



Exploring nitrogen release from urea fertilizer coated with biodegradable acetylated lignin sulfonate: A numerical analysis using the Crank-Nicolson method

Pouya Es'haghi¹, Hassan Seddighi¹, Keivan Shayesteh^{1*}, Navid Omrani¹

¹Department of Chemical Engineering, Faculty of Engineering, University of Mohaghegh Ardabili, Ardabil, Iran

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ABSTRACT

Soil alone cannot provide plants with all the vital nutrients they need. Chemical fertilizers are often used to supplement these nutrients but can introduce harmful contaminants. Fertilizers are coated to prevent wastage, cut costs, and minimize environmental pollution. Utilizing natural and biodegradable polymers is a highly viable option for coating fertilizers and producing slow-release fertilizers. These polymers, such as acetylated lignin sulfonate, offer an ideal solution owing to their natural abundance and efficient utilization. The system's behavior is comprehensively studied by modeling the nitrogen penetration process into the coating. The diffusion coefficient (D), concentration profile, and release rate are generally determined through modeling. Due to the thinness of the membrane, it is impossible to determine the concentration profile experimentally. Therefore, the total mass transferred through the membrane (M_t) is typically measured at specific intervals. The D , a parameter influencing M_t at specific times, is determined differently. This article aims to determine the concentration profile numerically using the Crank–Nicolson method for urea fertilizer coated with acetylated lignin sulfonate. Release charts are generated at various time points by solving M_t . Investigations indicate that at around 3000 seconds, the concentration profile becomes entirely linear and aligns with the concentration profile at 12000 seconds. Furthermore, beyond 3000 seconds, the stability of the concentration profile about time signifies a steady-state system. A comparative analysis between the experimental data and the numerical solution results demonstrates the high accuracy of the numerical solution, with the maximum relative error occurring at 7895 seconds.

1. Introduction

Due to its high nitrogen content, urea is widely used as a chemical fertilizer in agriculture to supply soil nitrogen. Nitrogen is among the main nutrients necessary for plant growth. Due to their high solubility in water, nitrogen fertilizers dissolve rapidly in water (in less than ten minutes) [1]. Because of the limited opportunity for nitrogen compounds to be absorbed, only a small portion of the nitrogen is absorbed as nitrate by the roots [2, 3]. Therefore, the majority of dissolved urea enters surface and groundwater sources. Nitrogen solubility in water,

evaporation, oxidation and regeneration, nitrification, and denitrification are among the influential factors in wasting nitrogen fertilizers. Nitrates and nitrites are considered the most significant pollutants in surface and groundwater [2]. These pollutants lead to various dangerous diseases, such as methemoglobinemia and human cancers [4]. To reduce the waste of nitrogen from nitrogen fertilizers and also to reduce the pollution of surface and underground water with nitrate and nitrite, it is recommended to use coated fertilizers (coating the fertilizer with polymer using matrix or coating methods such as fluidized bed method, rotary

* Corresponding author; e-mail: k.shayesteh@uma.ac.ir

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drama, etc.) [5, 6]. The use of polymers as a useful solution for reducing nitrogen leaching has attracted the attention of many researchers. Biodegradable natural polymers, due to their abundance in nature, contribute to cost reduction and help reduce environmental pollution. One of these substances is lignin, extracted from black liquor, a waste product of wood and paper industries. Lignin is hydrophilic, so its structure needs to be modified as a fertilizer coating [7-12].

