

A DYNAMIC MODELING OF THE PH OF SOILS AROUND ROOTS OF PLANTS

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Abstract. The relations between nutrients uptake, metabolism of the plants and pH are central in the study of the nutrition of plants and in particular the pH of the soil near the roots of plants has a great effect on different processes that occurs in the root rhizosphere. This work examines the capacity by the roots to change the pH of the soil around the roots by means of the formulation of a model of convection-diffusion for a growing root system. Unlike previous models (Nye, *Plant and Soil*, 61:7-26 (1981); Kim and Silk, *Plant, Cell & Environment*, 22: 1527-1538 (1999)), the model is formulated through a one-dimensional moving boundary model. The same is solved by immobilization of the domain and application of the finite element method. Using typical experimental values predictions for the profile of pH between the root surface and the outer edge of the rhizosphere versus the time as a function of typical parameters as the Peclet number and the initial pH of the soil are obtained. The obtained graphs show similar values in the magnitude of the change of pH predicted by previous models although a greater acidified volume is predicted as consequence of the increase of root density of the radical system.

1 INTRODUCTION

The relations between nutrients uptake, metabolism of the plant and pH of the soil are central in the study of the nutrition of plants. The capacity by the roots to change the pH of the soil in its vicinity affects the uptakes of beneficial nutrients like phytotoxic. It has been observed that the roots tend to acidify alkaline media as a calcareous soil as well as they can elevate the pH of acid media (Jenny and Overstreet, 1939), (Bledsoe and Zasoski, 1983). In fact, the interchange theory (Riley and Barber, 1971) proposed that the roots absorb cations from colloids of the soil interchanging them in their surface by provided protons by the root in order to balance the excess of influx of cations on anions and vice versa. Nye and colleagues (1981) developed a theory to predict the profiles of pH induced by the plant in the rhizosphere. Assuming that the ions hydrogen diffuse according to a modified Fick's law, Nye uses an analytical solution (Carslaw and Jaeger, 1959) for the diffusion equation in fixed domain with flow on the surface of a cylinder to find the pH as a logarithm function of the distance, r , from the surface of the root and the time t . The model of Nye with time predicts great effects on the pH profiles from initial values of pH and water content and a logarithmic dependency. The gradients of predicted pH are deep in the rhizosphere, whose extension is predicted so much as 0,5 to 3 mm from the surface of the root, particularly if the diffusion coefficient of acidity and the power buffer is low. Also, Kim and Silk (1999) have studied the pH profiles radially and longitudinally from the apex of a growing root having found through their predictions that the pH profile becomes stationary after 6 hours. In this work we propose to study the variation of the profiles of soil pH but considering the soil available to each root by means of the formulation of a moving boundary model (Reginato et al., 2000). To the aims to obtain a simplified model we only considers efflux and transport of protons $[H^+]$ in soil leaving the study of the effect of anions $[HCO_3^-]$ for a later study.

2 DEVELOPMENT OF THE MODEL

A fixed volume of soil in which our radical system is distributed like a homogenous piling up by roots is assumed. The equation of diffusive and convective transport of ions released (protons) from the root in cylindrical coordinates is:

$$\frac{\partial[H^+](r,t)}{\partial t} = \frac{\partial^2[H^+](r,t)}{\partial r^2} + \left(1 + \frac{s_o v}{D\theta f}\right) \frac{1}{r} \frac{\partial[H^+](r,t)}{\partial r} \quad (1)$$

where $[H^+](r,t)$ is th proton concentration, v is the speed of convective flow, D is the diffusion coefficient, θ is the water content of the soil and f is a tortuosity factor. The equation (1) can be noted:

$$[H^+]_t = D_e [H^+]_{rr} + D_e (1 + Pe) \frac{[H^+]_r}{r} \quad (2)$$

where $Pe = \frac{s_0 v}{D \theta f} = \frac{s_0 v}{D_e}$ is the Peclet number, $[H^+]_t = \frac{\partial [H^+](r, t)}{\partial t}$, $[H^+]_r = \frac{\partial [H^+](r, t)}{\partial r}$, $[H^+]_{rr} = \frac{\partial^2 [H^+](r, t)}{\partial r^2}$ and the product $D \theta f = D_e$ is the effective diffusion coefficient. For the boundary condition in the outer edge of rhizocylinder of our problem and whose radius is $R(t)$ prevails a null flow (i.e., they cannot leave protons nor enter protons released by neighboring roots) and for the condition on root surface the same condition of efflux of protons like the proposal by Nye is assumed:

