Original scientific papers UDK 631.431:546.21
doi: 10.7251/COMEN1601006J

NUMERICAL SOLUTION OF THE DIFFUSION EQUATION FOR OXYGEN DIFFUSION IN SOIL

Aco Janićijević[1], Svetislav Savović[2], Alexandar Djordjevich[3]*
[1] University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia
[2] University of Kragujevac, Faculty of Science, R. Domanovića 12, Kragujevac, Serbia
[3] City University of Hong Kong, 83 Tat Chee Avenue, Kowloon, Hong Kong, China

Abstract: By solving the diffusion equation using the explicit finite difference method, oxygen concentrations inside the soil are determined for various periods of time. Two different cases are investigated, with constant and daily changing air oxygen concentrations. It was concluded that the influence of the periodical change of the air oxygen concentration on the oxygen concentration in the soil was more pronounced for smaller diffusion times at smaller lengths of the soil profile.
Keywords: Oxygen diffusion; soil; diffusion equation; finite difference method.

1. INTRODUCTION

Soil productivity largely depends on the process of soil aeration. The air space in soil contains oxygen to provide for respiration of plant roots. Plant roots adsorb oxygen and release carbon dioxide in the process of respiration. In most plants, the internal transfer of oxygen from parts above the ground (leaves and stems) to those below the ground surface (roots) cannot take place at a rate sufficient to supply the oxygen requirements of the roots [1]. Adequate root respiration requires that the soil itself be aerated. Poor aeration can decrease the uptake of water and induce early wilting. Most plants depend on the transport through the soil of oxygen from and of carbon dioxide to the external air. Gases and vapors are transported in soil air by convection and diffusion, the latter being recognized as the main mechanism [2]. Most of the available research data indicate that excessive soil water reduces the exchange of air between the soil and the atmosphere and causes oxygen deficiency. There are several factors that affect the oxygen diffusion rate. It increases with decreasing soil water content or increasing suction up to a certain level and then declines with further depletion of water. Oxygen moves from the atmosphere to the plant roots mostly by the process of diffusion through air filled soil pores and subsequently through water films separating the root surfaces from the gas phase [3]. Compact layers in a soil profile can also influence transport of oxygen through the soil [4]. The oxygen diffusion rate of soil has been proposed as a good index of soil aeration [5,6].

Oxygen molecules in soil are in continuous thermal motion according to the kinetic theory of gases. The concentration gradient in soil causes net movement of molecules from high concentration to low concentration, this gives the movement of gas by diffusion. Analytical models are developed to describe transient-state oxygen diffusion in soil using Fourier Transforms [7]. An analytical solution to describe non steady-state oxygen transport from atmosphere to soil using the technique of Laplace transformation was also reported [8]. The analytical solutions have limited application since the solution is based on specific initial and boundary conditions. In general, analytical solutions are a very lengthy process. Numerical methods in solving diffusion equation are applicable with less efforts than analytical methods to accurately predict oxygen diffusion state in soil media [9].

Air is a mixture of several gases. When completely dry, it is about 78% nitrogen and 21% oxygen. The remaining 1% is other gases such as argon, carbon dioxide, neon, helium, and others. However, in nature, air is never completely dry. It always contains some water vapor in the amounts varying from almost none to 5% by volume. As water vapor content increases, the other gases decrease proportio-

* Corresponding author: savovic@kg.ac.rs

nately. The absolute oxygen concentration also continuously changes with daily change of barometric pressure. It is therefore of interest to investigate how a small periodical change of O_2 concentration in the air influences the diffusion dynamics of O_2 into the soil.

In this work, the diffusion dynamics of O_2 in the soil column has been investigated. By solving the relevant diffusion equation using the explicit finite difference method, the concentration profiles of O_2 inside the soil column are determined for various periods of time, for constant and periodically changing air oxygen concentration.

