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Mathematical Modeling of Pollutant Uptake by the Plant Root from the Soil

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Abstract. The classical model of plant root nutrient uptake given by Roose is modified and extended for pollutant uptake in plants. An explicit closed mathematical description is given for the pollutant uptake, by a single cylindrical root for all cases of practical interest, by solving the absorption-diffusion equation for the soil pollutant concentration asymptotically in the limit of large time. The theoretical results derived analytically.

Keywords: Pollutant uptake, ***a***bsorption-diffusion equation, mathematical model

AMS Mathematics Subject Classification (2010): 76Rxx, 76Sxx, 76Txx, 97M60

1. Introduction

The primary physiological function of root is uptaking the water as well as nutrients and transport to leaves for photosynthesis. Investigations and observation of the uptake of water and nutrient in plant root and stem can be traced back to many years ago, it possesses importance in point of view of agricultural production and economical development. Now a new trend of planting inedible plant emerge on industrial basis. The view of planting inedible plant are prevent the salinization, desertification of soil, to clean pollution of heavy metals, radioelement and plant's mining. To collect the valuable metals, like gold, in soil by planting some plants whose roots possess a special capability of absorbing the valuable metals. The plant of genus Bauhina have many species out of which Bauhinia variegata plant extract is analysed and found it contain micro-particles of gold [11]. Since ancient times Bauhinia racemosa Lam. family: Caesalpinaceae has been an integral part of life in India. Leaves of Bauhinia racemosa are traditionally used on occasion of Dashera festival as symbol of gold in India [3]. Recently proved that Bauhina racemosa extract also contain micro particles of gold.

In recent years, a number of researchers from various fields, such as physics, applied mathematics and plant physiology, paid more attention to develop mathematical model for water and nutrient uptake. The outstanding work in this field is done by T.Roose and proposed a mathematical model for uptake of water and nutrient. Roose work is development of Nye, Tinker and Barber model for water and nutrient uptake assuming that the root is an infinitely long cylinder [2,8,9,10].

It is also found that the plant root also uptake pollutant from the soil. The aim of the paper is to investigate relations between pollutant gradient in soil and its accumulation in plants through cylindrical roots.The classical model for uptake developed by T.Roose supposes a single cylindrical root to be surrounded by an infinite extent of soil, with prescribed far field soil water concentration. The pollutant diffuses through the soil water (via the pore water), and its uptake at the root is given by a Michaelis-Menten dependence on concentration (Jungk et al., 1997; Jensen, 1992). This absorption-diffusion model thus consists of a linear diffusion equation with the nonlinear root surface absorption condition [12]. In this paper we deal with this problem by providing a fully explicit approximation to the basic T.Roose model.

2. Pollutant uptake by a single root from a continuum soil

2.1. Model formulation

We assume that the soil consists of a solid phase, a liquid phase and a gas phase, and that the volume fraction of each phase stays constant, so,[1]

$$\theta_s + \theta_l + \theta_a = 1 \tag{1}$$

where θ_s is the volume fraction of the soil solid phase, θ_l is the volumetric water content and θ_a is the volume fraction of the air phase. The sum of θ_l and θ_a is the soil porosity Î¦. Typical values of Î¦ are 0.3-0.6 and typical values for θ_l in soils are 0.15 â€“ 0.4 (Richardson, 1995). We assume that pollutant is present in the solid (C_s) and liquid (C_l) phase and the total concentration of pollutant in soil $(C_T; soil)$ is

$$C_{T,Siol} = C_s + \theta_l C_l \tag{2}$$

Assuming equilibrium sorption according to a linear Freundlich isotherm and neglecting intra particle diffusion, the rate of change of C_s with respect to t is (Tinker, 1975, Morton et al.1994)

$$\frac{\partial C_s}{\partial t} = b_p \frac{\partial C_l}{\partial t} \tag{3}$$

where b_p is the buffer power of the soil. For a volume of soil V without internal sources or sinks, the conservation law gives

$$\theta \frac{\partial C_l}{\partial t} + \nabla . q = 0 \tag{4}$$

where the flux q is derived by assuming diffusive and convective transport and given by Fick's law that describes the movement of solutes in the direction of decreasing concentration gradient

$$q = -D_l \theta_l f_l(\theta_l) \nabla . C_l \tag{5}$$

where D_l is the diffusion coefficient of the solute in free water, $f_l(\theta_l)$ is the impedance factor of solute in the liquid phase and v is the Darcy flux.

