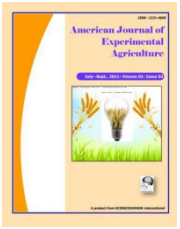

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A Mathematical Description of Pollutant Uptake in Plants by Single Cylindrical Root

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Research Article

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ABSTRACT

The classical model of plant root nutrient uptake given by Nye, Tinker and Barber is modified and extended for pollutant uptake in plants. An explicit closed mathematical description is given for the 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. This single root model can be used as a building block to construct a model for multiple root branching structure in a more realistic plant root system. The theoretical results derived analytically are compared with numerical results and experimental studies.

Keywords: Pollutant uptake; root system; mathematical model;

1. INTRODUCTION

The high concentration of pollutants in soils is reflected by higher concentrations of pollutants in plants, and consequently in animal and human bodies. The ability of some plants to absorb and accumulate xenobiotics makes them useful as indicators of environmental pollution. The study of excessive concentrations of pollutants in biological matrices has been reported in numerous publications (Jensen et al., 1992; Lynch et al., 1997; Marschner, 1995). Pine and spruce needles, mosses and grasses are widely used as a specific indicator in the study of a geographical and temporal pattern of pollutants. Streit and Strum et al. (1993) classified the exchange of chemicals between soil and plants and

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divided the most common methods of assessing toxicity to plants from soil into three categories in the conditions closed system:

(i) monitoring of the presence or absence of specific plant ecotypes and/or plant species (indicator plant),
(ii) measurements of pollutant concentration in tissues of selected species (accumulative bio-indicators),
(iii) recording of physiological and biochemical responses (biomarkers) in sensitive bio-indicators.

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 Nye and Tinker (1997) and Barber (1984) 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. In this paper we deal with this problem by providing a fully explicit approximation to the basic Nye–Tinker–Barber 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,

$$\theta_s + \theta_l + \theta_\alpha = 1 \tag{2.1}$$

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 Φ. Typical values of Φ are 0.3-0.6 and typical values for θ_l in soils are 0.15 – 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

$$C_{T,Soil} = C_s + \theta_l C_l \tag{2.2}$$

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)

$$\frac{\partial C_s}{\partial t} = b_p \frac{\partial C_l}{\partial t} \tag{2.3}$$

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

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

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:

$$q = -D_l \theta_l f_l(\theta_l) \nabla . C_l$$

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.

Hence

$$\frac{\partial(\theta_l C_l)}{\partial t} = \nabla(\theta_l D_l f_l \nabla . C_l) - \nabla . (v C_l) \quad (2.4)$$

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

$$\frac{\partial((b_p + \theta_l) C_l)}{\partial t} = \nabla(\theta_l D_l f_l \nabla . C_l) - \nabla . (v C_l) \quad (2.5)$$

Taking initial concentration $C_{l,0}$ ($\mu mol\ cm^{-3}$) 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

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

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

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 ($\mu mol\ cm^{-2}\ s^{-1}$) is the maximal root uptake rate and K_m ($\mu mol\ cm^{-3}$) 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

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

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

$$(b_p + \theta_l) \frac{\partial C_l}{\partial t} = \theta_l D_l f_l \frac{1}{r} \frac{\partial}{\partial r} (r \frac{\partial C_l}{\partial r}) + \frac{v_0}{r} \frac{\partial C_l}{\partial r}$$

$$\theta_l f_l D_l \frac{\partial C_l}{\partial r} - q_0 C_l = \frac{F_m C_l}{K_m + C_l} \ \ , \ r = r_0 \quad (2.6)$$

$C_l = C_{l,0}, \quad r = r_1$

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 ρ 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)

$$\frac{\partial C}{\partial t} - \frac{P_e}{r}\frac{\partial C}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right) \tag{2.7}$$

$$\frac{\partial C}{\partial r} + P_e C = \frac{\lambda C}{1+C} \quad on \;\; r = r_0 \tag{2.8}$$

$$C \to C_\infty \;\; as \;\; r \to \infty$$

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 $C_\infty = \frac{C_{l,0}}{K_m}$