2. OXYGEN DIFFUSION DYNAMICS

The governing equation describing the oxygen diffusion into soil is expressed by the following partial differential equation [8]:

$$\frac{\partial C(x,t)}{\partial t} = D\frac{\partial^2 C(x,t)}{\partial x^2} - \alpha \tag{1}$$

where $C(x,t)$ is the concentration of oxygen in the soil air at the depth x, t is the time, D is the diffusion coefficient of oxygen in the soil, α is the activity (the rate of oxygen consumption by the biological and chemical processes within the soil mass). In ref. [8] Eq. (1) is solved analytically for a semi-infinite homogenous soil profile, and for the following initial and boundary conditions:

$$C(x,t) = C_0, \quad 0 \le x \le L; \ \ t = 0 \tag{2}$$

$$C(x,t) = C_0, \quad x = 0; \ \ t > 0$$
$$\frac{\partial C(x,t)}{\partial x} = 0, \quad x \to \infty; \ \ t > 0 \tag{3}$$

where C_0 is the concentration of oxygen in the atmosphere. In Eq. (1) the assumption of constant and uniform activity α has only the merit of simplicity. If oxygen in a given soil is absorbed by biological action, then adsorption would presumably vary with time and position [8].

The analytical solution for this problem is [8]:

$$C(x,t) = C_0 + \alpha\left[\left(t + \frac{x^2}{2D}\right) erfc\left(\frac{x}{2\sqrt{Dt}}\right) - x\sqrt{\frac{t}{\pi D}}\exp\left(\frac{-x^2}{4Dt}\right)\right] \tag{4}$$

The concentrations of oxygen at any time and depth resulting from Eq. (4) were compared to the measured data obtained experimentally by [7], and a reasonably good agreement between measured and predicted oxygen concentrations was observed by [8]. In previously reported work by Kalita [9], Eq. (1) is solved numerically using the finite element method for a semi-infinite homogenous soil profile.

It is also of interest to study the problem of obtaining the O_2 concentration inside the soil in the case when the target O_2 concentration in the air is a periodic function of time, i.e. when the boundary condition at $x = 0$ is $C(x = 0,t) = C_0\left[1 + \varepsilon \sin(2\pi t / T)\right]$, where ε is the O_2 concentration oscillation amplitude and T the oscillation period. In that case, the analytical solution of diffusion equation (1) does not exist and numerical solution is needed.

3. NUMERICAL METHOD

Analytical solutions of diffusion equations with limited initial and boundary conditions have limited applicability and are very lengthy. Employing numerical methods does not have such limitations and also offers flexibility, especially for arbitrary initial distribution and boundary conditions [10,11]. In the 1970s and 1980s, implicit finite difference methods (IFDMs) were generally preferred over explicit finite difference methods (EFDMs). This trend has been changing with the advancement of computers, shifting the emphasis to EFDMs. Being often unconditionally stable, the IFDM allows larger step lengths. Nevertheless, this does not translate into IFDM's higher computational efficiency because extremely large matrices must be manipulated at each calculation step. We find that the EFDM is also simpler in addition to being computationally more efficient [11,12]. In this paper, EFDM is used to solve the diffusion equation (1). The central difference scheme was used to represent the term $\left(\partial^2 C(x,t) / \partial x^2\right)$

$$\left(\frac{\partial^2 C(x,t)}{\partial x^2}\right) = \frac{C_{i+1,j} - 2C_{i,j} + C_{i-1,j}}{(\Delta x)^2} + O(\Delta x)^2 \tag{5}$$

and a forward difference scheme for the derivative term $\left(\partial C(x,t) / \partial t\right)$ [12],

$$\left(\frac{\partial C(x,t)}{\partial t}\right) = \frac{C_{i,j+1} - C_{i,j}}{\Delta t} + O(\Delta t) \tag{6}$$

With these substitutions, equation (1) transforms into:

$$C_{i,j+1} = C_{i-1,j}\frac{D\Delta t}{\Delta x^2} + C_{i,j}\left(1 - \frac{2D\Delta t}{\Delta x^2}\right) + C_{i+1,j}\frac{D\Delta t}{\Delta x^2} - \alpha\Delta t \quad (7)$$

where indexes i and j refer to the discrete step lengths Δx and Δt for the coordinate x and time t, respectively. Equation (5) represents a formula for $C_{i,j+1}$ at the $(i, j + 1)^{th}$ mesh point in terms of the known values along the j^{th} time row. The truncation error for the difference equation (7) is $O(\Delta t, (\Delta x)^2)$. Using a small-enough value of Δt and Δx, the truncation error can be reduced until the accuracy achieved is within the error tolerance [12].

