Facilitated oxygen diffusion in muscle fibre

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This article highlights the problem arising from the diffusion of oxygen in living tissues, which continuously consumes oxygen. Oxygen not only diffuses into the muscle fibre, but also binds with the myoglobin to produce oxymyoglobin. In the absence of external oxygen supply, oxymyoglobin releases oxygen to meet its deficiency. However, the oxygen concentration at the centre of the muscle soon becomes zero, giving rise to oxygen debt, a highly undesirable condition. The condition which determines the movement of the boundary separating the oxygen and non-oxygen media, depends upon the rate of absorption of oxygen by the medium. The problem is solved using the explicit finite-difference scheme. The oxygen concentration has been obtained at any point in the medium as a function of rate of oxygen consumption and the facilitated diffusion parameter at any time. The results obtained have been compared with the modelling data available in the literature, and are found to be in close agreement.

Keywords: Diffusion, facilitated, living tissues, muscle fibre, oxygen concentration.

PROBLEMS in engineering, computation and applied sciences are increasingly addressed using sophisticated techniques of mathematics. A number of interdisciplinary applied mathematics research work is going on all over the world. The present study describes mathematical model with solution to describe the oxygen diffusion process in living tissues. It is of use to applied mathematicians, bioengineers and physiologists interested in theoretical approach to the subject. Physiologists such as Huxley[1] and Hodgkin[2] had taken a keen interest towards the mathematical approach to solve physiological problems.

The moving boundary is an essential feature of the present problem. The movement of boundary depends on the rate of absorption of oxygen by the medium. A number of research papers[3–24] dealing with moving boundary value problem are available in the literature due to its applications in various problems such as heat flow, diffusion process, pollution control, soil mechanics, decision theory, etc.

There are various reactions that are catalysed by enzymes which do not themselves change, but efficiently speed up the biological reaction[25]. It is often the case in reaction diffusion systems that the reactants in enzymatic reactions are free to diffuse into the medium. Therefore, one has to keep track of both reaction and diffusion. The subject is useful to understand the facilitated diffusion process[26]. Facilitated oxygen diffusion occurs when the flux of oxygen passing through the muscle fibre is amplified (catalysed) by the reaction taking place in the diffusing medium. In the muscle fibre, oxygen binds with myoglobin to produce oxymyoglobin. The transport of free oxygen is more in comparison to oxygen released by oxymyoglobin. However, in the case of oxygen debt, transport of oxygen is greatly enhanced in the presence of myoglobin. It happens because of the fact that molecular weight of myoglobin (16,890) is much greater than that of oxygen (32).

Muscle fibre uses oxygen even during the rest state of the body, because of the biological process taking place in the muscles. The consumption of ATP (adenosine triphosphate) by the medium requires metabolism of sugar, which consumes oxygen. Further, the oxygen at the exterior of the muscle cell must penetrate to the centre of the cell to prevent oxygen deficiency there (a case of oxygen debt). The problem of diffusion of oxygen was solved by Crank and Gupta[13] by considering the rate of absorption as constant. Marquina and Martinez[14], and Martinez *et al.*[15] extended the work of Crank and Gupta[13] by considering the rate of absorption as a function of distance from the outer surface for inhomogeneous media.

The present work is concerned with the diffusion of oxygen into the tissues, where the effect of biological reaction (myoglobin) is taken into account. The presence of oxymyoglobin protects the muscle at the farthest distance from oxygen debt by releasing the stored oxygen. In fact, the steady process is governed by a fourth-order nonlinear differential equation, which exists in real life.

$$s\varepsilon_2\frac{\mathrm{d}^4\sigma}{\mathrm{d}y^4}+\frac{\varepsilon_2}{y}\frac{\mathrm{d}^3\sigma}{\mathrm{d}y^3}+\left\{\left(\frac{\rho(\gamma-1)}{1+\sigma}\right)-(1+\sigma)-\frac{2\varepsilon_2}{y^2}\right\}\frac{\mathrm{d}^2\sigma}{\mathrm{d}y^2}$$
$$-\frac{\varepsilon_2}{(1+\sigma)}\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}y^2}\right)^2+2\left(\frac{\varepsilon_2}{y^3}-J'\right)\frac{\mathrm{d}\sigma}{\mathrm{d}y}-2\left(\frac{\mathrm{d}\sigma}{\mathrm{d}y}\right)^2$$
$$-\frac{\varepsilon_2}{(1+\sigma)y}\frac{\mathrm{d}\sigma}{\mathrm{d}y}\frac{\mathrm{d}^2\sigma}{\mathrm{d}y^2}+\left(\frac{\rho\gamma}{\varepsilon_2}+\frac{J'}{y}\right)(1+\sigma)=0\,, \tag{1}$$

where $J'(=Jak^{+}/D_sk^{-})$ is the oxygen flux parameter given by

$$-J'=\frac{\partial\sigma}{\partial y}+\rho\frac{\partial u}{\partial y}. \tag{2}$$

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All other terms are defined subsequently.

The models of Crank and Gupta[13] and Martinez *et al.*[15] can be obtained as particular cases. Free and bounded concentration of oxygen is obtained at any point in the medium as a function of rate of absorption of oxygen and facilitated diffusion parameter using the numerical method at any time. Explicit finite-difference scheme[13,27] derived from forward difference, central difference and Lagrange method is used to find the concentration of oxygen at the surface, intermediate points (between the surface and centre of the cylinder) and at the centre respectively.

Formulation of the problem

Consider the muscle fibre as a long circular cylinder of radius a where diffusion takes place in the radial direction only. Let the oxygen concentration at the surface (boundary) be kept constant s_a and distribution of the chemical species maintained radially symmetrical.

When oxygen [O_2] passes through the muscles, it reacts with myoglobin [Mb] to produce oxymyoblobin [MbO_2]

$$O_2 + \mathrm{Mb} \underset{k^-}{\overset{k^+}{\rightleftharpoons}} \mathrm{MbO}_2, \tag{3}$$

where k^+ and k^- are rate constants in the forward and backward direction respectively.

