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Analytical Method of Nitrogen Uptake Model for Plant Roots*

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Abstract The nitrogen uptake model for plant roots is an advection-diffusion equation subject to double Robin boundary conditions in Cartesian coordinates and its analytical method is expected to accurately estimate the quantity of nutrient uptake and fertilization. Firstly, the Michaelis-Menten (MM) kinetics function in the left boundary condition is changed into a function of time by numerical fitting and the nonlinear left Robin boundary condition then becomes a linear one in order to use traditional analytical methods. Based on the eigenfunction expansion method originally built by Golz and Dorroh, the nitrogen uptake model is homogenized and its eigenvalues are obtained from the Sturm-Liouville problem. Because the convergence of this eigenfunction expansion method is slow around the left boundary, i.e., root surface, we additionally consider the Laplace transform to solve the nitrogen uptake model. However, the solution after Laplace transform involves composite functions and numerical inverse Laplace transforms are introduced to obtain the final solutions. The analytical and numerical solutions show that the nitrogen concentration profiles along the distance from the root surface are convex upward and almost horizontal in the middle part with large gradients at both ends. The numerical simulation demonstrates that the eigenfunction expansion method can reach a satisfactory accuracy and the Laplace transform method with Stehfest inversion has higher calculation efficiency.

Keywords Nitrogen uptake, advection-diffusion equation, Robin boundaries, Golz and Dorroh's method, numerical inverse Laplace transform

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1. Introduction

Sufficient nutrient supply is important for the growth and harvest of crops [1]. Nitrogen is one of the most important nutrients for plants, and the main form of nitrogen absorbed by plant roots is inorganic [2]. On the contrary, excess nitrogen supply is detrimental to crops and wreaks havoc to N farmland [3, 4]. Hence, a

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thorough understanding of the nutrient absorption mechanism is of economic and scientific significance for the efficient use of chemical fertilizers and the increase of crop yields.

The movement of solutes from the surrounding soil into the roots can be effectively described by the advection-diffusion model (ADM) [5, 6, 7, 8, 9, 10]. Nutrient models of most plants took the root geometry into account and were built in cylindrical coordinates, otherwise in Cartesian coordinates, e.g., phytoplankton [11, 12, 13, 14]. Besides, most nutrient uptake models use Dirichlet or Neumann boundary conditions rather than Robin boundary condition which is in flux form and abided by mass conservation [15, 16, 17]. Therefore, it is still expected to build the analytical method for nutrient uptake models with double Robin boundary conditions in Cartesian coordinates.

Nutrient uptake models belong to the parabolic problem, more precisely to the advection-dispersion problem (ADP). Classical methods for solving one-dimensional ADE includes integral transforms, Green's function, variable separation, homotopy analysis, etc. [18, 19, 20, 21, 22, 23, 24]. Most analytical methods focused on ADE subject to the first or second type of boundary conditions [25, 26, 27, 28, 29]. There are fewer systematical results for ADE subject to double Robin boundary conditions in finite domain because of the mathematical and computational difficulty. Some researchers used the eigenfunction expansion method, and generalized integral transform technique to obtain the analytical solution of ADE with Robin boundary condition in finite domain [30, 31, 32, 33, 34, 35]. The nitrogen uptake model in this paper is an ADE subject to double Robin boundary conditions, but the right-hand side of left boundary condition is the Michaelis-Menten function of dependent variable. Golz and Dorroh [31] originally built an analytical method for the convection-diffusion equation with double Robin boundary conditions in Cartesian coordinates, which has been cited in [36, 37, 38], but none of them fully accomplished the application of this method. The nutrient uptake models conform to the general form proposed by Golz and Dorroh [31]. However, we still need to cope with the Michaelis-Menten function and the calculation. Because of the difficulty of this method, we will attempt to build another method with Laplace and inverse Laplace transforms for broader interest. [39, 40, 41].

The paper is organized as follows. Analytical methods are built to solve the nitrogen uptake model in Section 2. Analytical solutions and simulations are compared in Section 3. Finally, the conclusion of this paper is given in Section 4, and the numerical scheme is given respectively in Appendix A.

