Analytical solution of diffusion model for nutrient release from controlled release fertilizer

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Abstract. An analytical method has been developed to solve the initial value problem which arises from Fick’s diffusion equation encountered in the modelling of the Controlled Release Fertilizers. The proposed analytical solution is developed using the modified Adomian decomposition method. This method does not require the discretization method, reliability and efficiency of this method is more and it also reduces the calculation time. The model has predicted the effect of granule radius and diffusion coefficient on the nutrient release and total release time of Controlled Release Fertilizer. Model has predicted that increase in the radius of granule reduces the release and vice versa in case of diffusion coefficient. Detailed understanding of these parameters helps in improved designing of Controlled Release Fertilizer.

1. Introduction

In the 21st century the demand for food supply has increased drastically with increase in world population. To meet this demand, it is essential for farmers to use the synthetic fertilizers. This fertilizer has the low nutrient transport efficiency to plant and are very hazardous to the environment. The recent progress in the development of Controlled Release Fertilizer (CRF)[1]. CRF improve the current low efficient nutrient rate of fertilizers because controlled and timely release of nutrients. CRF granule are coated with polymers and biopolymers soluble in water.

Mathematical modeling of CRF is important to get a clear understanding of the release behavior of the nutrients, which benefit in developing highly efficient CRF. The model help will to comprehend the various parameters affecting the nutrient release like radius of the granule, diffusivity of the coating material and nutrient release rate. In this direction Baker [2] has developed two mathematical models to predict the release of drug from a sphere. Shaviv [3] has developed a mathematical model by the dividing the release stage in to three stages 1. Lag period – In this time there will not be any release of nutrient. 2. Constant release stage in this period release rate is constant and continuous until the majority of the nutrients (Approximately 80%) released from the granule. 3. Gradual decay release. [3] has given the formula to calculate the lag period based on their assumptions. They also given a statistical model for the group of granules together. [4] given a model for the release by assuming a non-homogenous diffusion equation by solving it with variable separable method. [5] has given a model and algorithm for the calculation of saturation time based on numerical method by using the two level explicit finite differencing scheme. Latest model on CRF is release from swelling polymer coated urea depends on swelling granule radius [6]. The mathematical model in the literature
requires a high knowledge of mathematics and computational technique. An analytical model with Adomian gives precise results for solving parabolic equations (diffusion/heat type) as compared to variable separable method [7]. In this work an analytical model is developed based on the Adomian decomposition method which is elegantly computable.

The Adomian decomposition method gives the solution in a series form which may converge to the exact solution is such a solution exists, otherwise the series can be used for computational purposes. The solution obtained from Adomian will be series solution [8]. Many researches have used Adomian decomposition method for variety of problems by Wazwaz [9], and Mehdi [10] and many more for parabolic differential equations with different initial and boundary conditions [11–13]. This method has been significantly used in physics, engineering and biology.

Even though much literature has been found on the application of Adomian decomposition method for the first time Adomian decomposition method has been used to solve the Fick’s second law of diffusion encountered in modelling the release characteristics of controlled release fertilizer. The Analytical solution obtained from in this work is very simply, reliable and easy to implement for industrial production of fertilizers and farmers. Results obtained from the model has been verified along with the experimental results from the literature.

2. Mathematical Model

The fertilizer granule considered in this study has the polymer coating and nutrient is release only through the diffusion. The fertilizer granule is spherical in shape and coating is uniform on the granule. The assumptions of the model are 1. Temperature effect on the release of nutrient is considered to be remain constant. 2. Effect of soil environment (both microbial and enzymatic effect) is considered to zero.

Let us consider a granule with radius ‘a’ and has the initial concentration of nutrient inside the fertilizer granule is \( C_{n0} \). When the granule saturate nutrient will release from the granule due to the process of diffusion. [14] has explained the diffusion phenomenon in the soil and represented them in the three-dimensional diffusion equation.

\[
\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left( D_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( D_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( D_z \frac{\partial C}{\partial z} \right)
\]

where \( C \) is the concentration of the nutrients and \( D_x, D_y \) and \( D_z \) are the coefficient of diffusion equation in the x, y and z direction respectively.

Release of the nutrient takes place after the saturation of the granules. Saturation time for the granule is studied by [5]. In this saturation coating is swelled due to diffusion of water after this stage the release of nutrient takes place. Release of the nutrient in three dimensions space with respect to time ‘t’ is given by

\[
\frac{\partial c_n}{\partial t} = D_n \left( \frac{\partial^2 c_n}{\partial x^2} + \frac{\partial^2 c_n}{\partial y^2} + \frac{\partial^2 c_n}{\partial z^2} \right)
\]

The initial condition is

\[
C_n(\alpha, y, z, t = 0) = C_{n0}
\]

Due to the radial symmetry in the three axis it can be written as

\[
x^2 + y^2 + z^2 = r^2
\]

Where ‘r’ is the position variable which is also called as the radius of diffusion in the coated fertilizer granule.

By substituting (4) in (2) we get the equation in the form of Fick’s second law of diffusion as

\[
\frac{\partial c_n}{\partial t} = D_n \left( \frac{\partial^2 c_n}{\partial r^2} + \frac{2}{r} \frac{\partial c_n}{\partial r} \right)
\]

with initial condition

\[
C_n(r, t) = C_{n0} \quad \text{when} \quad t = 0
\]

Equation (5) is the second order partial differential equation to solve this equation analytically hence new modified Adomian decomposition method has been used.