The law of mass action for uptake of oxygen f into oxymyoglobin is given by

$$f = -k^- c + k^+ se, \tag{4}$$

where s, e and c are the concentrations of oxygen, myoglobin and oxymyoglobin respectively, at a point r from the centre of the cylinder at any time t.

The governing diffusion equations for oxygen, oxymyoglobin and myoglobin are respectively given by:

$$\frac{\partial s}{\partial t} = D_s \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial s}{\partial r}\right) - g - f, \tag{5}$$

$$\frac{\partial c}{\partial t} = D_c \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right) + f, \tag{6}$$

$$\frac{\partial e}{\partial t} = D_e \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial e}{\partial r}\right) - f, \tag{7}$$

where g is the constant consumption rate of oxygen per unit volume in the medium, and D_s, D_c and D_e are the diffusion constants of oxygen, oxymyglobin and myoglobin respectively.

The boundary conditions to solve the differential equations are:

$$\text{At } r = a, \quad s = s_a, \quad \frac{\partial c}{\partial r} = 0, \ \frac{\partial e}{\partial r} = 0. \tag{8}$$

$$\text{At } r = 0, \quad \frac{\partial s}{\partial r} = 0, \ \frac{\partial c}{\partial r} = 0, \ \frac{\partial e}{\partial r} = 0. \tag{9}$$

Total myoglobin e_0 in the medium is conserved by the reaction. Therefore,

$$e + c = e_0. \tag{10}$$

The non-dimensionalized variables are:

$$\sigma = \frac{k^+ s}{k^-}, \ U = \frac{c}{e_0}, \ V = \frac{e}{e_0}, \ y = \frac{r}{a}, \ \frac{T}{t} = e_0 k^+. \tag{11}$$

Introducing the non-dimensional variables, eqs (5)–(7) and (10) reduce to:

$$\frac{\partial \sigma}{\partial T} = \varepsilon_1 \left(\frac{\partial^2 \sigma}{\partial y^2} + \frac{1}{y}\frac{\partial \sigma}{\partial y}\right) - \gamma + (U - \sigma V), \tag{12}$$

where $\varepsilon_1 = \dfrac{D_s}{a^2 k^+ e_0}$, $\gamma = \dfrac{g}{e_0 k^-}$.

$$\frac{e_0}{k}\frac{\partial U}{\partial T} = \varepsilon_2 \left(\frac{\partial^2 U}{\partial y^2} + \frac{1}{y}\frac{\partial U}{\partial y}\right) - U + \sigma V, \tag{13}$$

where $\varepsilon_2 = \dfrac{D_c}{a^2 k^-}$, $k = \dfrac{k^-}{k^+}$.

$$\frac{e_0}{k}\frac{\partial V}{\partial T} = \varepsilon_3 \left(\frac{\partial^2 V}{\partial y^2} + \frac{1}{y}\frac{\partial V}{\partial y}\right) + U - \sigma V, \tag{14}$$

where $\varepsilon_3 = \dfrac{D_e}{a^2 k^-}$.

And

$$U + V = 1. \tag{15}$$

The boundary conditions with respect to new variables are as follows:

$$\text{At} \quad y = 1, \quad \sigma = \sigma_1, \quad \frac{\partial U}{\partial y} = 0, \ \frac{\partial V}{\partial y} = 0. \tag{16}$$

And

$$\text{At} \quad y = 0, \quad \frac{\partial \sigma}{\partial y} = 0, \quad \frac{\partial U}{\partial y} = 0, \ \frac{\partial V}{\partial y} = 0. \tag{17}$$

Since molecular weight and structure of oxymyoglobin and myoglobin are similar, the constants ε_2 and ε_3 are approximately taken to be the same. Hence eq. (14) is superfluous. Therefore, the only differential equations to be solved are eqs (12) and (13).

Steady state

Oxygen diffuses into the muscle fibre freely, where some of the oxygen is absorbed by the medium, thereby being removed by the diffusion process. The concentration of oxygen at the surface of the medium is maintained constant. The first phase of the problem continues until steady state is reached, where the oxygen concentration does not change any further with time.

Thus the differential equations governing the steady-state process are:

$$\varepsilon_1 \left(\frac{\partial^2 \sigma}{\partial y^2} + \frac{1}{y}\frac{\partial \sigma}{\partial y} \right) - \gamma + (U - \sigma V) = 0, \tag{18}$$

$$\varepsilon_2 \left(\frac{\partial^2 U}{\partial y^2} + \frac{1}{y}\frac{\partial U}{\partial y} \right) - U + \sigma V = 0. \tag{19}$$

The explicit steady-state solution derived from Keener and Sneyd[28] for concentration distribution in the muscle fibre, using eqs (16) and (17) is:

$$\sigma(y,t) = \frac{1}{2}\left[\gamma_1 (y^2 - 1) + \sigma_1 + \rho U_1 - 1 - \rho \right.$$

$$\left. + \sqrt{\begin{matrix} (\gamma_1 (y^2 - 1) + \sigma_1 + \rho U_1 - 1 - \rho)^2 + \\ 4(\gamma_1 (y^2 - 1) + (\sigma_1 + \rho U_1)) \end{matrix}} \right], \tag{20}$$

where σ_1 and U_1 are free and bounded oxygen concentration at the surface respectively, while $\rho = \varepsilon_2/\varepsilon_1$ and $\gamma_1 = \gamma/4\varepsilon_1$ are the facilitated parameter and oxygen consumption parameter respectively.

Oxygen debt occurs when σ becomes zero, while marginal oxygen debt occurs when total oxygen concentration falls to zero. The oxygen concentration (critical oxygen concentration σ_0) at the boundary just enough to prevent oxygen debt at the centre is given by:

$$\sigma_0 + \rho \frac{\sigma_0}{1 + \sigma_0} = \gamma_1. \tag{21}$$

Extinction state

The supply of oxygen is cut-off by sealing the surfaces, so that no further oxygen passes in or out. The medium continues to consume the available oxygen present. Subsequently, oxygen debt occurs at the centre of the muscles and after sometime the boundary of zero concentration recedes towards the sealed surface.