2. Model and analytical methods

2.1. Nitrogen uptake model

McMurtrie and Näsholm built a nitrogen uptake model that simulated the balance between the supply of plant available nitrogen and losses associated with its uptake by plant roots, soil microbes and other mechanisms [9]. It takes the forms in Cartesian coordinates as

$$b\frac{\partial C_N}{\partial t} = Db\frac{\partial^2 C_N}{\partial x^2} + v_0\frac{\partial C_N}{\partial x} - mC_N + S_N, \qquad 0 \le x \le l, \quad t \ge 0, \tag{2.1}$$

$$v_0 C_N(0,t) + Db\frac{\partial C_N(0,t)}{\partial x} = \frac{j_{rmax} k_N C_{s0}}{k_N C_{s0} + j_{rmax}}, \qquad t \ge 0, \tag{2.2}$$

$$v_0 C_N(l,t) + Db\frac{\partial C_N(l,t)}{\partial x} = 0, \qquad t \geq 0, \tag{2.3}$$

$$C_N(x,0) = \frac{S_N}{m}, \tag{2.4}$$

where $C_N(x,t)$ is the concentration of soil N solution, b is the buffer power of soil, D is the effective diffusion coefficient of nutrient in soil, v_0 is the radial velocity of water at the root surface, m is the rate of solute loss through immobilization by soil microbes, S_N is the rate of supply of diffusible solute per unit soil volume, x is the distance from the root axis, j_{rmax} is the the maximum root-N influx, k_N is the root absorbing power for nutrient, and C_{s0} is the solute concentration of root surface [9]. Model (2.1)-(2.4) possesses complete and representative structure for nutrient uptake and we attempt to solve it by Golz and Dorroh's method, and Laplace transform method.

2.2. Golz and Dorroh's method

The heat transfer problem that Golz and Dorroh considered [31] is

$$R\frac{\partial u(x,t)}{\partial t} = D_g\frac{\partial^2 u(x,t)}{\partial x^2} - v_g\frac{\partial u(x,t)}{\partial x} - \mu u(x,t) + \delta, \qquad 0 \leq x \leq a, \tag{2.5}$$

$$v_g u(0,t) - D_g\frac{\partial u(0,t)}{\partial x} = v_g f(t), \quad t > t_0, \tag{2.6}$$

$$v_g u(l,t) - D_g\frac{\partial u(a,t)}{\partial x} = v_g C_E, \quad t > t_0, \tag{2.7}$$

$$u(x,t_0) = \phi(x), \tag{2.8}$$

where the parameters and functions in model (2.5)-(2.8) are referred to in [31].

The solution of model (2.5)-(2.8) is

$$u(x,t) = \sum_{n=0}^{\infty}\frac{\varphi_n(x)e^{rx-(p+(D_g/R)\lambda_n)t}}{\int_0^a \varphi_n^2(x)dx}\Bigg[e^{(p-(D_g/R)\lambda_n)t_0}\int_0^a \varphi_n(x)\Big(\phi(x)e^{-rx} - H(t_0)\Big)dx + \int_{t_0}^{t} e^{(p+(D_g/R)\lambda_n)\tau}\int_0^a \varphi_n(x)G(x,\tau)dxd\tau\Bigg] + e^{rx}H(x,t), \tag{2.9}$$

where

$$G(x,t) = \frac{\delta}{R}e^{-rx} - pH - H_t + \frac{D_g}{R}H_{xx}, \tag{2.10}$$

and

$$H(x,t) = (1+\cos\frac{\pi x}{a})f(t) + (1-\cos\frac{\pi x}{a})e^{-ar}C_E. \tag{2.11}$$

Compared with Eqs. (2.10) and (2.11), Eq. (2.7) in [31] lacks one term $-pH$ and e^{-ax} in Eq. (2.9) in [31] should be e^{-ar}.