3. APPROXIMATE SOLUTIONS

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

$$\frac{\partial C}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right) \tag{3.1}$$

$$\frac{\partial C}{\partial r} = \frac{\lambda C}{1+C} \quad on \;\; r = r_0 \tag{3.2}$$

$$C \to C_\infty \;\; as \;\; r \to \infty \tag{3.3}$$

3.1 Numerical Solution

For the numerical solution of Equations (3.1)-(3.3), we use a finite difference scheme with a centered discretisation in space and the θ-method in time (Ezawa et al., 2009). Let h be the step size of a uniform mesh in space, Δt be the time step and $J+1$ be the number of grid points. If $C(jh, n\Delta t) \approx U_j^n$ and $C_\infty(n\Delta t) \approx V_n$. Then the numerical scheme is given by

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \theta\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial U}{\partial r}\right)\right]^{n+1} + (1-\theta)\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial U}{\partial r}\right)\right]^{n} \quad n = 0,1,...N-1 \tag{3.4}$$

Where

$$\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial U}{\partial r}\right)\right] \approx \frac{1}{r_j h}\left[r_{j+\frac{1}{2}}\frac{U_{j+1}-U_j}{h} - r_{j-\frac{1}{2}}\frac{U_j - U_{j-1}}{h}\right] \quad j = 0,1,...J-1$$

The scheme can be rewritten as

$$-\frac{r_{j+\frac{1}{2}}}{r_j}\theta\mu U_{j+1}^{n+1} + \left(1+\frac{r_{j+\frac{1}{2}}+r_{j-\frac{1}{2}}}{r_j}\theta\mu\right)U_j^{n+1} - \frac{r_{j-\frac{1}{2}}}{r_j}\theta\mu U_{j-1}^{n+1} =$$

$$\frac{r_{j+\frac{1}{2}}}{r_j}(1-\theta)\mu U_{j+1}^{n} + \left(1-\frac{r_{j+\frac{1}{2}}+r_{j-\frac{1}{2}}}{r_j}(1-\theta)\mu\right)U_j^{n} + \frac{r_{j-\frac{1}{2}}}{r_j}(1-\theta)\mu U_{j-1}^{n}, \qquad j = 0,1,...J-1 \tag{3.5}$$

where $\mu = \frac{\Delta t}{h^2}$. We solve the tri-diagonal system of equations

$$(1-\theta\mu D)U^{n+1} = (I+(1-\theta)\mu D)U^n + b, \qquad j = 0,1,...J-1 \tag{3.6}$$

I is the (*J* + 1) × (*J* + 1) unit matrix, b is (*J* + 1) ×1 zero-vector used to implement the boundary conditions, *U* is the vector $(U_0;U_1;$ --- $U_J)^T$ and *D* is the differential operator, a tri-diagonal (*J* + 1) × (*J* + 1) matrix whose entries are zero except for

$$\left[\frac{r_{j-\frac{1}{2}}}{r_j}, \frac{r_{j+\frac{1}{2}}+r_{j-\frac{1}{2}}}{r_j}, \frac{r_{j+\frac{1}{2}}}{r_j}\right] \quad \text{at} \qquad j = 0,1,...J-1$$

The first and last rows of matrices $(1-\theta\mu D)$ and $I+(1-\theta)\mu D$ are modified according to the boundary conditions.

The numerical scheme for the initial condition and for flux equation (3.2) will be

$$U_j^0 = 1 \quad j = 0,1,...J-1 \tag{3.7}$$

$$\frac{U_1^{n+1}-U_0^{n+1}}{h} = \lambda\frac{\frac{1}{2}\left(U_1^n+U_0^n\right)}{1+\frac{1}{2}\left(U_1^n+U_0^n\right)} \qquad n = 0,1,...N-1 \tag{3.8}$$

and at every time step, we approximate C_∞ in equation (3.3) with an explicit Euler Scheme.

$$V^{n+1} = V^n + \Delta t\left(\frac{1}{2}\left(U_j^n + U_{j-1}^n\right) - V^n\right) \quad where\ V^0 = 1$$