According to the decomposition method, first let us multiply Adomian operators on both the sides of the equation no (5) then we get

\[
L_t(C_n) = L_{FP}(C_n)
\]
where \( L_t = \frac{\partial}{\partial t} \) and \( L_{FS} = \frac{\partial}{\partial r} A(r, t) + \frac{\partial^2}{\partial r^2} B(r, t) \)

\( L_{FS} \) is the Fick’s second law operator for space variable and the coefficient A and B are the time and space dependent variable, \( L_t \) is the time differential operator. To simplify the equation no (7) let us multiply inverse operator in time i.e \( L_t^{-1} \) on the sides of the equation

\[
L_t^{-1} L_t(C_n) = L_t^{-1} L_{FS}(C_n)
\]

where

\[
L_t^{-1} = \int_0^t (.) \, dt
\]

Using the initial condition and simplifying we get

\[
C_n(r, t) - C_n(r, 0) = L_t^{-1} L_{FS}(C_n)
\]

\[
C_n(r, t) = C_{n0} + L_t^{-1} L_{FS}(C_n)
\]

Now as per the decomposition method given by Adomian we decompose the unknown function \( C_n(r, t) \) by a sum of components series with \( C_{n0} \) identified as the initial condition \( C_n(r, 0) \).

\[
C_n(r, t) = D_n * \sum_{i=0}^\infty C_{ni}(r,t).
\]

The remaining terms of \( C_{ni}(r, t) \) for \( i \geq 1 \), can be completely determined by each term, which will be computed on the previous terms. Which will result in the components as \( C_{n0}, C_{n1}, C_{n2}, C_{n3} \ldots \) are identified and a series of solution is computed. The resulting solution converges in the closed form when the exact solution of the Fick’s second law diffusion equation.

Hence the determination of the terms \( C_{ni}(r, t) \) is given below

\[
C_{n0}(r, t) = C_{n0}
\]

\[
C_{ni+1}(r, t) = L_t^{-1} L_{FS}(C_n), i \geq 0
\]

Thus:

\[
C_{n1}(r, t) = L_t^{-1} L_{FS}(C_{n0})
\]

\[
C_{n2}(r, t) = L_t^{-1} L_{FS}(C_{n1})
\]

\[
C_{n3}(r, t) = L_t^{-1} L_{FS}(C_{n2})
\]

By calculating the terms \( C_{n0}, C_{n1}, C_{n2}, C_{n3} \ldots \), the solution \( C_n \) of Fick’s equation (5) which can be computed as follows from (12)

\[
C_{n0}(r, t) = C_{n0}.
\]

Substituting (12) in (14) and in the similar way (17) into (15) and (18) into (16), on simplifying we get

\[
C_{n3}(r, t) = -C_{n0} * \frac{t}{r^2} + C_{n0} * \frac{3t^2}{2r^4} - C_{n0} * \frac{8t^3}{r^6}.
\]

The exact solution of

\[
C_n(r, t) = D_n(C_{n0} - C_{n0} * \frac{t}{r^2} - C_{n0} * \frac{3t^2}{(x+a)^2} - C_{n0} * \frac{8t^3}{(x+a)^6}).
\]

The diffusion distance \( \chi^* \) in the membrane of coated fertilizer can be given by

\[
\chi = r - a
\]

Diffusion distance is depending on the coating thickness of the granule. In certain cases, when the coating of the material is very small in that diffusion distance will be negligible then \( r \approx a \). For larger coating thickness of the granule once diffusion of molecule starts fertilizer granule swell which can be approximately given as

Substituting (22) in (21) we get

\[
C_n(r, t) = D_n(C_{n0} - C_{n0} * \frac{t}{(x+a)^2} - C_{n0} * \frac{3t^2}{(x+a)^4} - C_{n0} * \frac{8t^3}{(x+a)^6}).
\]

Elimination the higher order terms we get

\[
C_n(r, t) = D_n C_{n0}.
\]

The quantity of diffusing substance \( Q_t \) can be given as[15]

\[
Q_t = 4\pi a b * C_n(r, t).
\]
\[ M_0 = \frac{4}{3} \pi r^2 \rho_s \]  

(26)

where \( \rho_s \) is nutrient density inside the granule.

Cumulative nutrient release is given by

\[ g = \frac{Q_t}{M_0} . \]  

(27)

Hence

\[ g = \frac{3 D t C_0}{\rho_s r} . \]  

(28)

Equation (28) gives the cumulative of nutrient release from the granule.

3. Results and Discussion

The simulation has been carried to understand the effect of influencing parameters on the release of the nutrients from the fertilizer granules. Figure 1 shows the variation in the release time when the diffusion coefficient increases the release time decreases. The trend in figure 1 indicates the importance of diffusion coefficient of coated material in order to have a controlled nutrient release from the granule. This will help in choosing the correct coating materials for different crop based required nutrient time. As the diffusion coefficient increases it allows more water to inter the coated material and diffuse the more nutrient. The trends in figure 1 and figure 2 are in Analogous results obtained by Basu et.al [5] after the solving equation (5) by the two level explicit finite difference schemes.

![Figure 1](image-url)

**Figure 1.** Variation of release time along with the change in the diffusion coefficient for three different radii of the granule.

Radius of the fertilizer is granule plays an important role in the release characteristics as it shows in the figure 2. As the radius of the granule increases the release time increases. This detail will be very critical in deciding the coating thickness of the granule. As the radius of granule increase nutrient distributed in the more area and takes more time to come out compared to the lesser radius of the granules.
Figure 2. Variation of release time along with the change in the different radius of the fertilizer granule.

4. Conclusion
ADM was applied successfully to solve the Fick’s second law of diffusion. This method has given the exact solution for the application of controlled release fertilizers. Model has predicted that increase in the granule radius will decrease cumulative nutrient release percentage and vice versa in case of diffusion coefficient. The results obtained with ADM has been in analogous with results from the existing literature results from the literature.

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