In order to apply the Golz and Dorroh's method to model (2.1)-(2.4), we temporarily take the nonlinear right-hand side of Eq.(2.2) as a function form of time $F(t)$,

$$v_0 C_N(0,t) + Db\frac{\partial C_N(0,t)}{\partial x} = v_0 F(t), \qquad t \geq 0, \tag{2.12}$$

where

$$F(t) = \frac{j_{rmax} k_N C_{s0}}{v_0 (k_N C_{s0} + j_{rmax})}. \tag{2.13}$$

The left boundary condition (2.12) is a linear one, and we will explain how to get $F(t)$ later. Models (2.1), (2.3), (2.4) and (2.12) conform to the general form (2.5)-(2.8) and the former's solution can be expressed by Eq. (2.9),

$$C_N(x,t) = A_1(x,t) + A_2(x,t) + A_3(x,t), \tag{2.14}$$

where

$$A_1(x,t) = \sum_{n=0}^{\infty} \frac{\varphi_n(x)\, e^{-(q_1 + D\lambda_n)t}}{\int_0^l \varphi_n^2(x)dx} \int_0^l \varphi_n(x) \left[\frac{S_N}{m}\, e^{-q_2 x} - (1 + \cos\frac{\pi x}{l})F(0)\right] dx, \tag{2.15}$$

$$A_2(x,t) = \sum_{n=0}^{\infty} \frac{\varphi_n(x)}{\int_0^l \varphi_n^2 dx} \int_0^t e^{-(q_1 + D\lambda_n)(\tau - t)} \int_0^l \varphi_n(x) \Big[\frac{S_N}{b}\, e^{-q_2 x} + \ldots$$

$$q_1(1 + \cos\frac{\pi x}{l})F(\tau) - \frac{D\pi^2}{l^2}\cos\frac{\pi x}{l} F(\tau) - (1 + \cos\frac{\pi x}{l})F'(\tau)\Big] dx d\tau, \tag{2.16}$$

$$A_3(x,t) = (1 + \cos\frac{\pi x}{l})F(t), \tag{2.17}$$

where

$$q_1 = -\frac{v_0}{2Db},\ q_2 = \frac{1}{b}(\frac{v_0^2}{4Db} + m).$$

Solutions (2.14)-(2.17) can be applied to other simpler models [42, 43]. However, the calculation of solutions (2.14)-(2.17) involves eigenfunctions, integration, series, and iteration in time and space. Moreover, MM function (2.13) will be fitted by numerical concentration at the root surface. Laplace transform is more acceptable in many fields. We attempt to build another analog with Laplace transform, and compare their efficiency and precision.

2.3. Laplace transform method

The Laplace transform of nitrogen uptake models (2.1), (2.3) and (2.12) is

$$\frac{S_N}{s} + b\frac{S_N}{m} + Db\frac{\partial^2 \overline{C_N}(x,s)}{\partial^2 x} + v_0 \frac{\partial \overline{C_N}(x,s)}{\partial x} - (m + bs)\overline{C_N}(x,s) = 0, \tag{2.18}$$

$$Db\frac{\partial \overline{C_N}(0,s)}{\partial x} + v_0 \overline{C_N}(0,s) = v_0 \bar{F}(s), \tag{2.19}$$

$$Db\frac{\partial \overline{C_N}(l,s)}{\partial x} + v_0 \overline{C_N}(l,s) = 0, \tag{2.20}$$

where s and $\overline{C_N}(x,s)$ are the Laplace transforms of t and $C_N(x,t)$. The solution of model (2.18)-(2.20) is

$$\overline{C_N}(x,s) = \frac{S_N}{ms} + c_1(x,s)n_1(x,s) + c_2(x,s)n_2(x,s), \tag{2.21}$$