$$-D_e [H^+]_r(s_0, t) - v [H^+](s_0, t) = F \tag{4}$$

where F is the efflux of protons. As our radical system increases its length (increases the roots density) the radius of rhizocylinder available to each root decreases with time according to Reginato, 2000:

$$R(t) = R_0 \sqrt{\frac{l_0}{l(t)}} \tag{5}$$

Finally our first approach of the problem, but now in variable domain, is given by the following moving boundary model:

$$\begin{aligned} [H^+]_t &= D [H^+]_{rr} + D_e (1 + Pe) \frac{[H^+]_r}{r}, & 0 < r < R(t), & 0 < t < T \\ [H^+](r, 0) &= [H^+]_0(r), & 0 \leq r \leq R(0) = R_0 \\ [H^+]_r(R(t), t) &= 0, & 0 < t < T \\ -D_e [H^+]_r(s_0, t) - v [H^+](s_0, t) &= F, & 0 < t < T \\ R(t) &= R_0 \sqrt{\frac{l_0}{l(t)}}, & 0 < t < T \end{aligned} \tag{6}$$

In order to obtain the solution of the problem (1.6), previously we propose the following change of variables:

$$\begin{aligned} [H^*](r^*, t^*) &= \frac{v_0}{F} [H^+](r, t), & r^* &= \frac{r - s_0}{R(t) - s_0}, & t^* &= \frac{v_0^2}{D} t, \\ l^*(t^*) &= \frac{l(t)}{s_0}, & R^*(t^*) &= \frac{R(t)}{s_0} = \frac{R_0}{s_0} \sqrt{\frac{l_0}{s_0}} \frac{1}{\sqrt{l^*(t^*)}} \end{aligned} \tag{7}$$

With this change of variables, our problem (6) in variable domain is transformed in an adimensionless and fixed boundary model, which is given by:

$$\begin{aligned}
 [H^*]_{t^*} &= \frac{1}{Pe^2} \frac{[H^*]_{r^*,t^*}}{[R^*(t^*)-1]^2} + \left[r^* \frac{dR^*}{dt^*} + \frac{(1+Pe)}{Pe^2} \frac{1}{1+r^*[R^*(t^*)-1]} \right] \frac{[H^*]_{r^*}}{[R^*(t^*)-1]}, \\
 & \quad 0 < r^* < R^*(t^*), 0 < t^* < T^* \\
 [H^*](r^*, 0) &= [H_o^*](r^*), \quad 0 \leq r^* \leq R^*(0)=1 \\
 [H^*]_{r^*}(1, t^*) &= 0 \quad 0 < t^* < T^* \\
 [H^*]_{r^*}(0, t^*) &= -Pe[R^*(t^*)-1][1+[H^*](0, t^*)], \quad 0 < t^* < T^* \\
 R^*(t^*) &= \frac{R_o}{s_o} \sqrt{\frac{l_o}{s_o} \frac{1}{\sqrt{l^*(t^*)}}}, \quad 0 < t^* < T^*
 \end{aligned} \tag{8}$$

The solution to our problem (8) is obtained by through of the finite element method (FEM), which was implemented in this first approach to the problem by means of software FlexPDE (<http://www.pdesolutions.com>). For the simulation, data was extracted from literature (Nye, 1981, Kim, 1999) according to the following table (Table 1):

Parameter	Value	Dimension s
Simulation period	259200 (30 days)	sec
Root radius (s_o)	0.05	cm
Initial root length (l_o)	7.05	cm
Rhizosphere radius (R_o)	2	cm
Velocity of convective flux (v_o)	1×10^{-5}	cm/s
Velocity or root growth (k_i) [$l(t) = l_o + k_i t$]	6.66×10^{-5}	cm/s
Proton efflux from the root (F)	3×10^{-12}	mol/cm ² -s
Effective diffusion coefficient (D_e) (slow diffusion) $Pe=2.5$ (fast diffusion) $Pe=0.0053$	2×10^{-7} 9.4×10^{-5}	cm ² /s
Initial concentration of protons according initial pH ([H ⁺]) pH = 6.8 (neutral soil) pH = 8 (soil moderately alkaline)	1.5849×10^{-10} 1×10^{-11}	mol/cm ³