3.2 Approximate Analytic Solutions

3.2.1 Analytic solutions for the limit $c_\infty < 1$

3.2.1.1 Approximations for λ >> 1

(1) When *λ* >> 1 i.e., pollutant uptake is high, we expect the gradient of pollutant concentration near the root surface to be big i.e.

$$\left.\frac{\partial C}{\partial r}\right|_{r=1} \approx \lambda \rangle\rangle 1 \tag{3.9}$$

Thus, there is a boundary layer near *r = 1* and by rescaling the independent variables *r* and *t* to stretched variables *R* and *T*, i.e., $r = 1 + R/\lambda$ and $t = T/\lambda^2$, the problem reduces to

$$\frac{\partial C}{\partial T} = \frac{\partial^2 C}{\partial R^2} + \frac{1}{R+\lambda}\frac{\partial C}{\partial R} \tag{3.10}$$

since 1/(λ + R) << 1 for λ >> 1. The rescaled boundary conditions are

$$\frac{\partial C}{\partial R} = C \;\; at \;\; R = 0, \;\; and \;\; C \to 1 \;\; as \;\; R \to \infty \tag{3.11}$$

and the initial condition is *C = 1 at T = 0 for 0 < R <* ∞.
The solution to this leading order problem (3.10)-(3.11) is given by

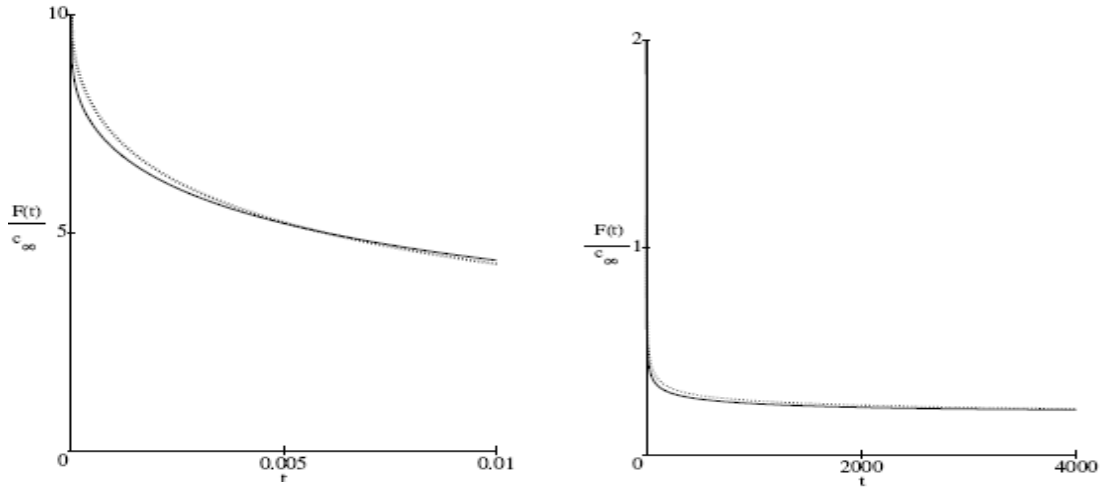
$$C(R,T) = erf\left(\frac{R}{2\sqrt{T}}\right) + e^{R+T} erfc\left(\frac{R}{2\sqrt{T}} + \sqrt{T}\right), \tag{3.12}$$

with the flux, $F(T) = \frac{\partial C}{\partial R}\frac{\partial R}{\partial r}\Big|_{R=0}$, of pollutant into the root given by

$$F(T) = \lambda e^T erfc(\sqrt{T}) \tag{3.13}$$

as $T \to \infty$, the concentration of pollutant at the root surface C → 0 and F→ 0, since $e^T erfc(\sqrt{T}) \to 0$

For $t \le \frac{1}{\lambda^2}$ the comparison of analytic solution with numerical simulations of the model is given in Fig 1 (a)



(a) (b)

Fig. 1. Comparison of numerical experiments (solid lines) for pollutant flux *F(t)* for λ = *10 and C∞=0.1* with the full non-linear model and asymptotic approximations (dashed lines)

Analytic solution given by the equation (3.13) for short time (a), and by the equation (3.20) for long time (b).