where

$$
\begin{aligned}
c_1(x,s) &= \frac{2[e(s)(d_2(x,s)-1)-d_2(x,s)\bar{F}(s)]}{\beta_1(s)(d_1(x,s)-d_2(x,s))},\\
c_2(x,s) &= \frac{2[e(1-d_1(x,s))+d_1(x,s)\bar{F}(s)]}{\beta_2(s)(d_1(x,s)-d_2(x,s))},\\
n_1(x,s) &= exp\left(\frac{-v_0+x\sqrt{4Dbm+4b^2Ds+v_0^2}}{2Db}\right),\\
n_2(x,s) &= exp\left(\frac{-v_0+x\sqrt{4Dbm+4b^2Ds+v_0^2}}{2Db}\right),\\
d_1(x,s) &= exp\left(\frac{-v_0l-l\sqrt{4Dbm+4b^2Ds+v_0^2}}{2Db}\right),\\
d_2(x,s) &= exp\left(\frac{-v_0x+x\sqrt{4Dbm+4b^2Ds+v_0^2}}{2Db}\right),\\
\beta_1(s) &= v_0-\sqrt{4Dbm+4b^2Ds+v_0^2},\\
\beta_2(s) &= v_0+\sqrt{4Dbm+4b^2Ds+v_0^2},\ e(s)=\frac{v_0S_N}{ms}.
\end{aligned}
$$

Eq. (2.21) has a complicated structure and it is difficult to directly take the inverse Laplace transform using the Residue theorem and complex integration. Thus, we plan to adopt numerical inverse Laplace transform to get the final solution. Because of the uncertainty of the numerical inverse transform, we will consider three inversion algorithms. i.e., Zakain, Stehfest and Weeks inversions and find an appropriate one.

The Zakain inverse Laplace transform of Eq.(2.21) is

$$
\begin{aligned}
C_N(x,t) =&\frac{2}{t}\sum_{j=1}^{n} Re\Bigg[K_j\Bigg(\frac{S_Nt}{m\alpha_j}+c_1\Big(x,\frac{\alpha_j}{t}\Big)n_1(x,\frac{\alpha_j}{t})\\
&+c_2\Big(x,\frac{\alpha_j}{t}\Big)n_2(x,\frac{\alpha_j}{t})\Bigg)\Bigg],
\end{aligned}
\tag{2.22}
$$

where the coefficients K_j, α_j and n are referred to [44].

The Stehfest inverse Laplace transform of Eq.(2.21) is

$$
\begin{aligned}
C_N(x,t) =&\frac{\ln 2}{t}\sum_{j=1}^{N} V_j\Bigg[\frac{S_Nt}{mj\ln 2}+c_1\Big(x,\frac{\ln 2}{t}j\Big)n_1(x,\frac{\ln 2}{t}j)\\
&+c_2\Big(x,\frac{\ln 2}{t}j\Big)n_2(x,\frac{\ln 2}{t}j)\Bigg],
\end{aligned}
\tag{2.23}
$$

where

$$
V_j=(-1)^{(\frac{N}{2}+j)}\sum_{k=\left[\frac{j+1}{2}\right]}^{\min(j,\frac{N}{2})}\frac{k^{\frac{N}{2}}2k!}{(\frac{N}{2}-k)!k!(k-1)!(j-k)!(2k-j)!}.
$$

The Weeks inverse Laplace transform of Eq.(2.21) is

$$
C_N(x,t)=e^{\sigma t}\sum_{j=0}^{\infty}a_jL_j(\frac{t}{w}),
\tag{2.24}
$$

where L_j is the Laguerre polynomial, a_j is the Taylor coefficient, w is a scale factor,

$$\sigma = \Psi - \frac{1}{2w},\ w = \frac{t_{max}}{N},\ \Psi = 1 + \frac{1}{t_{max}},\ \theta_k = \frac{\pi}{2}\frac{2k+1}{N+1},$$

$$a_0 = \frac{1}{N+1}\sum_{k=0}^{N} h(\theta_k),\ a_j = \frac{2}{N+1}\sum_{k=0}^{N} h(\theta_k)\cos(j\theta_k),$$

$$h(\theta_k) = \frac{1}{T_n}\left\{Re\left[\overline{C_N}\left(x, \Psi + \frac{i\cot\frac{\theta_k}{2}}{2w}\right)\right] - \cot\frac{\theta_k}{2} Im\left[\overline{C_N}\left(x, \Psi + \frac{i\cot\frac{\theta_k}{2}}{2w}\right)\right]\right\},$$

and the other parameters are referred to [39].