Table 1: Input parameters

3 RESULTS AND CONCLUSIONS

Once we have obtained the proton concentrations $[H^+]$ we obtain the pH like $\log [1/[H^+]]$, where \log is \log_{10} and $[H^+] = 10^3 F[H^*]/v_0$ (in order to obtain our physical proton concentration in Molar from the dimensionless concentration). The factor 10^3 results from the transformation of moles/cm³ to molar)

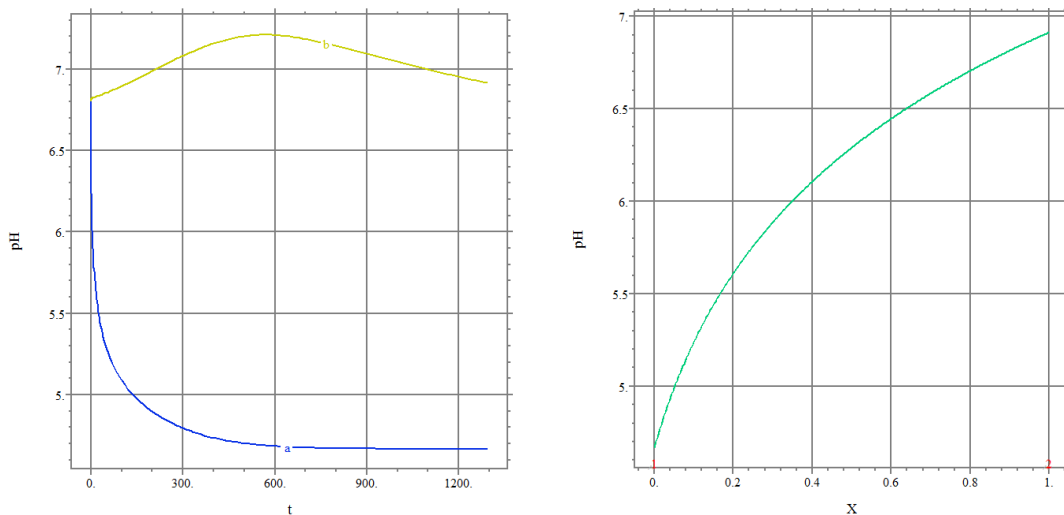


Figure 1. Variation of the pH in $r = s_0$ (blue) and $r = R(t)$ (yellow) versus the time, and the final profile between s_0 and $R(t)$ (after the three days and in dimensionless domain) being both graphs for a neutral soil (initial pH = 6,8) and slow diffusion ($D_e = 2 \times 10^{-7} \text{ cm}^2/\text{s}$)

The simulations run for neutral soils (pH = 6.8) and slow diffusion ($D_e = 2 \times 10^{-7} \text{ cm}^2/\text{s}$) for a time of 30 days and during which the rhizosphere radius has been reduced approximately to half (from 2 to 1 cm) show a noticeable acidification on the root of approximately 2 units and which becomes stationary after almost two days, while the profile of the pH between the root and the rhizosphere edge is distributed in all the radial distance (Figure 1). These results are similar to those of Nye [4] although with an acidification more homogenous in all the profile between the root and the rhizosphere edge $R(t)$ which is decreasing. This difference in the pH profiles is owing to the Nye's results has been obtained for an infinite rhizosphere. For the same soils and fast diffusion ($D_e = 9,4 \times 10^{-5} \text{ cm}^2/\text{s}$), variations of pH significantly smaller are obtained (Figure 2) and again the acidification profile is distributed in all the radial length of the rhizosphere.