(2) For $\tilde{t} > t_c \sim 1/\lambda^2$ the root surface pollutant concentration has dropped to a very low level so the boundary condition at the root surface at the leading order will be *C = 0 at r = 1*

so, $$\frac{\partial C}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial C}{\partial r}), \qquad (3.14)$$

C = 0 at r = 1; and C → 1 as r → ∞.

The initial condition for this problem would be given by the approximate solution (3.7) evaluated at *t≈ 1/λ ^{2} i.e.*

$$C \approx erf(\lambda\frac{r-1}{2}) + e^{\lambda(r-1)+1}erfc(\lambda\frac{r-1}{2}+1) \qquad at\ t = t - t_c \approx t - \frac{1}{\lambda^2} = 0 \qquad (3.15)$$

The analytical solution to the model can be derived as

$$C(r,t) = -\frac{2}{\pi}\int_0^\infty e^{-u^2 t}\,\frac{J_0(ur)Y_0(u) - Y_0(ur)J_0(u)}{J_0^2(u) + Y_0^2(u)}\,\frac{du}{u} \qquad (3.16)$$

and the flux at the root surface *r = 1* is

$$F(\tilde{t}) = \frac{4}{\pi^2}\int_0^\infty e^{-u^2 t}\,\frac{du}{u[J_0^2(u) + Y_0^2(u)]} \qquad (3.17)$$

According to (Richardson, 1993) the small time flux approximation is given by

$$F_{small}(\tilde{t}) \approx (\pi\tilde{t})^{-1/2} + \frac{1}{2} + ... \tag{3.18}$$

and large time flux approximation is

$$F_{large}(\tilde{t}) \approx 2[\frac{1}{ln(4\tilde{t}) - 2\gamma} - \frac{\gamma}{(ln(4\tilde{t}) - 2\gamma)^2} - O(\frac{1}{ln(4\tilde{t}) - 2\gamma)^3})] \tag{3.19}$$

where $\gamma \approx 0.57722..$ is Euler's constant. Hence at the leading order without singularity at $t=0$ (by taking time shift $t_0=(1/4)e^{\gamma}$) the approximation can be written as

$$F_{large}(t) \approx \frac{2}{ln(4e^{-\gamma}t) + 1)} \tag{3.20}$$

and the all time solution can be found by taking the uniform interpolation in the form

$$F(t) = \frac{F_{small}(t)F_{large}(t)}{\left[F^{\alpha}_{small}(t) + F^{\alpha}_{large}(t)\right]^{1/\alpha}}, \tag{3.21}$$

α is some positive number. Though it is not unique, but for the purposes of current research possibly quite satisfactory.

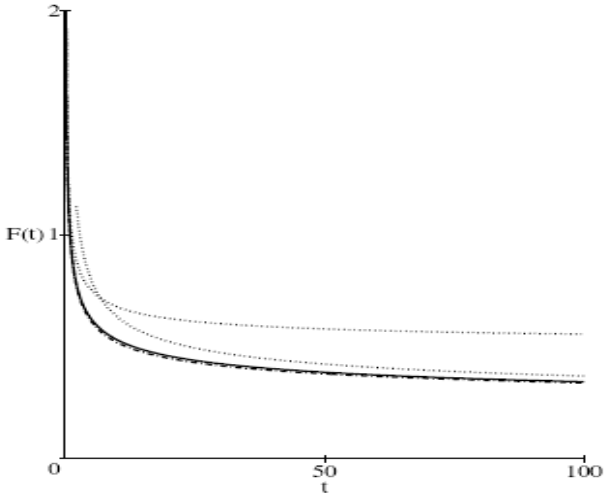


Fig. 2. Comparison of numerical experiments with model (solid line) at large (3.20) and small time (3.18) approximations (dashed lines) together with interpolation (3.21) for $\alpha = 3$ (dotted-dashed line)

3.2.1.2 Approximations for λ <<1

For λ<<1, we expect the region (where C is less than order 1) to be larger. The asymptotic behaviour of this system turns out to be mathematically similar to that of Oseen type of problems of flow past cylinder (Greenwood et al. 1997, Richardson 1995) and is derived in terms of two length scales $r \approx 1$ and $r >> 1$. In the first case i.e. the inner (near root surface) expansion has *ln r* terms which make it impossible to satisfy the boundary condition. This is overcome by considering the variables of second case (Outer expansion) such that to the first approximation the radius of the root is negligible. Hence the first term in the outer expansion is the solution in the absence of the disturbance from the root. The second term in the outer expansion represents the disturbance to the far-field due to a thin root. By matching the inner and outer solutions, a uniformly valid approximation can be derived.