The initial condition (2) for equation (1) can be expressed in the finite difference form as:

$$C_{i,0} = C_0, \quad 0 \le x \le L; \quad t = 0 \quad (8)$$

In the case of constant boundary condition at the soil surface, it can be written in the finite difference form as:

$$C_{0,j} = C_0, \quad x = 0; \quad t > 0 \quad (9)$$

In the case of periodic boundary condition at the soil surface, it can be written in the finite difference form as:

$$C_{0,j} = C_0\left[1 + \varepsilon\sin(2\pi t_j / T)\right], \quad x = 0; \quad t > 0 \quad (10)$$

Boundary condition at $x \to x_\infty$ in the finite difference form becomes:

$$C_{N,j} = C_{N-1,j}, \ x \to x_\infty; \quad t > 0 \quad (11)$$

where $N = x_\infty / \Delta x$ is the grid dimension in the x direction and x_∞ is the distance in the direction x at which $\partial C / \partial x = 0$ (x_∞ replaces $x \to \infty$ in equation (3)).

4. NUMERICAL AND ANALYTICAL RESULTS

To facilitate the comparison of results, we applied our numerical method to the diffusion of oxygen in a soil column with the geometry used in the work by Kalita [9], Figure 1. The following values of diffusion coefficient (D) and activity (α) are used: D = 259.2 cm^2 h^{-1} and α = 0.002125 cm^3 cm^{-3} h^{-1}[7]. We first investigate the case when the air oxygen concentration at x = 0 is $C(0,t) = C_0$ = 0.21 cm^3 cm^{-3}.

Shown in Figure 2 are numerical results for relative oxygen concentration at five different times obtained by solving the diffusion equation (1) by EFDM in the case of constant air oxygen concentration. In the numerical calculations, the step lengths Δx = 5 cm and Δt = 0.00005 h have been used to achieve the stability of the finite difference scheme. In equation (11) we used $x_\infty = 10$ m as the distance at which there is no change in the oxygen concentration. Increasing x_∞ further affected the solution a little but greatly increased the grid size and therefore the computation time. In Figure 2 the filled squares represent an analytical solution (4) of the diffusion equation (1). A good agreement between the numerical and analytical solution is obtained. The deviations are less than 0.5%. Figure 2 illustrates the O_2 concentration profile, $C(x, t)$ inside the soil column with lapse of time. The oxygen concentration decreases with increasing the soil depth, approaching the steady-state distribution for t = 160 h.

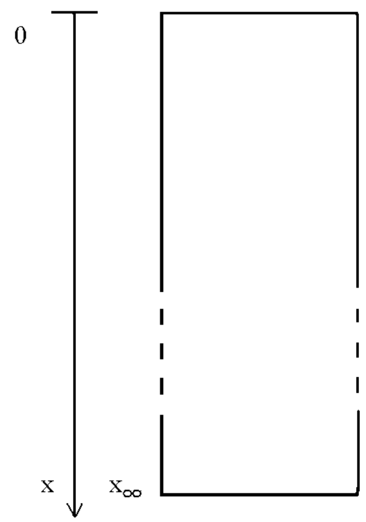

Figure 1. A schematic diagram of a soil column.