$$\frac{\partial(\theta_l C_l)}{\partial t} = \nabla(\theta_l D_l f_l \nabla . C_l) - \nabla . (v C_l) \tag{6}$$

The rate of change of $C_{T;soil}$ with time is given by:

$$\frac{\partial(b_p + \theta_l) C_l}{\partial t} = \nabla(\theta_l D_l f_l \nabla . C_l) - \nabla . (v C_l) \tag{7}$$

2.2. Boundary condition

Taking initial concentration $C_{l,0}$(Î¼$molcm^{-3}$) in soil solution as constant and assuming the uptake of pollutant at the root surface follows Michaelis-Menten kinetics, the conditions at the root surface will be

$$C_l = C_{l,0} \text{ at } t = 0$$

$$\theta_l f_l D_l \frac{\partial C_l}{\partial n} - v_n C_l = \frac{F_m C_l}{K_m + C_l}$$

where $\frac{\partial}{\partial n}$ is the operator for the outward normal derivative, v_n is the Darcy flux of water normal to the root surface, F_m(Î¼$molcm^{-2}s^{-1}$) is the maximal root uptake rate and K_m(Î¼$molcm^{-3}$) is the Michaelis Menten constant.

If there is no competition between roots then concentration far away from the root surface stays constant. So, the boundary condition far away from the root surface will be

$C_i = C_{l,0}$ at $|x| \to \infty$

For simulating radial flow into a cylindrical root, the model is

$$(b_p + \theta_l)\frac{\partial C_1}{\partial t} = \theta_l D_l f_l \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_1}{\partial r}\right) + \frac{v_0}{r}\frac{\partial C_1}{\partial r} \quad (8)$$

$$\theta_l f_l D_l \frac{\partial C_l}{\partial r} - q_0 C_l = \frac{F_m C_l}{K_m + C_l}, r = r_0 \quad (9)$$

$$C_l = C_{l,0}, r = r_l \quad (10)$$

where r_0 is the radius of the root, r_1 is the half distance between two roots ($r_1 = 1/\sqrt{\pi\rho}$, where Ï is root length density) and v_0 is the Darcy flux of water into the root surface (Fowler, 1997; Varney et al. 1993).

let $r = r_0 r^*, t = \frac{r_0^2(b_p+\theta_l)}{\theta_l D_l f_l} t^*$ and $C_l = K_m C^*$

Then the non-dimensional model is (dropping asterisks)

$$\frac{\partial C}{\partial t} - \frac{P_e}{r}\frac{\partial C}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right) \quad (11)$$

$$\frac{\partial C}{\partial r} + P_e C = \frac{\lambda C}{1+C} \;\; on \;\; r = r_0 \quad (12)$$

$$C \to C_\infty \;\; as \;\; r \to \infty \quad (13)$$

Hence dimensionless parameters are Peclet number, $P_e = \frac{r_0 v_0}{D_l f_l \theta_l}$,uptake parameter $\lambda = \frac{F_m r_0}{K_m D_l f_l \theta_l}$ and concentration in soil $C_\infty = \frac{C_{l,0}}{K_m}$.

2.3. Initial condition and boundary condition

Initial condition can be write as for $t = 0$

$$c = c_0 \;\; at \;\; t = 0 \;\; for \;\; a < r < \infty \quad (14)$$

for later time

$$c \to c_0 \;\; as \;\; r \to \infty \;\; for \;\; t > 0 \quad (15)$$

3. Approximate solutions

At $P_e << 1$, neglecting convective transport, the model becomes

$$\frac{\partial C}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right) \quad (16)$$

with boundary condition

$$\frac{\partial C}{\partial r} = \frac{\lambda C}{1+C} \;\; on \;\; r = r_0 \quad (17)$$

$$C \to C_\infty \;\; as \;\; r \to \infty \quad (18)$$

and initial conditions

$$c = c_0 \;\; at \;\; t = 0 \;\; for \;\; a < r < \infty \tag{19}$$

4. Pollutant uptake equation with $c_\infty << 1$ and $P_e << 1$

In this section we consider P_e and c_∞ are negligible. If Michaelis-Menten coefficient K_∞ much larger than the far field concentration $c_{0,}$ i.e., $c_\infty << 1$, the equation (16) reduces to the form[7]

$$\frac{\partial c}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right). \tag{20}$$