1. Rescaling, the space variable r to large scale variable R by $r = R/\sigma$ and time variable τ by $t=\tau/\sigma^2$ where σ << 1. To find concentration gradient far away from the root surface we choose $\sigma = e^{-1/\lambda}$ <<1 for λ <<1 so the diffusion equation will be

$$\frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial C}{\partial R}\right)=\frac{\partial C}{\partial \tau} \tag{3.22}$$

At the root surface $r = 1$ gives $R = \sigma << 1$, we find that far away from the root, the root acts as an infinitely thin line sink at the origin. This suggests that we should look for a similarity type solution with similarity variable $\eta = R^2/(4\tau)$. The solution satisfying the far-field boundary condition C → 1 as η → ∞ is the outer expansion of the problem and given by:

$$C = 1 + BE_1(\eta) = 1 + BE_1(\frac{R^2}{4\tau}) \tag{3.23}$$

Where $E_1(\eta)=\int_{\eta}^{\infty}\frac{e^{-y}}{y}dy$ and the unknown coefficient B is determined from the solution that is valid in the near root surface.

2. For inner expansion we again rescale the space variable near root surface region, *i.e.,* $r = R\sigma$, and keeping long time-scale variable τ, we have

$$\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial C}{\partial r}) = \sigma^2\frac{\partial C}{\partial \tau} \tag{3.24}$$

The leading $O(\sigma^0)$ solution satisfying the root surface boundary condition at r = 1, is given by

$$\mathrm{C} \approx \mathrm{C}(1, \tau) + \mathrm{F}(\tau)\ \ln\ r + \mathrm{O}(\sigma^2) \tag{3.25}$$

In order to satisfy the boundary condition at the root surface we choose $F(\tau) = \lambda C(1, \tau)$. $C(1, \tau)$ and $F(\tau)$ can be determined via matching with the outer solution.

To match the above solutions in the overlap region, we expand the outer solution at the small, near root surface, limit and the expansion at small argument η limit will be

$E_1(\eta) \approx -\gamma - ln\,\eta + O(\eta)$, for $\eta << 1$ (3.26)

Thus, the outer solution at the inner limit will be

$$C \approx 1 + B\left[-\gamma - 2ln\left(\frac{R}{2\sqrt{\tau}}\right) + O\left(\frac{R}{\sqrt{\tau}}\right)\right] \quad (3.27)$$

which is equal to the inner solution. So by, matching the $O(ln\ R)$ terms in the expansions we find that

$$-2B(\tau) = F(\tau)\ i.e.\ B(\tau) = -\frac{F(\tau)}{2} \quad (3.28)$$

and matching the remaining leading order terms we get

$$C(1,\tau) = 1 - \frac{F(\tau)}{2}\left[-\gamma - 2ln(\sigma) + 2ln(2\sqrt{\tau})\right] \quad (3.29)$$

The flux F in terms of root surface pollutant concentration can be estimated as $F(\tau) = \lambda C(1, \tau)$, so the root surface Pollutant concentration is given by

$$C(1,\tau) = \frac{1}{1 - \lambda(\frac{\gamma}{2} + ln(\sigma) - \frac{1}{2}ln(4\tau))} \quad (3.30)$$

Scaling back into the natural time variable $\sigma^2\tau = t$, after introducing the small time shift $t_0 = (1/4)e^{\gamma}$ such that $C(1, t) = 1$ at $t = 0$, we get

$$C(1,t) = \frac{1}{1 + \frac{\lambda}{2}ln(4e^{-\gamma}t + 1)} \quad (3.31)$$

To obtain the approximation of the flux we use this approximation to the root surface concentration and substitute it into the full non-dimensional flux condition $F = \lambda C_1/(1 + C_1)$ where $C_1 = C_\infty\ C(1, t)$. Hence we obtain

$$F(t) \approx \frac{\lambda C_\infty}{1 + C_\infty + \frac{\lambda}{2}ln(4e^{-\gamma}t + 1)} \quad (3.32)$$

The results of numerical experiments in comparison to the approximations derived, are shown in Fig. 3. The solution agrees reasonably well with the numerical experiments conducted with the full non-linear model. The slight error at larger times is due to the leading order approximation of the non-linear boundary condition.