To predict the system's behavior, measuring the value of M_t at a specific time is necessary. Molecular diffusion is the process wherein molecules or particles move randomly from higher concentration to lower concentration areas. This phenomenon profoundly impacts various processes, such as the dispersion of medications, the flow of mass and heat, chemical reactions, and membrane separation. Several factors, including the medium, temperature, pressure, and the properties of the diffusing species, influence the D , which measures the diffusion rate [13]. Understanding this parameter is crucial for gaining insights into the underlying processes. Data related to mass transfer flux, release rate, partition coefficient (k), and permeability rate are all encompassed in this study [14]. In the following, the methods of determining D will be examined. Yum et al. [15] introduced a practical technique for D_s from single-component steady-state evaporative penetration studies. This method involves fitting experimental porosity data to a numerical diffusion equation solution. Huang et al. [16] developed a theoretical model to determine liquid D_s in polymer membranes, evaluating it with literature data from hexane-polyethylene and benzene-polyethylene systems. Walcher et al. [17] proposed a technique using a two-parameter function, $D = D_0 \cdot e^{\gamma c}$, where D_0 represents the intrinsic D , and γ is the plasticization parameter. The calculation of D_0 is obtained by fitting the asymptotic solution of the ideal diffusion theory to experimental infiltration data during the initial transient. The parameter γ can be determined only when evaporation reaches a steady condition. Dudek and Borys [18] presented a method for determining the D in solution diffusion models of hydrophilic membranes used in evaporation-based purification studies. Crank [19] calculated D based on the concentration-distance curve during an unsteady one-dimensional permeation process. The sample's concentration profile at time "t" is determined as a distance function. [20]. Rouholahnejad and Tabrizchi [21] introduced ion mobility spectroscopy to measure D_s rapidly in binary gas mixtures. This technique injects a brief sample pulse into the drift gas, forming a Gaussian concentration profile inside the drift area. A swarm of swiftly moving electrons irradiates this Gaussian cloud, producing negative ions. The spatial distribution of

molecules in the drift area is tracked, and D_s are derived from the gathered spectra using Gaussian functions. Sequential ion mobility spectroscopy spectra illustrate the temporal development of the cloud. Hamada and Anna [22] employed an approach based on directly measuring the spatial profile of a tracer's concentration using optical methods in a diffusion chamber. The peak width, height, and residence duration of the tracer concentration profile are used to compute the D . Additionally, they introduced a method based on the Einstein-Stokes Equation for calculating D . This involves directly measuring the spatial profile of the concentration of a tracer using optical techniques in a diffusion chamber. The concentration profile is obtained by recording images from the emission front of the tracer at different times, and these profiles are fitted by analytically solving the diffusion equation with D as the fitting parameter. The method was tested on a monodisperse suspension of spherical colloids, providing an estimate for D based on the Einstein-Stokes equation (Equation 1).

$$D = \frac{kT}{6\pi\mu r} \quad (1)$$

In this equation, k is the Boltzmann constant (J/K), μ is the dynamic viscosity (pa.s), and r is the radius of the particle (m).

Kouzoudis et al. [23] employed an experimental approach to ascertain the D by utilizing absorption data from magnetoelastic sensors, onto which a zeolite layer was synthesized. The D was determined by fitting the data with Fick's diffusion rules.

Payne and Morison [24] employed the Stefan-Maxwell model to simulate the diffusion of salt and water in cheese. This model represents the chemical potential gradient as a linear function of the flux of matter, as illustrated by Equation 2:

$$\frac{x_i}{RT} \left(\frac{\partial \mu_i}{\partial x} \right) = \sum_{j=1}^n \frac{x_i x_j}{D_{ij}^{SM}} (v_j - v_i) \quad (2)$$

In this equation, D_{ij}^{SM} is Stefan-Maxwell D ($m^2 \cdot s^{-1}$), R is the ideal gas constant ($8.314 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$), T , x_i , μ_i , and v_i are temperature (K), molar fraction, molar chemical potential ($\text{J} \cdot \text{mol}^{-1}$), and velocity relative to stationary coordinates ($\text{m} \cdot \text{s}^{-1}$), respectively [25].

In determining the D using the steady-state diffusion method, two situations are usually done [26-28]:

1. Fick's first law, shown in equation 3, describes the flux density (j_x) in the x direction against the concentration gradient as the partition coefficient. When the concentration gradient is divided by the concentration difference (ΔC_i) by the membrane thickness (δ), the j in the x direction is obtained according to equation 4, in which D_T is the transport diffusion.

$$j_i = -D_T \frac{\partial c}{\partial x} \quad (3)$$

$$j_x = -D_T \frac{\partial c}{\partial x} \approx -D_T \frac{C_i}{\delta} \quad (4)$$

2. From equation 5, from independent measurements of membrane permeability (P_i) and the adsorption constant (amount of gas adsorbed at each pressure, called solubility (S_i), which can be obtained from adsorption isotherms), D_T can be estimated.

$$P_i = S_i D_T \quad (5)$$

Dinesh [29] employed the time lag method for determining the D . This method utilizes experimental data and a mathematical equation associated with the asymptotic solution of the substance release graph from the membrane over time [30]. A more detailed explanation of this method is provided in Section 2.2.