Figure 3 shows numerical results for the oxygen concentration inside the soil column for various diffusion times, when the air oxygen concentration periodically changes as $C(x=0,t) = C_0 \cdot [1 + \varepsilon\sin(2\pi t / T)]$, where C_0 = 0.21 cm^3 cm^{-3}, ε = 0.05, and T = 24 h are assumed. In Figure 3 O_2 concentration in the soil column in the case of constant air oxygen concentration C_0=0.21 cm^3 cm^{-3} is also shown.One can see in Figure 3 that due to the periodical change of air oxygen concentration, the transient oxygen concentrations after 12 h is slightly larger if compared to the case of constant air oxygen concentration. With increasing the diffusion time, the oxygen concentrations in soil for the case of periodical change of the air oxygen concentration are smaller than those when air oxygen concentration is constant. These differences are more pronounced for smaller x and smaller diffusion times. Finally, the same steady-state oxygen concentration in the soil profile is obtained for different air oxygen concentrations analyzed.

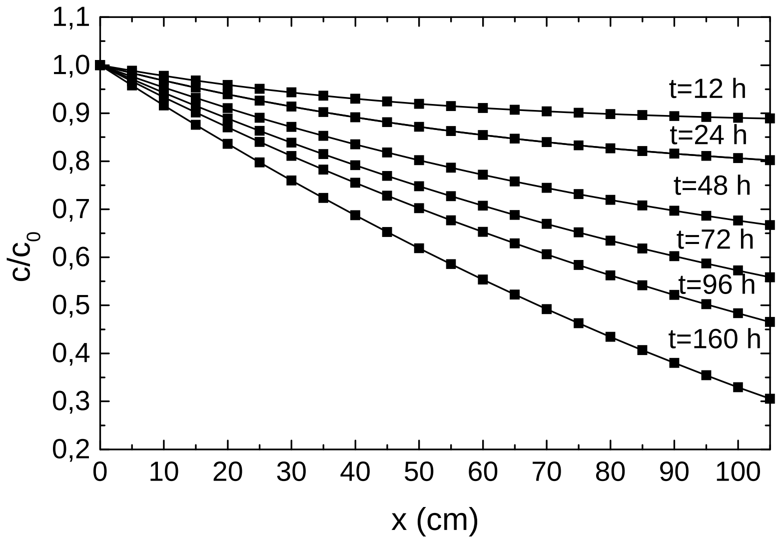

Figure 2. Relative oxygen concentration vs. depth of the soil column at different diffusion times for constant air oxygen concentration C_0=0.21 cm^3 cm^{-3}. Solid squares represent analytical solution (4).

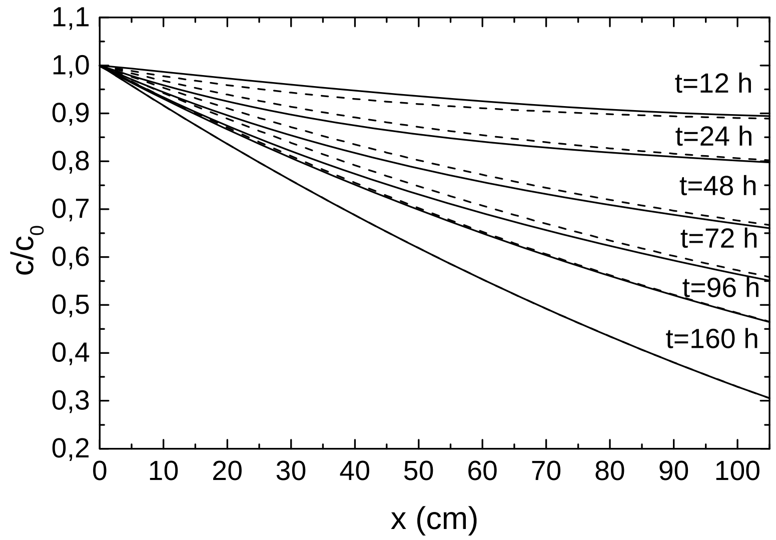

Figure 3. Relative oxygen concentration vs. depth of the soil column at different diffusion times obtained for periodically changing air oxygen concentration $C(x=0,t)=C_0\cdot(1+\varepsilon\sin(2\pi t/T))$, *$C_0$ = 0.21 cm^3 cm^{-3}, ε = 0.05 and T = 24 h (solid line) and for constant air oxygen concentration C_0 = 0.21 cm^3 cm^{-3} (dashed line).*