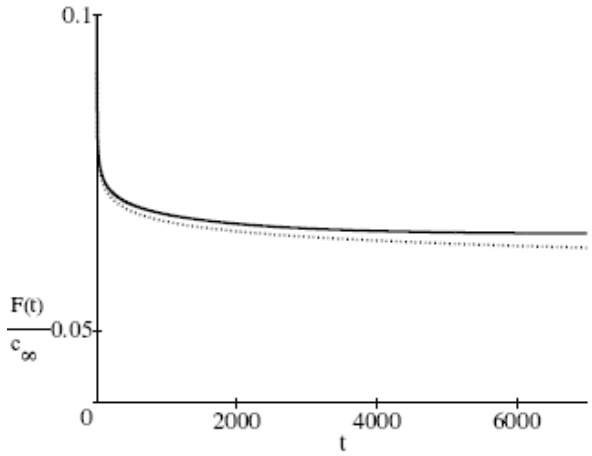


Fig. 3. Comparison of numerical experiments (solid line) with the full non-linear model and asymptotic approximation (dashed line) given by (3.27) for C_∞ = 0.1 and λ = 0.1.

3.2.2 Analytic solutions for the limit $C_\infty \geq 1$

We will now investigate the case when the Pollutant far-field concentration is large, i.e., and $C_\infty \geq 1$ thus $C_0 >> K_m$. we rescale C $= C_\infty C$, so the equation and boundary conditions become

$$\frac{\partial C}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right), \tag{3.33}$$

$$\frac{\partial C}{\partial r} = \frac{\lambda}{C_\infty}\frac{C}{(C+1/C_\infty)} \quad at \quad r=1, \tag{3.34}$$

and $C \to 1 \quad as \quad r \to \infty$ (3.35)

The solution to this model can be found using Laplace transformations

$$C(r,t) = 1 + \frac{2\lambda}{C_\infty \pi}\int_0^\infty (1-e^{-u^2 t})\frac{J_0(ur)Y_1(u) - Y_0(ur)J_1(u)}{u^2\left[J_1^2(u)+Y_1^2(u)\right]}du. \tag{3.36}$$

with small time approximation given by

$$C(r,t) = 1 - 2\frac{\lambda}{C_\infty}\sqrt{\frac{t}{r}}\left[ierfc\frac{r-1}{2\sqrt{t}} - \frac{(3r+1)\sqrt{t}}{4r}i^2 erfc\frac{r-1}{2\sqrt{t}} + ...\right] \tag{3.37}$$

and Large time approximation is

$$C(r,t) = 1 + \gamma - \frac{\lambda}{2C_\infty}ln\frac{4t}{r^2} + O\left(\frac{1}{t}\right) \tag{3.38}$$

where γ ≈ 0.57722.. is Euler's constant.

3.2.2.1 Approximate solution for λ >> 1

If *λ* >> 1 mean that there is a boundary layer near the root surface *r =1* where *∂C/∂r >>1.* Therefore, we define $t=T/\lambda^2$ and $r = 1 + R/\lambda$. Hence, the equations (3.33) and (3.34) becomes

$$\frac{\partial C}{\partial T} = \frac{1}{R+\lambda}\frac{\partial C}{\partial R} + \frac{\partial^2 C}{\partial R^2}, \tag{3.39}$$

together with the boundary conditions

$$\frac{\partial C}{\partial R} = 1 \; at \; R = 0, \; and \; C \to 1 \; as \; R \to \infty, \tag{3.40}$$

and the initial condition

$C = 1$ *at* $T = 0$ *for* $0 < R < \infty$. (3.41)