This article will calculate the concentration profile numerically using the Crank-Nicolson method. Then, the total transferred nitrogen will be determined numerically. The following compares the mass of output from the modeling with the values calculated by Kjeldahl.

2. Material and Methods

The D of urea fertilizer coated with acetylated lignin sulfonate was determined using the time lag method. Initially, experimental data was employed to investigate M_t at specific time points. The intersection of the asymptote of this graph with the time axis provides the time lag, facilitating the calculation of D . Subsequently, utilizing the determined D , the concentration profile from the analyzed system was numerically solved. The parameters 'a' and 'b' denote the inner and outer average diameters of urea fertilizer coated with acetylated lignin sulfonate, measuring 0.2 and 0.219576 cm, respectively. The Kjeldahl method was utilized for nitrogen release measurement. The Crank-Nicolson method numerically determined the concentration profile and M_t .

2.1. Kjeldahl method

This method includes three stages: digestion, distillation, and titration. In digestion, sulfuric acid is first added to the sample to obtain the nitrogen as ammonium sulfate. In the distillation stage, ammonium sulfate is combined with some NaOH solution to release ammonia gas. Then, liquid ammonia enters the boric acid container by performing the refrigeration operation. The color change of the boric acid container (which contains methyl red and bromocresol green catalyst) indicates the formation of ammonium borate. In the titration step, ammonium borate is titrated

with sulfuric acid. Finally, the amount of acid consumed determines the sample's nitrogen percentage.

2.2. Modeling of the release process and the method of determining the D

Urea coated with acetylated lignin-sulfonate is slowly released into water or soil. The coating is a physical barrier that prevents the release of nitrogen. First, water must penetrate the coating to start the release. Therefore, it penetrates the membrane through the microscopic pores in the membrane. The water diffuses the acetylated lignin-sulfonate membrane, causing swelling of the coating. Swelling causes small cracks to be created in the lignin-sulfonate membrane, and as a result, the passage of water from the outside of the membrane to the inside expands. After the water reaches urea, urea dissolves in water according to its solubility. As long as solid urea is present in the membrane, the concentration of urea dissolved in the aqueous solution inside the membrane will always remain constant, according to the solubility of urea in water (if the temperature remains constant). Therefore, the diffusion process of dissolved urea into the environment begins [1, 31]. Urea can be dissolved in acetylated lignin-sulfonate coating depending on its preference. According to Figure 1, at $r=a$, if C_s is the solubility of urea in water, the equilibrium concentration of urea in the membrane is k times the equilibrium concentration of urea. Also, due to the aqueous environment's infinity, the membrane's concentration at $r=b$ equals zero. It should be mentioned that the membrane does not contain any effective substance before urea penetration. Figure 1 shows the membrane and an element of the membrane on which the mass balance of urea is written. Assuming the uniformity of the release from the coated urea fertilizer and writing the mass balance around the spherical element in the acetylated lignin-sulfonate coating, the PDE (Equation 6) of urea penetration into the coating is obtained. This equation is a function of time and radius.

$$\text{PDE: } \frac{\partial C}{\partial t} = \frac{D}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial C}{\partial r} \right) \quad (6)$$

Equation 1's initial and boundary conditions are written as equation 7, considering that no urea is present in the membrane at the beginning of the release process.

$$\left\{ \begin{array}{l} \text{B. C's} = \begin{cases} C = kC_s & \text{at } r = a \\ C = 0 & \text{at } r = b \end{cases} \\ \text{I. C: } C = 0 & \text{at } t = 0 \end{array} \right. \quad (7)$$