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial r^2} + \frac{1}{r}\frac{\partial c}{\partial r}. \tag{21}$$

Corresponding boundary condition reduces to the form

$$\frac{\partial c}{\partial r} = \lambda\frac{c}{1+c}, \tag{22}$$

re-scaling $c = c_\infty C$ then the model in scaled concentration is written as

$$\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial r^2} + \frac{1}{r}\frac{\partial C}{\partial r}, \tag{23}$$

scaled boundary condition are as follows

$$\frac{\partial C}{\partial r} = \lambda\frac{C}{1+c_\infty C}, \;\; r = 1 \;\; and \;\; C \to 1 \;\; as \;\; r \to \infty. \tag{24}$$

for $c_\infty << 1$ we can approximate the root surface boundary condition, using the binomial expansion,at the leading order given by

$$\frac{\partial C}{\partial r} \approx \lambda C \; at \; r = 1. \tag{25}$$

Initial condition scaled in following manner

$$C = 1 \;\; at \;\; t = 0 \;\; for \;\; 1 < r < \infty. \tag{26}$$

We solve the above boundary value problem by separation of the variables. Substituting the substitution $C(r,t) = T(t)U(r)$ the value in equation(23) we have

$$\frac{1}{U}\left[\frac{\partial^2 U}{\partial r^2} + \frac{1}{r}\frac{\partial U}{\partial r}\right] = \frac{1}{T}\left[\frac{\partial T}{\partial t}\right] = -\beta^2. \tag{27}$$

Now consider the boundary value problem

$$\frac{\partial^2 U}{\partial r^2} + \frac{1}{r}\frac{\partial U}{\partial r} + \beta^2 U = 0. \tag{28}$$

With the boundary condition

$$\frac{dU}{dr} - \lambda U = 0. \tag{29}$$

The complete solution is given by, see [4],

$$C(r,t) = \int_{\beta=0}^{\infty}\frac{\beta}{N(\beta)}e^{-\beta^2 t}U(\beta,r)d\beta\int_{r=1}^{\infty} r'U(\beta,r')dr', \tag{30}$$

where $U(\beta_m, r)$ is eigenvalue function.

$$U(\beta,r) = J_0(\beta r)[\beta Y_1(\beta) + \lambda Y_0(\beta)] - Y_0(\beta r)[\beta J_1(\beta) + \lambda J_0(\beta)]. \tag{31}$$

$$N(\beta) = [\beta J_1(\beta) + \lambda J_0(\beta)]^2 + [\beta Y_1(\beta) + \lambda Y_0(\beta)]^2. \tag{32}$$

So the general solution of equation is given by

$$c(r,t) = c_\infty\int_{\beta=0}^{\infty}\frac{\beta}{N(\beta)}e^{-\beta^2 t}U(\beta,r)d\beta\int_{r=1}^{\infty} r'U(\beta,r')dr'. \tag{33}$$

5. Pollutant uptake equation with $\lambda << 1$

Equation (11) write as

$$\frac{\partial c}{\partial t} - (\frac{P_e+1}{r})\frac{\partial c}{\partial r} = \frac{\partial^2 c}{\partial r^2}, \tag{34}$$

implies

$$\frac{\partial c}{\partial t} = (\frac{P_e+1}{r})\frac{\partial c}{\partial r} + \frac{\partial^2 c}{\partial r^2}, \tag{35}$$

re-scaling with $r = (1 + P_e)R$, then $\partial r = (1 + P_e)\,\partial R$. Then equation (34) become

$$(1 + P_e)\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial R^2} + \frac{1}{R}\frac{\partial c}{\partial R}, \tag{36}$$