The governing differential equations of extinction state are:

$$\frac{\partial \sigma}{\partial T} = \varepsilon_1 \left(\frac{\partial^2 \sigma}{\partial y^2} + \frac{1}{y}\frac{\partial \sigma}{\partial y} \right) - \gamma + (1 + \sigma)U - \sigma, \tag{22}$$

$$\frac{e_0}{k}\frac{\partial U}{\partial T} = \varepsilon_2 \left(\frac{\partial^2 U}{\partial y^2} + \frac{1}{y}\frac{\partial U}{\partial y} \right) - (1 + \sigma)U + \sigma, \tag{23}$$

The boundary conditions are:

$$\text{At}\, y = 1, \quad \frac{\partial \sigma}{\partial y} = 0, \quad \frac{\partial U}{\partial y} = 0, \quad T \geq 0. \tag{24}$$

$$\text{At}\, y = 0, \quad \frac{\partial \sigma}{\partial y} = 0, \quad \frac{\partial U}{\partial y} = 0, \quad T \geq 0. \tag{25}$$

The free and bounded oxygen concentration σ and U obtained in steady state can be taken as the initial distribution of oxygen for the solution of extinction state.

$$\sigma(y, 0) = \sigma, \quad U(y, 0) = U, \text{ at time } T = 0. \tag{26}$$

The objective of the problem is to trace the movement of the boundary and determine the distribution of oxygen in the medium as a function of time and distance. The change in concentration of oxygen and movement of the boundary point in different time stages are found to be different. Hence, different methods have been proposed for different time stages by earlier researchers, like integral, finite difference, Laplace transformation, etc. Crank and Gupta[13] suggested an appropriate numerical method to find the concentration of oxygen at any time at the surface, intermediate points (between the surface and centre of the cylinder) and at the centre of the cylinder.

Method of solution: Numerical method

The continuous absorption of oxygen by the medium results in oxygen debt at the centre of the muscle fibre in extinction state. Subsequently, the boundary of zero concentration of oxygen moves towards the sealed surface. Abrupt sealing of the surface causes discontinuity in the derivative boundary condition and hence numerical methods based on the finite differences are liable to give inaccurate solution in the surface neighbourhood for short times.

Several numerical methods have been proposed earlier to obtain the approximate solution. Douglas and Gallie[22] introduced a method of variable time-step, keeping the size of the space mesh fixed. Ehlrich[24] employed implicit formula at the intermediate points and Taylor's expansions near the moving boundary in both time and space directions. Crank[27] suggested a Lagrange interpolation formula near the moving boundary to obtain the concentration.

In the present analysis, the concentrations at the intermediate points have been calculated using explicit finite-difference formula, as suggested by Crank[27]. The location of the moving point is determined by the Taylor's series. The whole region, $0 \le y \le 1$ is subdivided into M intervals each of width δy, such that $y_r = r\delta y$, where $0 \le r \le M$ $(M\delta y = 1)$.

Let the concentration at each of the grid points at the jth time level be known. The position of the moving boundary at that time is somewhere in the rth interval between y_{r-1} and y_r, given by $y_0 = (r-1)\delta y + p^j\delta y$, $0 \le p^j < 1$ along the radial direction. Figure 1 shows the boundary point y_0.

Then the concentration at the $(j+1)$th time level can be calculated using the explicit formula:

$$\sigma_{ij+1} = \sigma_{ij} + \delta t \times \left[\frac{\varepsilon_i(\sigma_{i+1j} - \sigma_{ij})}{\mathrm{d}y}\left(\frac{2}{\mathrm{d}y} + 1\right) - \gamma + (1+\sigma_{ij})U_{ij} - \sigma_{ij} \right], \quad (27)$$

while at the other intermediate points the explicit formula becomes

$$\sigma_{ij+1} = \sigma_{ij} + \delta t \left[\frac{\varepsilon_1}{\mathrm{d}y}\left(\frac{(\sigma_{i+1j} - 2\sigma_{ij} + \sigma_{i-1j})}{\mathrm{d}y} + \frac{(\sigma_{i+1j} - \sigma_{i-1j})}{2y_i} \right) - \gamma + (1+\sigma_{ij})U_{ij} - \sigma_{ij} \right]. \quad (28)$$

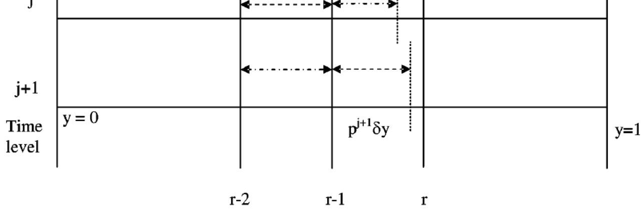

Figure 1. Movement of boundary separating oxygen and non-oxygen media.

Concentrations in the neighbourhood of the boundary as suggested by Crank and Gupta[13] using the appropriate finite-difference replacement leads to the following equations.

