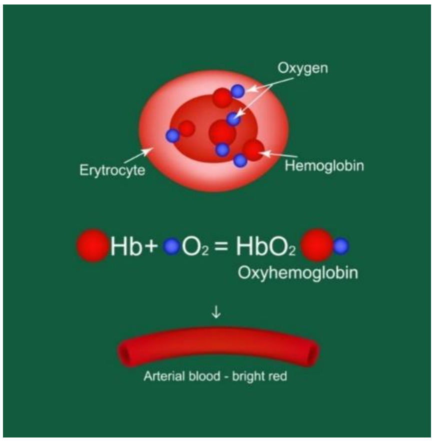
The ratio of hemoglobin and oxyhemoglobin has various medical applications such as diagnosis of respiratory disorders such as asthma, COPD, pneumonia, assessment of hypoia, monitoring oxygen therapy for selecting appropriate blood products and assessing a balanced oxygen carrying capacity of the patients.

The objective of this study is to use a computational technique that captures the dynamic relationship between oxygen and hemoglobin. Analyzing the reversible binding and release of oxygen with hemoglobin and simulating the blood's oxygen transport mechanisms are the goals of the model.

The study specifically responds to the following research questions:

1. How do variable oxygen concentrations in the environment affect the concentrations of hemoglobin and oxyhemoglobin over time?
2. How the blood's oxygenation status impacted by the association and dissociation of oxygen with hemoglobin?
3. How reliable is the computational technique used in estimation of the peripheral capillary oxygen saturation (SpO_2)?

In this paper time-dependent behavior of hemoglobin and oxyhemoglobin concentrations is discussed. First-order kinetics are considered to govern the binding and release of oxygen from hemoglobin, allowing for a reversible association and dissociation process.



2. Mathematical Formation of the Model

The oxyhemoglobin H_o and hemoglobin H_b concentrations over time are represented as a mathematical model by a pair of ordinary differential equations. The model takes into account the association and dissociation of oxygen with hemoglobin, which are controlled by rate constants k1 and k3, respectively and the oxygen content in the environment (S).

The system of differential equations can be represented by

$$d[H_o]/dt= k_1*[H_b]*S-k3*[H_o]$$
$$d[H_b]/dt= k3*[H_o]-k_1*[H_b]*S$$

The concentration of hemoglobin and oxyhemoglobin values are calculated by solving the above equations by using R-K method of 4^{th} order.

3. Assumptions

Throughout the simulation, the oxygen concentration (S) in the surrounding air is assumed to be constant.

The following initial values are assumed for the parameters to solve the model.

$$k_1= 0.5,\ k_3= 0.3,\ S=0.8,\ H_o=1.0,\ H_b=0.0\ h=0.01\ t=0.01\ \text{(endpoint)}$$

4. Notations

The following notations are used to solve the mentioned model.

H_b: Concentration of hemoglobin in the blood (mol/L).

H_O: Concentration of oxyhemoglobin in the blood(mol/L).

k_1: Association constant (L/mol/s).

k_3: Dissociation constant (1/s).

S: Concentration of oxygen in the surroundings (mol/L).

H_S: Saturation of Peripheral Oxygen (SpO_2).

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5. Methodology Used

In solving an ordinary differential equation numerically, the R-K method is a potent numerical technique renowned for its high accuracy and stability. It guarantees closer estimates of the H_o and H_b concentrations at each time step, producing accurate simulation results.

The usage of complex mathematical models is facilitated by MATLAB which is user-friendly and effective environment for scientific computing. A better comprehension of the simulation findings is also made possible by MATLAB visualization capabilities, which enable the graphical representation of the data.

5. Numerical Analysis

The mathematical representation of the model required to estimate the hemoglobin and oxyhemoglobin values is given as follows.

$$d[H_o]/dt = f1(k_1*[H_b]*S - k3*[H_o])$$
$$d[H_b]/dt = f2(k3*[H_o] - k_1*[H_b]*S)$$

6. Numerical Solution

ITERATIONS	$[H_o]$	$[H_b]$
1	1.00	0.003
2	1.006	0.006
3	1.009	0.009
4	1.012	0.012
5	1.015	0.015
6	1.018	0.018
7	1.021	0.021
8	1.024	0.024
9	1.027	0.027
10	1.030	0.030