5. CONCLUSION

Diffusion of oxygen in the soil is investigated based on a simple diffusion equation. By solving the diffusion equation using the explicit finite difference method, the oxygen concentration profiles inside the soil column are determined for various periods of time. Two different cases are investigated, with constant and periodically changing air oxygen concentration. We have inferred that the influence of a daily periodical change of the air oxygen concentration on the oxygen concentration in the soil is more pronounced for smaller diffusion times at smaller lengths of the soil profile. Finally, we have shown that the explicit finite difference method is effective and accurate for solving the equation that describes the oxygen diffusion in the soil, which is especially important when arbitrary initial and boundary conditions are required.

6. ACKNOWLEDGMENT

The work described in this paper was supported by the Strategic Research Grant of City University of Hong Kong (Project No. CityU 7004069) and by a grant from the Serbian Ministry of Education, Science and Technological Development (Project No. 171011, 171021, 44002).

7. REFERENCES

[1] D. Hillel, *Fundamentals of Soil Physics*, Academic Press, New York 1980.

[2] J. C. Refsgaard, T. H. Christensen, H. C. Ammentrop, *A model for oxygen transport and consumption in the unsaturated zone*, J. Hydrol., Vol. 129 (1991) 349–369.

[3] R. S. Kanwar, S. Mukhtar, P. Singh, *Transient state oxygen diffusion through undisturbed soil columns*, Trans. ASAE 32 (1989) 1644–1650.

[4] C. H. Huang, Y. Ouyang, J. En. Zhang, *Effects of a compact layer on soil O_2 diffusion*, Geoderma, Vol. 135 (2006) 224–232.

[5] J. Letey, L. H. Stolzy, N. Valoras, T. E. Szuskiewicz, *Influence of soil oxygen on growth and mineral concentration of barley*, Agron. J., Vol. 54 (1962) 538–540.

[6] A. E. Erickson, *Tillage effects on soil aeration*, In: Predicting Tillage Effects on Soil Physical Properties and Processes, ch. 6. Am. Soc. Agron., Madison, WI (1982) 91–104.

[7] R. I. Papendick, J. R. Runkles, *Transient state oxygen diffusion in soil: I. The case when rate of oxygen consumption is constant*, Soil Sci., Vol. 100 (1965) 251–261.

[8] R. S. Kanwar, *Analytical solutions of the transient-state oxygen diffusion equation in soil with a production term*, J. Agron. Crop. Sci., Vol. 156 (1986) 101–109.

[9] P. K. Kalita, *Transient finite element method solution of oxygen diffusion in soil*, Ecol. Modell., Vol. 118 (1999) 227–236.

[10] S. Savović, J. Caldwell, *Finite difference solution of one-dimensional Stefan problem with periodic boundary conditions*, Int. J. Heat Mass Transfer, Vol. 46 (2003) 2911–2916.

[11] S. Savović, J. Caldwell, *Numerical solution of Stefan problem with time-dependent boundary conditions by variable space grid method*, Thermal Science, Vol. 13 (2009) 165–174.

[12] J. D. Anderson, *Computational Fluid Dynamics*, McGraw-Hill, New York 1995.

НУМЕРИЧКО РЕШЕЊЕ ДИФУЗИОНЕ ЈЕДНАЧИНЕ ЗА ДИФУЗИЈУ КИСЕОНИКА У ЗЕМЉИ

Сажетак: Решавајући дифузиону једначину користећи експлицитни метод коначних разлика, одређене су концентрације кисеоника у земљи за различита времена дифузије. Испитивана су два различита случаја, са константним и дневно-промењљивим концентрацијама кисеоника у ваздуху. Добијено је да је утицај периодичне промене концентрације кисеоника у ваздуху на концентрацију кисеоника у земљи израженији код краћих времена дифузије на мањим дубинама у земљи.

Кључне речи: дифузија кисеоника, земља, дифузиона једначина, експлицитни метод коначних разлика.