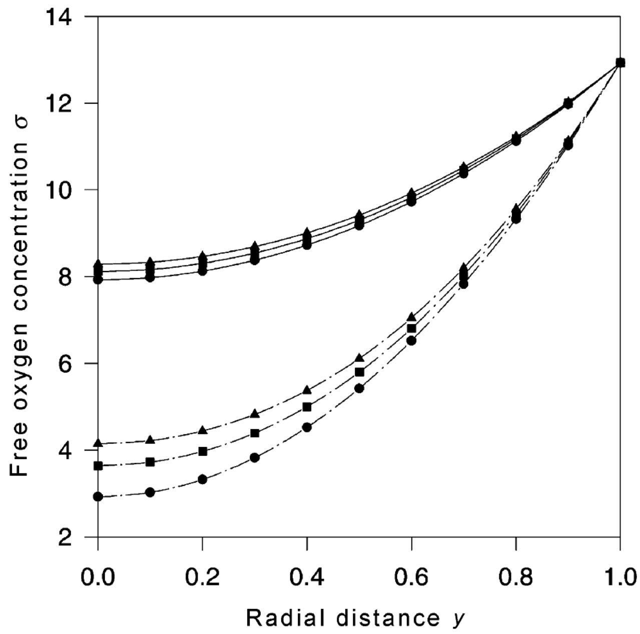

Figure 2. Free oxygen distribution in steady state. Free oxygen concentration in steady state for oxygen consumption $\gamma_1 = 5.0$: ———, and $\gamma_1 = 10.0$: -·-·-·-·-·-. Key symbol $\rho = 0.0$: ●●●; $\rho = 5.0$: ■ ■ ■, and $\rho = 10.0$: ▲▲▲.

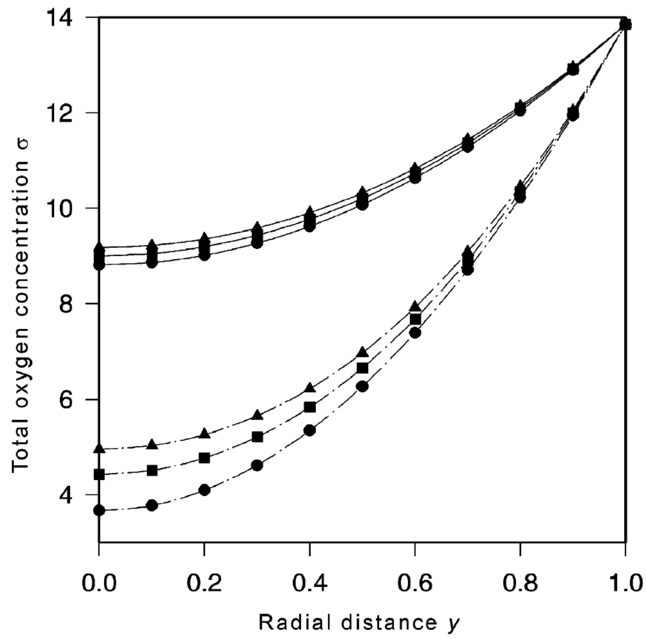

Figure 3. Total oxygen distribution in steady state. Total oxygen concentration in steady state for oxygen consumption $\gamma_1 = 5.0$: ———, and $\gamma_1 = 10.0$: -·-·-·-·-·-. Key symbol $\rho = 0.0$: ●●●; $\rho = 5.0$: ■ ■ ■, and $\rho = 10.0$: ▲▲▲.

When the boundary does not move within the specified degree of accuracy,

$$\sigma_{ij+1} = \sigma_{ij} + \delta t \times \left[\frac{\varepsilon_1}{\mathrm{d}y} \frac{2}{\mathrm{d}y} \left(\frac{\sigma_{i-1j}}{p_s + 1} - \frac{\sigma_{ij}}{p_s} \right) - \gamma + (1 + \sigma_{ij}) U_{ij} - \sigma_{ij} \right], \quad (29)$$

where $p_s = \dfrac{\sqrt{2\sigma_{ij}}}{\mathrm{d}y}$.

When the boundary starts moving,

$$\sigma_{ij+1} = \sigma_{ij} + \delta t \left[\frac{\varepsilon_1}{\mathrm{d}y} \left(\frac{2}{\mathrm{d}y} \left(\frac{\sigma_{i-2j}}{p_s + 1} - \frac{\sigma_{i-1j}}{p_s} \right) + \frac{\sigma_{i-1j} - \sigma_{i-2j}}{y_i} \right) - \gamma + (1 + \sigma_{ij}) U_{ij} - \sigma_{ij} \right], \quad (30)$$

where $p_s = \dfrac{\sqrt{2\sigma_{i-1j}}}{\mathrm{d}y}$.

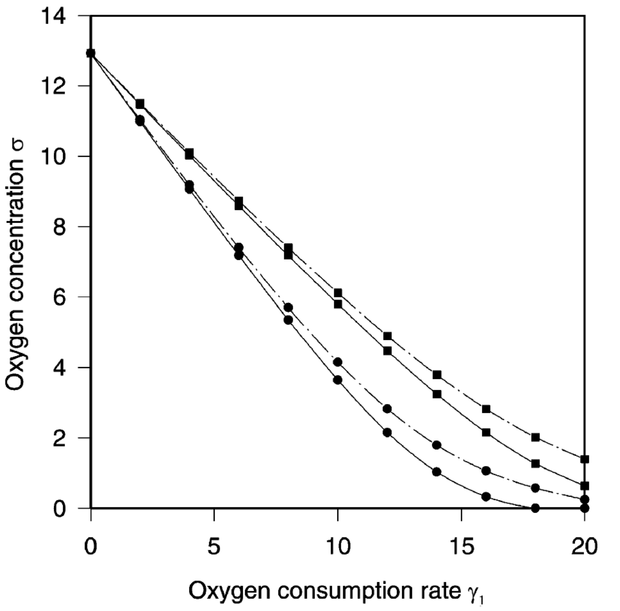

Figure 4. Oxygen concentration σ for $\rho = 5$: ——— and $\rho = 10$: –·–·–, in steady state. Key symbol $y = 0.0$: ••• and $y = 0.5$: ■ ■ ■.