The solution to equations (3.39)-(3.41) taking $1/(\lambda + R) << 1$, is given by

$$C(R,T) = 1 - 2\left(\sqrt{\frac{T}{\pi}}e^{-R^2/4T} - \frac{R}{2}erfc\frac{R}{2\sqrt{T}}\right) \tag{3.42}$$

In particular, at *R = 0, i.e., r = 1*, we have $C = 1 - 2(T/\pi)^{1/2}$, which implies that C = 0 when $T_c = \pi/4$ and hence $t_c \approx \pi/(4\lambda^2)$ for *λ>> 1.* Hence we can find approximation for pollutant concentration and flux for time $t<t_c=\pi/4\lambda^2$ as

$$C(1,t) = C_\infty\left(1 - 2\lambda\sqrt{\frac{t}{\pi}}\right) \tag{3.43}$$

$F(t)=C_\infty\lambda$ and for $t > t_c$ we have

$$C \approx 1 - \sqrt{\pi}\, erfc\frac{\lambda(r-1)}{\sqrt{\pi}} \tag{3.44}$$

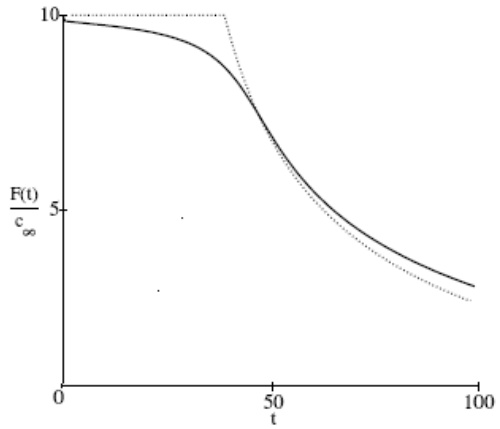


Fig. 4. Comparison of numerical experiments (solid line) with the full non-linear model (3.1)-(3.3) and asymptotic approximation (dashed line) given by 3.43) for C_∞ = *100* and λ = 1000. *C(1, t)* is the root surface Pollutant concentration.

3.2.2.2 Approximate solution for λ <<1

For the case λ<< 1we have $\partial C/\partial r|_{r=1} \approx \lambda << 1$, we expect the region, where C is less than order 1, to be larger. Similar to Section 3.1.2 we use the Oseen type expansion to find the approximate solution.

Thus, after rescaling to large time and space variables τ and R, i.e., $t = \tau/\sigma^2$ and $r = R/\sigma$ with $\sigma << \lambda << 1$ and $\sigma = e^{-1/\lambda}$, we find that the outer similarity solution satisfying boundary conditions

$$C(R,\tau) \approx 1 + BE_1(\frac{R^2}{4\tau}), \tag{3.45}$$

Where $E_1(x) = \int_x^\infty e^{-y}\frac{dy}{y}$

and the unknown coefficient B is determined from the solution that is valid in the near root surface. Similar to the $C_\infty << 1$ case, the inner long time solution is given by

$$C(r,\tau) \approx C(1,\tau) + \lambda\, ln(r) + O(\sigma^2) \tag{3.46}$$

By expanding the outer solution for small argument and matching *ln(R)* terms in the inner and outer expansions we find that $B = -\lambda/2$. The matching of the leading order terms gives

$$C(1,t) \approx 1 - \frac{\lambda}{2} ln(4e^{-\lambda}t). \tag{3.47}$$

Thus, the critical time when the root surface pollutant concentration has reached zero is given by $t_c = \frac{1}{4}e^{\gamma+\frac{2}{\lambda}}$ i.e., the concentration at the root. For the case λ<< 1 we have