We have hitherto given the solution expressions for two methods, i.e., solutions (2.14)-(2.17), solutions (2.22)-(2.24) for models (2.1), (2.3), (2.4) and (2.12). Even if solutions (2.14)-(2.17) are exact, its calculation is approximate because of the truncation of series and the fitting of MM function $F(t)$. The performance of numerical inverse Laplace transforms closely depends on the preceding Laplace transform and their adaptions are not universal. We have to discuss their precision and efficiency.

3. Precision and efficiency of solutions

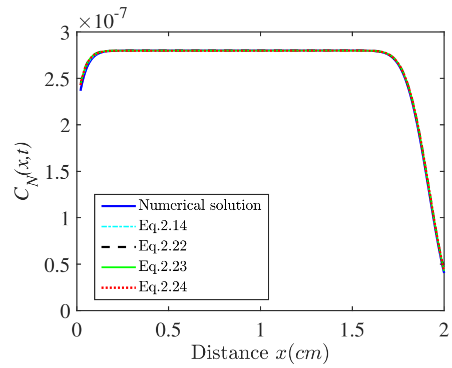
Models (2.1)-(2.4) are a typical parabolic problem, its numerical scheme is reliable and highly accurate, and then it can be taken as the precision benchmark. The numerical scheme adopts the first-order forward difference for time, the first-order forward difference for the first derivative in space, and the second-order central difference for the second derivative in space (Appendix A). We set the space step $\Delta x = l/1000$ and time step $\Delta t = 0.1(\Delta x)^2$ for satisfying the consistency and convergence conditions. The parametric values can be found in [9], i.e., $b = 1$, $D = 0.05\, cm^2\, d^{-1}$, $v_0 = 1\, cm\, d^{-1}$, $m = 0.05\, cm\, d^{-1}$, $S_N = 1.4 \times 10^{-8}\, g\, N\, cm^{-3}\, d^{-1}$ and $l = 1.98\ cm$. $F(t)$ is fitted by the numerical concentration on the root surface of model (2.1)-(2.4) in MALTAB.

The mean absolute percent error (MAPE) is used to evaluate the deviation between the numerical solution C_i^n and the analytical solutions C_N, i.e., (2.14), (2.22), (2.23) and (2.24) [45]:

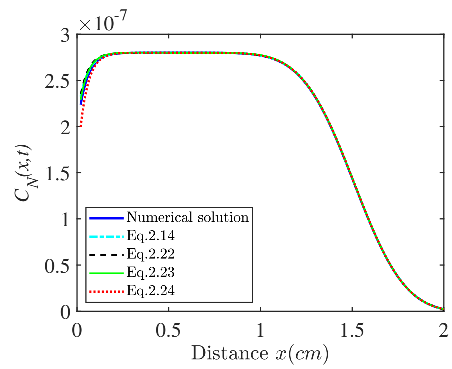
$$MAPE = \frac{1}{M}\sum_{i=1}^{M}\left|\frac{C_i^n - C_N(x_i, t_n)}{C_N(x_i, t_n)}\right| \times 100\%.$$

$C_N(x, t)$ will be statistically approximate enough to numerical solution if MAPE is less than or equal to 10%.

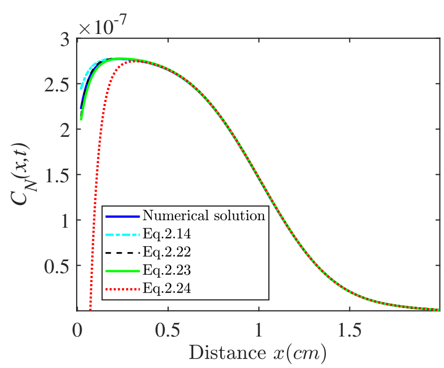
The profiles of numerical and analytical solutions are displayed in Fig. 1. The overall trends of solutions increase monotonically near the root surface, level off in the middle, and decrease steeply at the right end. The trends primarily result from the advection effect and Robin boundary conditions. At three moments 0.1 day, 0.5 day and 1 day, all solutions are close except for solution (2.24) in Fig. 1(c). The subtle divergence of solution near the root surface should be rechecked in Tab. 1, where the solutions of Golz and Dorroh's method and the Laplace transform with Stehfest inversion are more approximate to numerical solution. However, the computation efficiency of Golz and Dorroh's method falls behind that of the Laplace transform method because the former contains a lot of integrations and iteration.