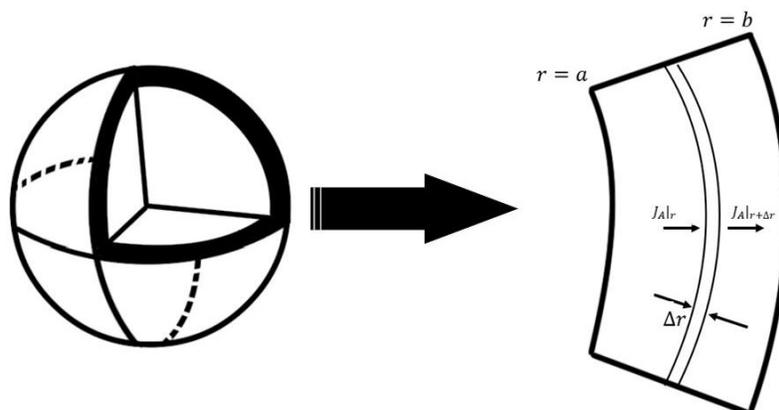


Fig. 1. Nitrogen balance in acetylated lignin-sulfonate biopolymer membrane

By examining the rate of urea release from the membrane to the aqueous environment in the laboratory, the graph of the output mass in terms of time for the fertilizer is obtained according to Figure 2. As mentioned before, the Kjeldahl device measured the concentration of nitrogen released in the water environment. According to the container volume in which the experiment was performed, the mass of nitrogen released per unit of time is determined by multiplying the volume by the nitrogen concentration in the container. Since each sample's release time is known, the total mass of released nitrogen is determined at a specific time. Due to the almost constant concentration inside and outside the membrane during the release time and the constant path of entering and leaving the water containing nitrogen from the membrane, most of the time, the amount of mass exiting the membrane per unit time is constant. Therefore, the amount of mass released after t is linearly related to time. Therefore, the amount of mass released after t is linearly related to time. Therefore, based on the time lag method, plotting M_t against t , a line

whose slope is $\frac{4\pi abDkC_s}{(b-a)}$ and its intercept is $-\frac{2\pi abkC_s(b-a)}{3}$ was obtained [30, 32]. According to Figure 2, the linearity of the shape can be seen most of the time. Therefore, the value of k is obtained from the intercept, and the value of D from the slope of the line is obtained from the modified lignin-sulfonate membrane. Also, in the beginning, and according to Figure 2, it takes time for water to find pores to penetrate the membrane. Then, the dissolution of nitrogen in water should happen. Finally, the reverse diffusion of water-soluble nitrogen from inside the membrane to the water environment occurs. This time, according to Figure 2, is known as time lag. The Kjeldahl test can only measure the concentration of the effective substance once it reaches a certain level. Therefore, after more time, the concentration of the effective substance can be measured with the help of the Kjeldahl test. Therefore, D in this method is slightly smaller than the actual value. It should be noted that the higher the sensitivity of the analyzer, the lower the measurement error of D by the time lag method.

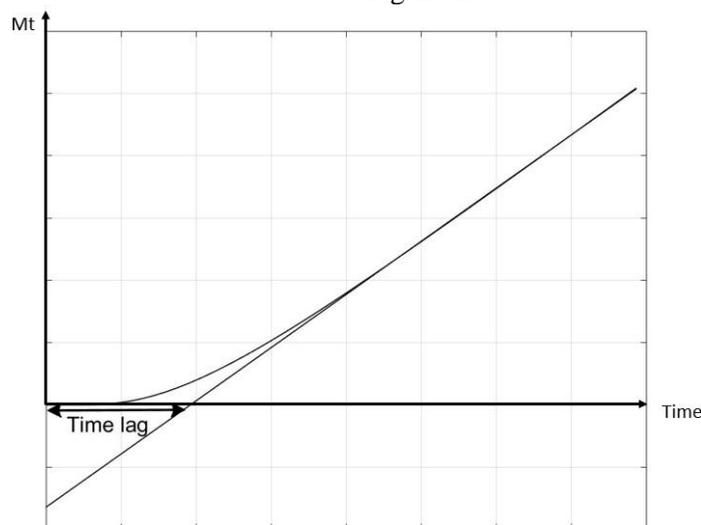


Fig. 2. The diagram of the time lag method

2.3. Determining the concentration profile by Crank–Nicolson method

It is usually suggested that numerical methods be used to solve PDEs. Because with a slight change in PDE, boundary and initial conditions, molecular diffusion coefficient, thermal diffusion coefficient, or kinematic viscosity, it is rarely possible to solve PDE analytically. Therefore, this article used the Crank-Nicolson method to solve PDE. One of the great merits of the Crank-Nicolson method is its permanent stability. To solve PDE, first, the distance between points a and b is divided into N equal parts (Equation 8). Therefore, the total number of unknown nodes can be N+1 in the direction of the radius. Considering the stability of the Crank-Nicolson method,

the time step can be chosen as a large number. However, Δt should be selected so that the changes in nitrogen concentration with time are noticeable and specific.