Corresponding boundary condition changes

$$\frac{\partial c}{\partial R} + (1 + P_e)P_e c = \lambda(1 + P_e)[\frac{c}{1+c} - \varepsilon],\ at\ \ R = \frac{1}{1+P_e}, \tag{37}$$

for $\lambda = \frac{F_m a}{D K_m \Phi_l}$ value of λ with large value of ϕ and small radius R we have

$$\lambda \equiv 0. \tag{38}$$

Then the boundary condition becomes

$$\frac{\partial c}{\partial R} + (1 + P_e)P_e c = 0, \tag{39}$$

Consider $c(R, t) = U(R)T(t)$ substituting in (36) and (39) then it becomes

$$\frac{1}{T}(1 + P_e)\frac{\partial T}{\partial t} = \frac{1}{U}[\frac{\partial^2 U}{\partial R^2} + \frac{1}{R}\frac{\partial U}{\partial R}], \tag{40}$$

corresponding boundary condition becomes

$$\frac{\partial U}{\partial R} + (1 + P_e)P_e U = 0. \tag{41}$$

From the equation (36) we can write

$$\frac{1}{T}(1 + P_e)\frac{\partial T}{\partial t} = \frac{1}{U}[\frac{\partial^2 U}{\partial R^2} + \frac{1}{R}\frac{\partial U}{\partial R}] = -\beta^2. \tag{42}$$

We have the Bessel equation with boundary condition

$$\frac{\partial^2 U}{\partial R^2} + \frac{1}{R}\frac{\partial U}{\partial R} + \beta^2 U = 0. \tag{43}$$

$$\frac{\partial U}{\partial R} + (1 + P_e)P_e U = 0,\ at\ \ R = \frac{1}{1+P_e} \tag{44}$$

and

$$\frac{\partial T}{\partial t} = -\frac{\beta^2}{1+P_e}T. \tag{45}$$

$$c = c_\infty \;\; at \;\; t = 0 \;\; as \;\; 1 < R < \frac{1}{1+P_e} \tag{46}$$

Solution of Bessels equation is given by,

$$U(\beta, R) = J_0(\beta R)[\beta Y_1(\beta \frac{1}{(1+P_e)}) + P_e(-1 - P_e)Y_0(\beta \frac{1}{(1+P_e)})]$$
$$-Y_0(\beta R)[\beta J_1(\beta \frac{1}{(1+P_e)}) + P_e(-1 - P_e)J_0(\beta \frac{1}{1+P_e})], \tag{47}$$

also

$$N(\beta) = [\beta J_1(\beta \frac{1}{(1+P_e)}) + (-1 - P_e)J_0(\beta \frac{1}{(1+P_e)})]^2$$
$$+[\beta Y_1(\beta \frac{1}{(1+P_e)}) + (-1 - P_e)Y_0(\beta \frac{1}{(1+P_e)})]^2. \tag{48}$$

Replacing R by $R = \frac{r}{(1+P_e)}$ in equation (47).
Above solution of Bessels equation become

$$U(\beta, r) = J_0(\beta \frac{r}{(1+P_e)})[\beta Y_1(\beta \frac{1}{(1+P_e)}) + P_e(-1 - P_e)Y_0(\beta \frac{1}{(1+P_e)})]$$
$$-Y_0(\beta \frac{r}{(1+P_e)})[\beta J_1(\beta \frac{1}{(1+P_e)}) + P_e(-1 - P_e)J_0(\beta \frac{1}{1+P_e})]. \tag{49}$$

Then the complete solution is given by, see [4]

$$c(r,t) = \int_{\beta=0}^{\infty} \frac{\beta}{N(\beta)} e^{-\frac{1}{(1+P_e)}\beta^2 t} U(\beta, r) d\beta \int_{r'=1}^{\infty} r' U(\beta, r') c_\infty dr'. \tag{50}$$

Amount of pollutant absorb by root is given as, [5][6]

$$M = 2\pi r t \frac{\partial c}{\partial t}. \tag{51}$$

6. Discussion

The pollution in the environment occur in the soil and atmosphere. In the both phase plant absorb the pollutant and maintain the quality of soil i.e of water and air. Soil pollutant affect the quality of water. To increase purity of water there is no other convenient way to purify the soil. In this paper we try to developed the mathematical model for pollutent uptake by plant root assuming that Michaelis-Menten boundary condition hold. The above described expression hold if flow is not turbulent flow occurring at higher velocities. In the first section, we have calculated the pollutant uptake in case $P_e << 1$ and the case $C_\infty << 1$. Also for ϕ_l is considerable large and Root radius is small the the parameter λ is negligible. In the later section for the negligible value of λ, we also calculated the pollutant uptake by the plant root.

This model is not valued in the soil, where the flow of the pollutant is Laminar and is also not valued water flow is turbulent.

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