7. Matlab Solution

```
t: 0, HbO2: 1, Hb: 0
t: 0.01, HbO2: 0.99701, Hb: 0.0029895
t: 0.02, HbO2: 0.99404, Hb: 0.0059582
t: 0.03, HbO2: 0.99109, Hb: 0.0089062
t: 0.04, HbO2: 0.98817, Hb: 0.011834
t: 0.05, HbO2: 0.98526, Hb: 0.014741
t: 0.06, HbO2: 0.98237, Hb: 0.017627
t: 0.07, HbO2: 0.97951, Hb: 0.020494
t: 0.08, HbO2: 0.97666, Hb: 0.02334
t: 0.09, HbO2: 0.97383, Hb: 0.026167
t: 0.1, HbO2: 0.97103, Hb: 0.028974
t: 0.11, HbO2: 0.96824, Hb: 0.031761
t: 0.12, HbO2: 0.96547, Hb: 0.034529
t: 0.13, HbO2: 0.96272, Hb: 0.037278
t: 0.14, HbO2: 0.95999, Hb: 0.040008
t: 0.15, HbO2: 0.95728, Hb: 0.042718
t: 0.16, HbO2: 0.95459, Hb: 0.04541
t: 0.17, HbO2: 0.95192, Hb: 0.048082
t: 0.18, HbO2: 0.94926, Hb: 0.050736
t: 0.19, HbO2: 0.94663, Hb: 0.053372
t: 0.2, HbO2: 0.94401, Hb: 0.055989
t: 0.21, HbO2: 0.94141, Hb: 0.058588
t: 0.22, HbO2: 0.93883, Hb: 0.061169
t: 0.23, HbO2: 0.93627, Hb: 0.063732
t: 0.24, HbO2: 0.93372, Hb: 0.066277
t: 0.25, HbO2: 0.9312, Hb: 0.068804
t: 0.26, HbO2: 0.92869, Hb: 0.071314
t: 0.27, HbO2: 0.92619, Hb: 0.073806
t: 0.28, HbO2: 0.92372, Hb: 0.07628
t: 0.29, HbO2: 0.92126, Hb: 0.078738
t: 0.3, HbO2: 0.91882, Hb: 0.081178
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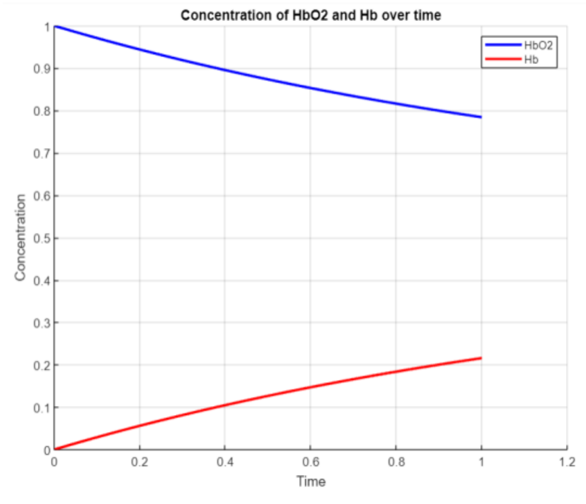
From the concentration of the H_o and H_b, saturation of the peripheral oxygen is calculated as follows:

$$Hs = (H_o/(H_o+H_b))*100$$

Saturation of the peripheral oxygen at H_o=1.00 and H_b= 0.003is: Hs=99.7%.

Thus the saturation of the peripheral oxygen (SpO2) is in the normal range (the ideal range of the SpO_2 is at 95-100%).

8. Graphical Representation



The graph reveals that the concentration of oxyhemoglobin and total hemoglobin first rise quickly over time. This increase is the result of hemoglobin's absorption of oxygen in the lungs, where oxygen-rich air is converted to carbon dioxide during respiration. Oxygen is released to tissues that require it when the oxygenated blood circulates through the body, gradually lowering the concentration of oxyhemoglobin. As it contains both oxyhemoglobin and deoxyhemoglobin, the total hemoglobin content is steady throughout the process.

9. Conclusion

The results provides an insight into oxygen transport process in the blood under varying oxygen concentrations. Additionally, the study allowed the estimation of peripheral capillary oxygen saturation (SpO_2) as an indirect measure of arterial oxygen saturation. The findings of the model may have implications for understanding oxygenation under different physiological conditions and diagnosing oxygenation status in clinical settings[7].

10. Future Work

The model can be further developed to examine the effects of various hemoglobin variations, including fetal hemoglobin (HbF), on oxygen transport and the behavior of the model[6]. Variants of hemoglobin could alter oxygen saturation patterns and have different oxygen-binding characteristics. It can also be used to analyze the total circulation and oxygen delivery within the cardiovascular system using the hemoglobin-oxyhemoglobin model in conjunction with a hemodynamic model.

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