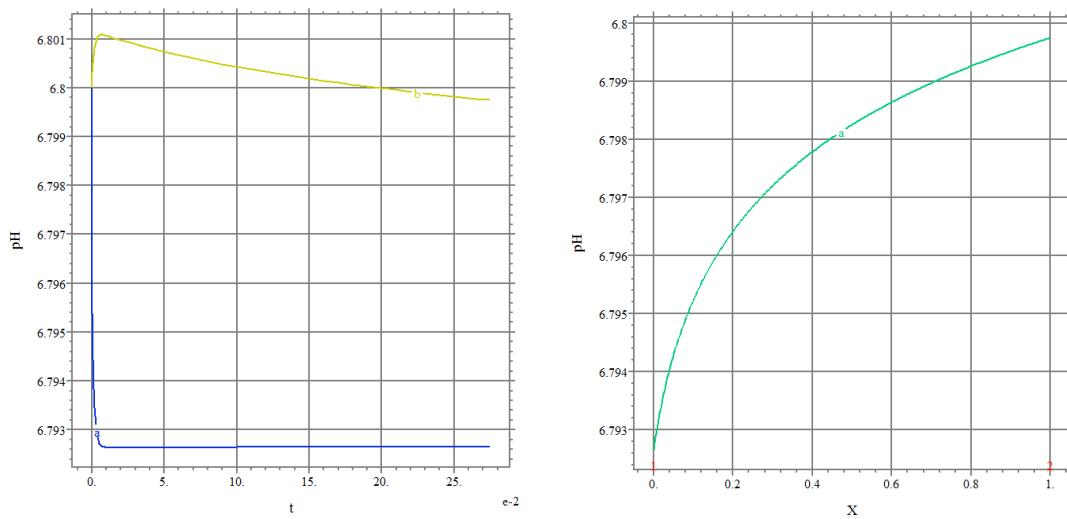


Figure 2. Variation of the pH in $r = s_0$ (blue) and $r = R(t)$ (yellow) versus the time and the final profile between s_0 and $R(t)$ (dimensionless domain) being both graphs for a neutral soil (pH = 6,8) and fast diffusion ($D_e = 9,4 \times 10^{-5} \text{ cm}^2/\text{s}$)

In Figure 3 are shown analogous results to the obtained in the Figure 1 but for moderately alkaline soils (initial pH = 8) and slow diffusion.

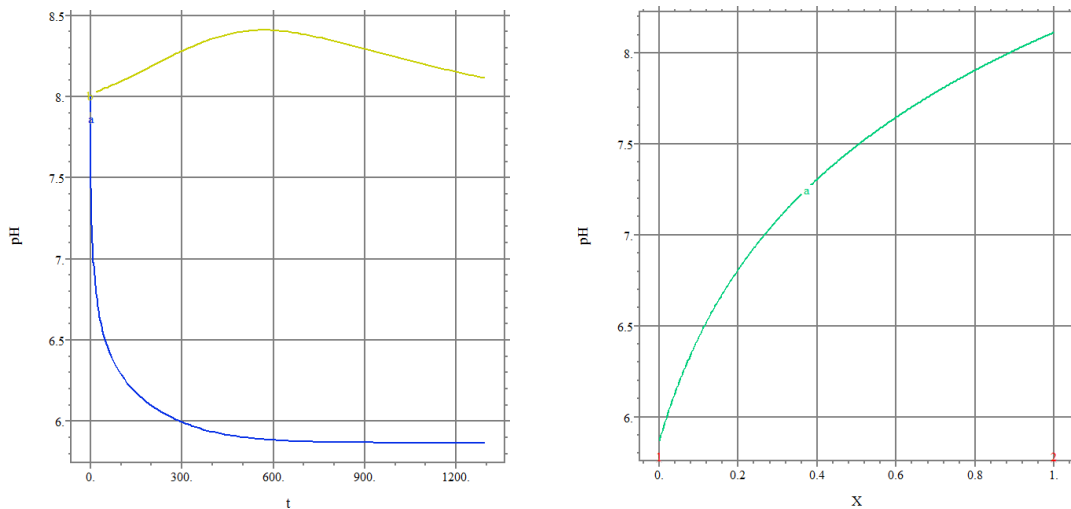


Figure 3. Variation of the pH in $r = s_0$ (blue) and $r = R(t)$ (yellow) versus the time, and the final profile between s_0 and $R(t)$ (after 30 days for the dimensionless domain) being both graphs for a moderately alkaline soils (initial pH = 8) and slow diffusion ($D_e = 2 \times 10^{-7} \text{ cm}^2/\text{s}$)

In Figure 4 the variation of the radius of rhizocylinder below which the soil is acidified (with a smaller pH to the initial) and the variation of the half-distance between roots $R(t)$ versus the time are shown simultaneously. As it can be appreciated of the same, of the volume of soil available to time t , a part acidifies, another one remains neutral (conserves the initial pH) and other is alkalized although after three days the neutral zone disappears and only the acidified and the alkalized zones remains, of which the last one is reduced as the root density

increases ($R(t)$ decreases) while the acidified zone is increasing until practically to include all the soil available to each root. These conclusions are valid for a homogenous occupation of the soil by the roots.