$\partial C/\partial r|_{r=1} \approx \lambda << 1$, we expect the region, where C is less than order 1, to be larger. Similar to Section 3.1.2 we use the Oseen type expansion to find the approximate solution. Thus, after rescaling to large time and space variables τ and R, i.e., $t = \tau/\sigma^2$ and $r = R/\sigma$ with $\sigma << \lambda << 1$ and $\sigma = e^{-1/\lambda}$, we find that the outer similarity solution satisfying boundary conditions

$$C(R,\tau) \approx 1 + BE_1(\frac{R^2}{4\tau}), \tag{3.45}$$

Where $E_1(x) = \int_x^\infty e^{-y}\frac{dy}{y}$

and the unknown coefficient B is determined from the solution that is valid in the near root surface. Similar to the $C_\infty << 1$ case, the inner long time solution is given by

$$C(r,\tau) \approx C(1,\tau) + \lambda\, ln(r) + O(\sigma^2) \tag{3.46}$$

By expanding the outer solution for small argument and matching *ln(R)* terms in the inner and outer expansions we find that $B = -\lambda/2$. The matching of the leading order terms gives

$$C(1,t) \approx 1 - \frac{\lambda}{2} ln(4e^{-\lambda}t). \quad (3.47)$$

Thus, the critical time when the root surface pollutant concentration has reached zero is given by $t_c = \frac{1}{4} e^{\gamma + \frac{2}{\lambda}}$ i.e., the concentration at the root surface drops to zero on exponentially large time scale.

The approximation becomes invalid when $\tau \leq \sigma^2 = e^{-2/\lambda}$. But if we choose $C(1, t) = 1$ for $t = 0$, i.e., $t_0 = (1/4) e^{\gamma}$,
we arrive at

$$C(1,t) = C_\infty [1 - \frac{\lambda}{2} ln(4e^{-\lambda}t + 1)] \quad (3.48)$$

The approximation to the flux, which is given in this approximation by $F(t) = \lambda C_\infty$, is even worse than the approximation to the root surface concentration (Fig. 5). This is due to the leading order approximation of the nonlinear boundary condition.

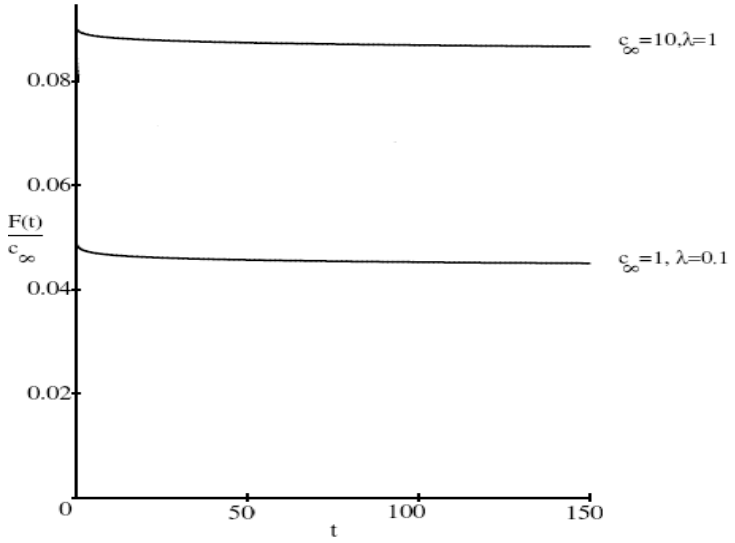


Fig. 5. Comparison of numerical experiments (solid line) with the full non-linear model and asymptotic approximation (dashed line) given by (3.48)

4. CONCLUSION

In this paper the derivation of the model for pollutant uptake, initially developed by Nye, Tinker and Barber is presented together with its non-dimensionalisation and mathematical analysis at different dimensionless parameter limits. We estimated the critical time t_c after

which the pollutant flux into the root starts decreasing due to the deficiency of pollutants at the root surface. This critical time is relatively large for the case when the far-field concentration $c_0$is much larger than the Michaelis-Menten uptake coefficient K_m, and also when the dimensionless pollutant uptake coefficient $\lambda = \frac{F_m a}{DK_m \phi_1}$ is very small compared to the far-field concentration. When the pollutant uptake coefficient λ is large compared to the far-field concentration C_∞, the flux starts decaying very rapidly after a short transition time, which is approximately of order $1/\lambda^2$, and in the case of the small uptake coefficient λ, the decrease in root surface Pollutant concentration takes place over the exponentially large time-scale, more specifically of order $e^{2/\lambda}$ corresponding to times larger than the average vegetative period of agriculturally important plants.

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