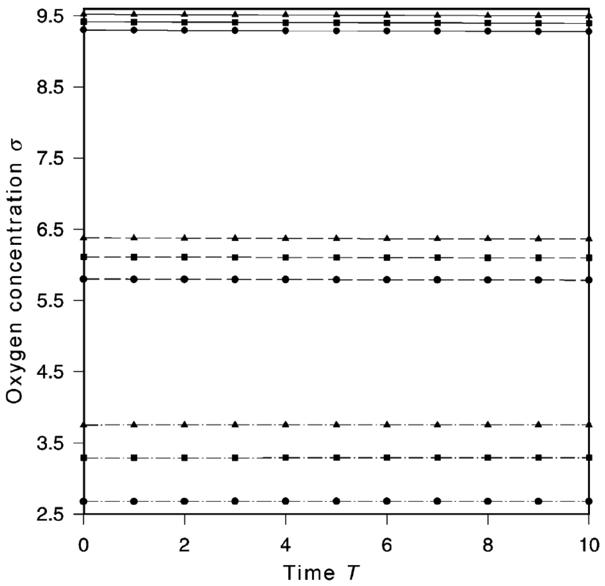

Figure 6. Oxygen concentration σ vs time T at midpoint $y = 0.5$ as a function of consumption rate $\gamma_1 = 5.0$: ———, $\gamma_1 = 10.0$: – – – –; $\gamma_1 = 15$: –·–·–. Key symbol $\rho = 5$: •••; $\rho = 10$: ■ ■ ■, and $\rho = 15$: ▲▲▲.

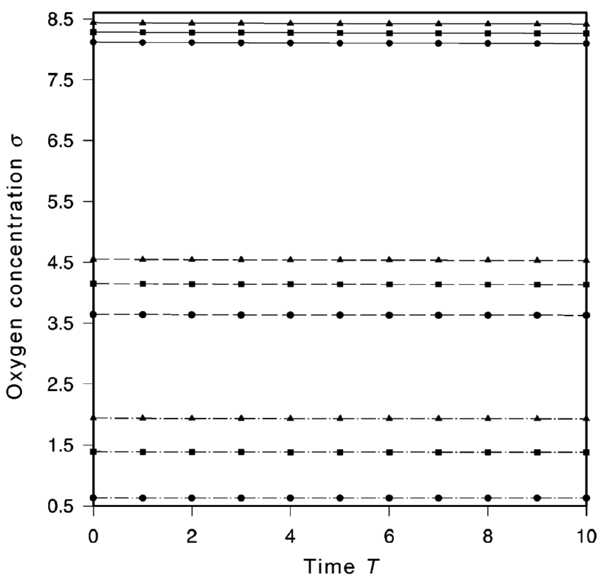

Figure 5. Oxygen concentration σ vs time T at the centre $y = 0.0$ as a function of consumption rate $\gamma_1 = 5.0$: ———, $\gamma_1 = 10.0$: – – – –; $\gamma_1 = 15$: –·–·–. Key symbol $\rho = 5$: •••; $\rho = 10$: ■ ■ ■, and $\rho = 15$: ▲▲▲.

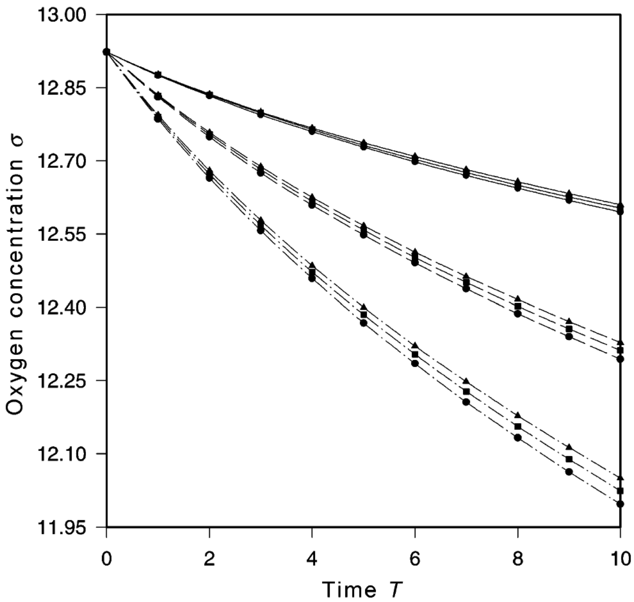

Figure 7. Oxygen concentration σ vs time T at the surface $y = 1.0$ as a function of consumption rate $\gamma_1 = 5.0$: ———, $\gamma_1 = 10.0$: – – – –; $\gamma_1 = 15$: –·–·–. Key symbol $\rho = 5$: •••; $\rho = 10$: ■ ■ ■, and $\rho = 15$: ▲▲▲.

Similarly, the bound oxygen concentration at the sealed surface, intermediate points and in the neighbourhood of the moving boundary becomes respectively,

$$U_{ij+1} = U_{ij} + \delta t \frac{k}{e_0}\left[\frac{\varepsilon_2(U_{i+1j} - U_{ij})}{\mathrm{d}y}\left(\frac{2}{\mathrm{d}y} + 1\right) - (1 + \sigma_{ij})U_{ij} + \sigma_{ij}\right], \tag{31}$$

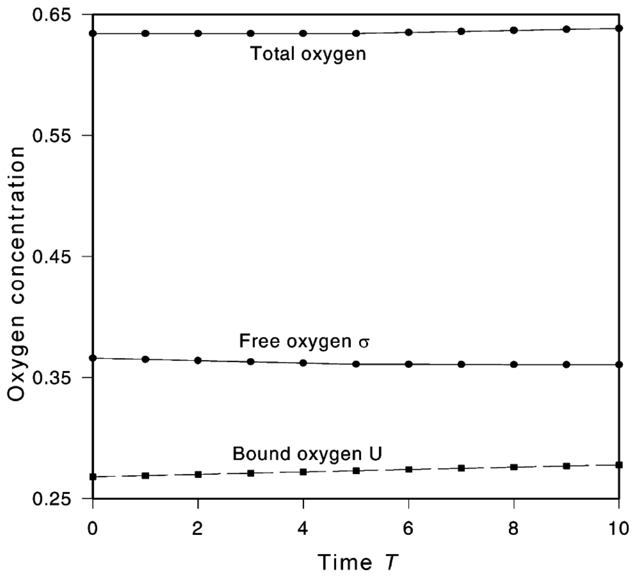

Figure 8. Release of bounded oxygen by oxymyoglobin when free oxygen is reduced to a low level for $\gamma_1 = 16.0$ and $\rho = 5.217$ at the centre.