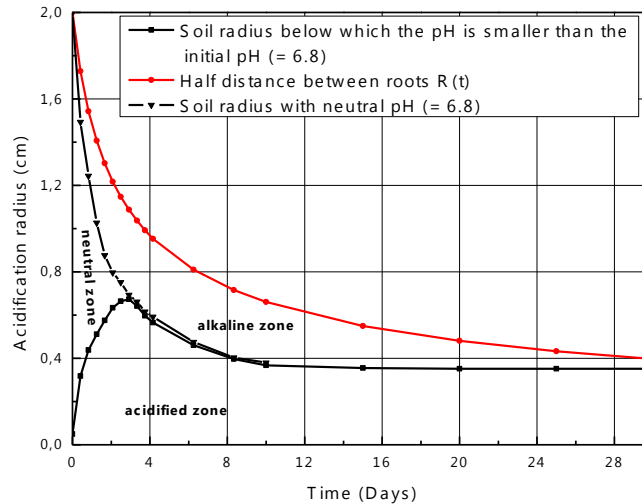


Figure 4. Variation of the distance from the axis of the root below which the soil is acidified versus the time for a neutral soil (initial pH = 6,8) and slow diffusion ($D_e = 2 \times 10^{-7} \text{ cm}^2/\text{s}$)

In Figure 5 the variation of the fraction of volume of soil acidified with respect to the volume of soil available to each root versus the time is shown.

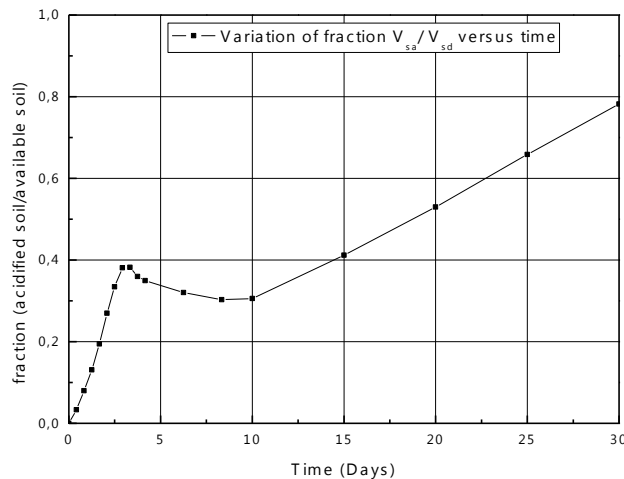


Figure 5. Variation of the fraction of volume of acidified soil (V_{sa}) with respect to the volume of available soil (V_{sd}) versus the time for a neutral soil (initial pH = 6,8) and slow diffusion ($D_e = 2 \times 10^{-7} \text{ cm}^2/\text{s}$)

Again, figure 5 shows that the zone of acidification is distributed in more homogenous form between the surface of the root and the outer edge of the rhizocylinder than the predicted one's by the model of Nye showing that modeling with a variable rhizosphere has a significant effect in the degree in which others factors in the rhizosphere like the bioavailability of nutrients and toxic elements,

physiology of the root and microorganisms can be affected. For example, phosphorus is the least mobile major nutrient in many soils and is frequently the prime limiting factor for plant growth in terrestrial and aquatic ecosystems. Many studies have tried to model P bioavailability, i.e. the actual flux of P taken up by the plant. Barber (1995) showed that the concentration of P in soil solution which is made available for the plant was the second variable controlling P bioavailability, after root elongation rate. However those models systematically underestimate P uptake by plants under conditions of low P supply (Mollier et al., 2008). This failure to predict P bioavailability may be caused by the use of the P availability obtained for bulk soil chemistry in such models, with little account of rhizosphere chemistry. Roots and microorganisms are however well known to induce dramatic chemical changes in the rhizosphere, which ultimately determine P uptake. For inorganic P, a number of chemical properties of soils, such as pH, concentrations of inorganic ligands, redox potential, and ionic strength can indeed alter P availability in the rhizosphere (e.g. Hinsinger, 2001). Many studies have measured changes of some of those chemical parameters in the rhizosphere and attempted to relate them to P bioavailability. Amongst them, a major chemical change observed in the rhizosphere is a pH variation which can reach up to several units as measured by Solaiman et al (2007) for wheat plants in response of low P supply. Even the few models which considered root-induced chemical changes failed at adequately predicting P uptake by plants (Kirk, 2002). Thus, our model can contribute to a more quantitative explanation of the effect of the pH on the availability of P taking into account the soil occupation model (given by the variable rhizosphere radius $R(t)$) by the radical system.

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