(a) t = 0.1 day



(b) t = 0.5 day



(c) t = 1 day

Figure 1. The profiles of numerical solution and analytical soltions of N concentration distributions vs. distance in t = 0.1 day, 0.5 day, and 1 day.

The convergence between numerical solution of original model (2.1)-(2.4) and the analytical solution of models (2.1), (2.3), (2.8) and (2.12) demonstrates that the linearization of MM function does not alter the quality of solution.

In Tab. 1, the convergence speed of the eigenfunction expansion method is far behind that of the Laplace methods because its solution (2.14) is a series with integrations and the series needs more than thousands of eigenfunctions to be convergent

Table 1. The comparison of accuracy and efficiency between Golz and Dorroh's method and the Laplace transform methods with different numerical inversions.

	T = 0.1	T = 0.5	T = 1
Golz and Dorroh's method	MAPE(%) = 0.27 CPU t = 4307 s	MAPE(%) = 0.25 CPU t = 44207 s	MAPE(%) = 0.42 CPU t = 44241 s
Zakain inversion	MAPE(%) = 0.3 CPU t = 0.09 s	MAPE(%) = 0.83 CPU t = 0.92 s	MAPE(%) = 9.20 CPU t = 0.18 s
Stehfest inversion	MAPE(%) = 0.30 CPU t = 0.18 s	MAPE(%) = 0.29 CPU t = 0.21 s	MAPE(%) = 0.38 CPU t = 0.19 s
Weeks inversion	MAPE(%) = 0.34 CPU t = 1.01 s	MAPE(%) = 0.36 CPU t = 1.03 s	MAPE(%) = 25.09 CPU t = 1.03 s

near the nonlinear left boundary. The Laplace transform method with the Stehfest inversion has satisfactory performance in convergence and efficiency compared with the Zakain and Weeks inversions.

4. Conclusion

In this paper, we have proposed two analytical methods to solve the nitrogen uptake model. The nonlinear nitrogen uptake model is linearized by replacing the MM function of concentration with the MM function of time, making it suitable for traditional analytical methods. The Golz and Dorroh's method has been rectified and examined by the investigated plant nutrient uptake model. The Golz and Dorroh's method and the Laplace transform method with Stehfest inversion both perform best in terms of accuracy, and the latter also has the fastest efficiency. The analytical procedures for solving the plant nutrient uptake model in this paper are illuminating for other advection-diffusion problems with double Robin boundary conditions.

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Appendix A

In this appendix, we will give the numerical scheme of models (2.1)-(2.4). C_i^n is the value of $C_N(x,t)$ at grid points in models (2.1)-(2.4). The crossing point ($x_i = i\Delta x$,

$t_n = n\Delta t$ for $i = 0, 1, \ldots, J$, $n = 0, 1, \ldots$).

$$b\frac{C_i^{n+1} - C_i^n}{\Delta t} = Db\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2} + v_0\frac{C_{i+1}^n - C_i^n}{\Delta x} - mC_i^n + S_N, \tag{A.1}$$

$$v_0 C_0^n + Db\frac{C_1^n - C_0^n}{\Delta x} = \frac{k_N\ j_{rmax} C_0^n}{k_N\ C_0^n + j_{rmax}}, \tag{A.2}$$

$$v_0 C_J^n + Db\frac{C_J^n - C_{J-1}^n}{\Delta x} = 0, \tag{A.3}$$

$$C_i^0 = \frac{S_N}{m}. \tag{A.4}$$

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