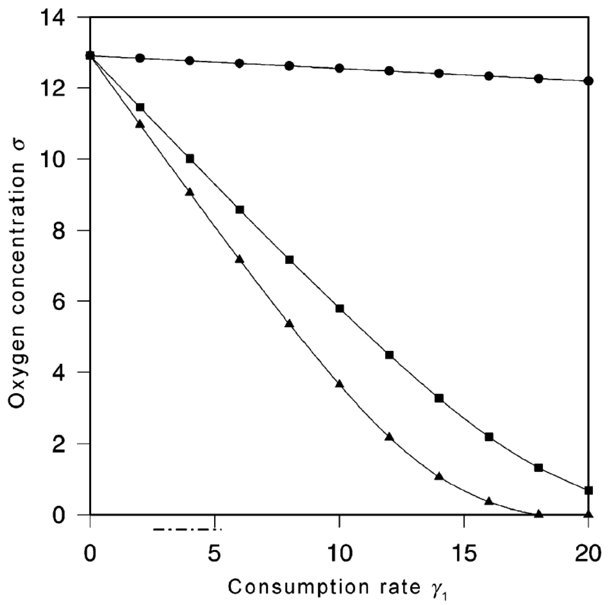

Figure 9. Free oxygen concentration as a function of consumption rate γ_1 at time $T = 5.0$ and $\rho = 5.217$. Key symbol $y = 1.0$: ●●●; $y = 0.5$: ■ ■ ■, and $y = 0.0$: ▲▲▲.

$$U_{ij+1} = U_{ij} + \delta t \frac{k}{e_0}\left[\frac{\varepsilon_2}{\mathrm{d}y}\left(\frac{(U_{i+1j} - 2U_{ij} + U_{i-1j})}{\mathrm{d}y} + \frac{(U_{i+1j} - U_{i-1j})}{2y_i}\right) - (1 + \sigma_{ij})U_{ij} + \sigma_{ij}\right]. \tag{32}$$

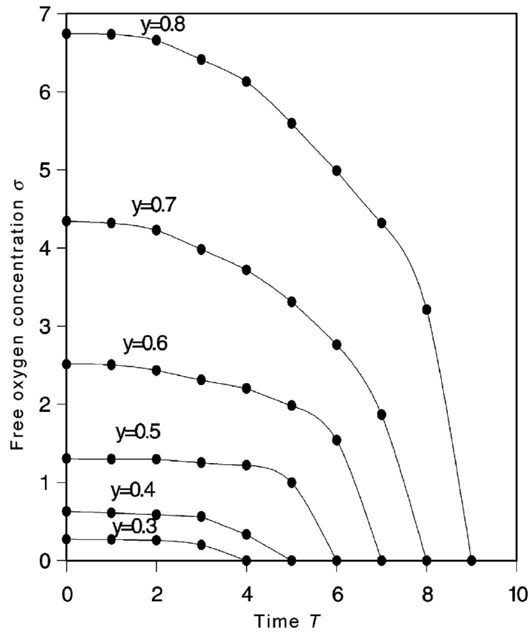

Figure 10. Position of moving boundary with respect to time for faciliated diffusion parameter $\rho = 5.215$ and consumption rate parameter $\gamma_1 = 18.0$.

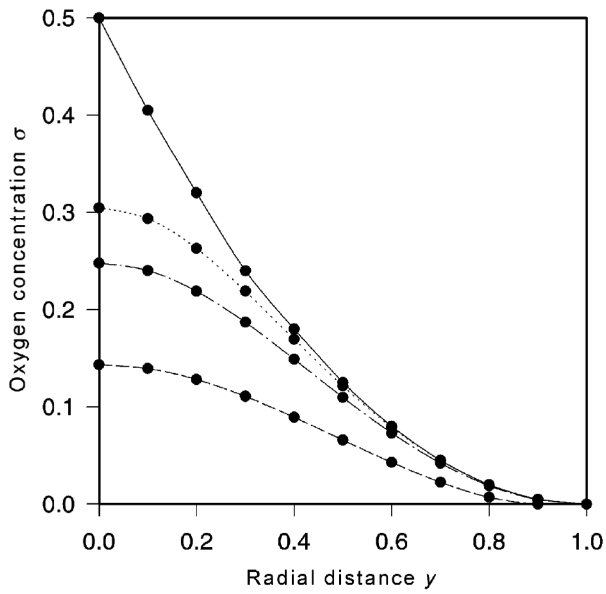

Figure 11. Comparison of oxygen concentration (•) with Crank and Gupta[13] for $T = 0.00$: ——; $T = 0.03$: ··········; $T = 0.05$:-·-·-·-·-·-·- and $T = 0.10$: ---------.

When the boundary does not move,

$$U_{ij+1} = U_{ij} + \delta t \frac{k}{e_0} \times \left[\frac{\varepsilon_2}{\mathrm{d}y} \frac{2}{\mathrm{d}y} \left(\frac{U_{i-1j}}{p_u + 1} - \frac{U_{ij}}{p_u} \right) - (1 + \sigma_{ij}) U_{ij} + \sigma_{ij} \right], \tag{33}$$

where $p_u = \dfrac{\sqrt{2U_{ij}}}{\mathrm{d}y}$.

When the boundary starts moving,

$$U_{ij+1} = U_{ij} + \delta t \frac{k}{e_0} \left[\frac{\varepsilon_2}{\mathrm{d}y} \left(\frac{2}{\mathrm{d}y} \left(\frac{U_{i-2j}}{p_u + 1} - \frac{U_{i-1j}}{p_u} \right) + \frac{U_{i-1j} - U_{i-2j}}{y_i} \right) - (1 + \sigma_{ij}) U_{ij} + \sigma_{ij} \right], \tag{34}$$

where $p_u = \dfrac{\sqrt{2U_{i-1j}}}{\mathrm{d}y}$.

Numerical results

Free and bounded oxygen concentration eqs (22) and (23) are solved by explicit finite-difference method for various values of reaction diffusion parameters, such as facilitated diffusion parameter ρ(= 0, 5, 10), rate of consumption parameter γ_1 (= 0, 5, 10) at different times T. Time $T = 0$ corresponds to the result of steady state. Total myoglobin e_0, diffusion constants ε_1, ε_2 and rate constants k^+ and k^- are taken as 2.8×10^{-7} mol/cm^3, 2.3×10^{-4}, 1.2×10^{-3}, 2.4×10^{10} cm^3/mol s and 65/s respectively, to compute the entire results.

Results and discussion

Oxygen concentration has been obtained for the facilitated oxygen diffusion process for different values of facilitated parameter ρ, oxygen consumption parameter γ_1 at any time T, and at any point in the medium. Finite-difference numerical techniques have been utilized to find the concentration of oxygen at the centre, intermediate points and on the surface of the medium. The work presented here analyses how myoglobin facilitates the oxygen diffusion process and prevents oxygen debt in the muscle fibre. The combined effect of diffusion and myoglobin in oxygen consumption is presented in Figures 2–13. Figure 2 presents the graph of free oxygen concentration vs radius vector y for facilitated oxygen distribution at steady state for facilitated parameter $\rho = 0.0$, 5.0 and 10.0, and oxygen consumption parameter $\gamma_1 = 5.0$ and 10.0. Figure 2 shows that oxygen concentration gradually decreases from the surface to the centre of the muscle, keeping other parameter values fixed. The concentration of oxygen is greater for higher values of ρ. The role of ρ is found to increase the concentration of oxygen at all points in the medium. Thus presence of myoglobin reduces the chances of occurrence of oxygen debt. But reverse is the case with the increase of γ_1. Figure 3 shows the total oxygen concentration due to free and bounded oxygen released by oxymyoglobin for the same parameter values as in Figure 2. Figure 4 presents the graph of free oxygen concentration vs consumption rate parameter γ_1 at $y = 0.0$ and 0.5 for facilitated parameter $\rho = 5.0$ and 10.0. The

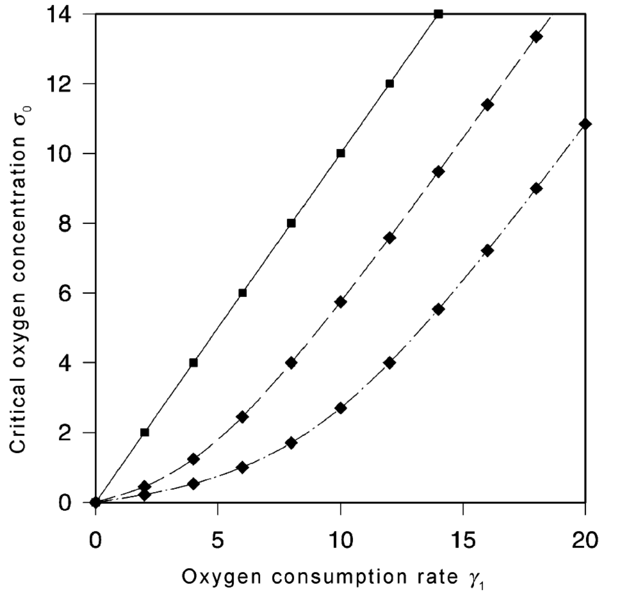

Figure 12. Comparison of critical oxygen concentration (■) with that of Keener and Sneyd[26] for $\rho = 0$:——; $\rho = 5$: — — and $\rho = 10$: -·-·-·-·-·.

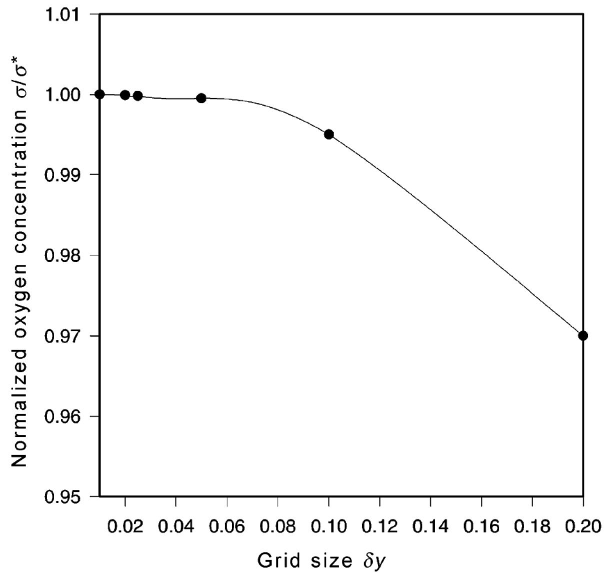

Figure 13. Convergence of normalized oxygen concentration σ/σ^* with grid size δy for $\gamma_1 = 2.0$ and $\rho = 5.217$ at the origin. σ^*, Concentration obtained at $\delta y = 0.01$.

Table 1. Free oxygen concentration in facilitated oxygen diffusion in extinction state as a function of radius y and time T

ρ = 5.0 and γ_1 = 5.0											
T/y	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.0	8.113	8.160	8.302	8.538	8.871	9.299	9.826	10.451	11.175	11.999	12.923
2.0	8.106	8.156	8.296	8.533	8.865	9.294	9.820	10.445	11.169	11.992	12.833
4.0	8.101	8.152	8.292	8.528	8.860	9.289	9.815	10.440	11.164	11.982	12.760
6.0	8.097	8.149	8.289	8.524	8.856	9.285	9.811	10.435	11.159	11.971	12.698
8.0	8.094	8.146	8.285	8.521	8.852	9.281	9.807	10.431	11.154	11.960	12.644
10.0	8.090	8.143	8.283	8.518	8.849	9.277	9.803	10.427	11.149	11.947	12.595
ρ = 10.0 and γ_1 = 5.0											
T/y	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.0	8.282	8.327	8.462	8.687	9.004	9.415	9.921	10.523	11.223	12.023	12.923
2.0	8.276	8.323	8.457	8.682	8.999	9.409	9.915	10.517	11.217	12.016	12.835
4.0	8.271	8.319	8.452	8.677	8.994	9.404	9.910	10.512	11.212	12.007	12.764
6.0	8.266	8.316	8.449	8.673	8.990	9.400	9.906	10.508	11.207	11.996	12.703
8.0	8.263	8.313	8.445	8.670	8.986	9.396	9.902	10.503	11.203	11.984	12.650
10.0	8.260	8.310	8.443	8.666	8.983	9.393	9.898	10.500	11.198	11.972	12.603
ρ = 5.0 and γ_1 = 10.0											
T/y	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.00	3.641	3.723	3.970	4.391	4.998	5.799	6.805	8.018	9.443	11.078	12.923
2.00	3.635	3.720	3.966	4.387	4.993	5.795	6.800	8.014	9.438	11.071	12.749
4.00	3.632	3.718	3.964	4.384	4.990	5.792	6.797	8.010	9.433	11.058	12.609
6.00	3.629	3.717	3.962	4.382	4.988	5.789	6.793	8.006	9.429	11.041	12.491
8.00	3.627	3.716	3.961	4.381	4.986	5.787	6.791	8.003	9.425	11.023	12.387
10.00	3.626	3.715	3.960	4.379	4.984	5.784	6.788	8.000	9.420	11.003	12.294
ρ = 10.0 and γ_1 = 10.0											
T/y	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.00	4.148	4.220	4.442	4.822	5.374	6.111	7.047	8.193	9.552	11.129	12.923
2.00	4.141	4.218	4.438	4.818	5.370	6.107	7.044	8.189	9.548	11.123	12.754
4.00	4.137	4.215	4.436	4.815	5.367	6.104	7.040	8.185	9.544	11.111	12.617
6.00	4.135	4.214	4.434	4.813	5.364	6.101	7.038	8.182	9.540	11.095	12.502
8.00	4.133	4.212	4.432	4.811	5.362	6.099	7.035	8.179	9.536	11.077	12.402
10.00	4.131	4.211	4.431	4.810	5.361	6.097	7.033	8.177	9.532	11.058	12.312

oxygen concentration decreases with increase of γ_1. The decrease of oxygen concentration causes oxygen debt at the centre of the muscle, which can be avoided for higher values of ρ. Figures 5–7 show the graph of oxygen concentration vs time T at ρ = 5, 10 and 15 in extinction state for different values of γ_1 (=5.0, 10.0, 15.0) at the centre, intermediate points and surface of the muscle fibre respectively. It can be seen from Figures 5–7 that the concentration of oxygen not only decreases with increase in γ_1, but also with the increase in T, keeping other parameters fixed. The rate of decrease of oxygen concentration is more at points towards the surface. The same can be seen from Table 1. When free oxygen concentration drops, oxygen is released by the myoglobin. Thus even bound oxygen diffuses slowly compared to free oxygen; the quantity of bound oxygen is high (Figure 8). But in the absence of external oxygen supply, oxygen debt occurs after a certain time, keeping all other parameters fixed (Figure 9). Subsequently, boundary of zero concentration recedes towards the sealed surface (Figure 10). Consumption of oxygen is faster at the end of the process.

Figure 11 compares oxygen concentration with the result obtained by Crank and Gupta[13], when rate of consumption per unit volume is constant in the one-dimension Cartesian coordinate system, in the absence of oxygen uptake function f. The obtained results are in good agreement with those of Crank and Gupta[13]. The model presented by Martinez *et al.*[15] can be obtained as a special case of the present model, by taking rate of consumption per unit volume as a function of distance (i.e. $\sqrt{\text{distance}}$) in the one-dimension Cartesian coordinate system, in the absence of oxygen uptake function f. A comparative study with different models presented by Martinez *et al.*[15], Crank and Gupta[13] and Hansen and Hougaard[19] is shown in Table 2. Figure 12 compares the critical oxygen concentration at the surface vs oxygen consumption rate parameter γ_1 for facilitated parameter ρ = 0, 5 and 10 with the result of Keener and Sneyd[28]. Figure 12 shows that as the consumption rate increases, the critical oxygen concentration at the surface has to be increased to prevent oxygen debt, but reverse is the case for higher values of ρ. There is a linear increase of critical oxygen concen-

Table 2. Comparative study of free oxygen concentration in extinction state as a function of time T at the surface

Time T	Matinez *et al.* model[15]	Present study	Crank and Gupta model[13]	Present study	Hansen and Hougaard model[19]	Present study
0.04	0.2759	0.2758	0.2759	0.2743	0.2743	0.2741
0.10	0.1449	0.1445	0.1449	0.1432	0.1432	0.1430
0.18	0.0235	0.0238	0.0235	0.0213	0.0218	0.0217
0.19	0.0109	0.0111	0.0109	0.0082	0.0090	0.0091

tration in the absence of facilitated myoglobin, but the increase is parabolic in its presence. Concentration of oxygen has been obtained for grid size $\delta y = 0.05$ and 0.1. It has been observed that there is no change in the result up to three places of decimal. A convergence of results with respect to grid size is also presented in Figure 13.

Conclusion

Thus the boundary value problem has wide applications in applied sciences, engineering, metallurgy, soil mechanics, decision theory, etc. The problem is of immediate interest in medical research concerning uptake of oxygen in the tissues. The present problem analyses the combined effect of diffusion and myoglobin on oxygen diffusion process. Presence of myoglobin prevents the deficiency of oxygen in the muscle fibre. The results obtained are in good agreement with the modelling results available in the literature.

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