$$\Delta r = \frac{b-a}{N} \quad (8)$$

Figure 3 shows the finite difference discretization for the PDE solution. According to Figure 3, the nodes are presented in the radial direction and at different two times. The concentration values at $i=1$ and $i=N+1$ for $m>0$ are the boundary conditions of the problem. According to equation 7, the concentration values of the boundaries at $t>0$ are fixed numbers; Therefore, with the determination of the concentration in $i=1$ and $i=N+1$, the number of unknowns in each time step $m+1$ is equal to $N-1$.

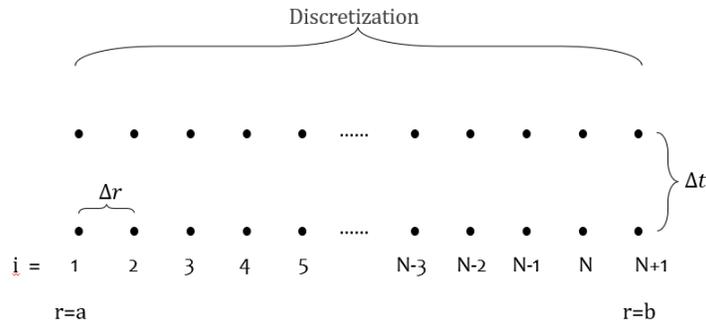


Fig. 3. Finite difference discretization

Now, for the $\partial C/\partial t$ term, the Forward Difference Method is used, and for the $(\partial^2 C)/(\partial r^2)$ and $\partial C/\partial r$ terms, the Central Difference Method is used based on the past and present average (Equations 9-11).

$$\frac{\partial C}{\partial t} = \frac{C_i^{m+1} - C_i^m}{\Delta t} \quad (9)$$

$$\frac{\partial C}{\partial r} = \frac{1}{2} \left[\frac{C_{i+1}^{m+1} - C_{i-1}^{m+1}}{2\Delta r} + \frac{C_{i+1}^m - C_{i-1}^m}{2\Delta r} \right] \quad (10)$$

$$\frac{\partial^2 C}{\partial r^2} = \frac{1}{2} \left[\frac{C_{i+1}^{m+1} - 2C_i^{m+1} + C_{i-1}^{m+1}}{\Delta r^2} + \frac{C_{i+1}^m - 2C_i^m + C_{i-1}^m}{\Delta r^2} \right] \quad (11)$$

Similarly, the value of 'r' is calculated from equation 12, where 'i' is the counter of the space unit that starts from one and ends at N+1.

$$r = a + i\Delta r \quad (12)$$

A System of linear equations is obtained by placing equations 9-12 in equation 6, shown in equation 13.

$$\left(\frac{D \Delta t}{2(a+i \Delta r) \Delta r} + \frac{D \Delta t}{2\Delta r^2} \right) C_{i+1}^{m+1} + \left(\frac{-D \Delta t}{\Delta r^2} - 1 \right) C_i^{m+1} + \left(\frac{-D \Delta t}{2(a+i \Delta r) \Delta r} + \frac{D \Delta t}{2\Delta r^2} \right) C_{i-1}^{m+1} = - \left(\frac{D \Delta t}{2(a+i \Delta r) \Delta r} + \frac{D \Delta t}{2\Delta r^2} \right) C_{i+1}^m - \left(\frac{-D \Delta t}{\Delta r^2} + 1 \right) C_i^m - \left(\frac{-D \Delta t}{2(a+i \Delta r) \Delta r} + \frac{D \Delta t}{2\Delta r^2} \right) C_{i-1}^m \quad (13)$$

Also, for nodes 1 and N+1, boundary conditions in $r=a$ and $r=b$ are used (Equations 14 & 15).

$$C_1^{m+1} = k C_A^* \quad (14)$$

$$C_{N+1}^{m+1} = 0 \quad (15)$$

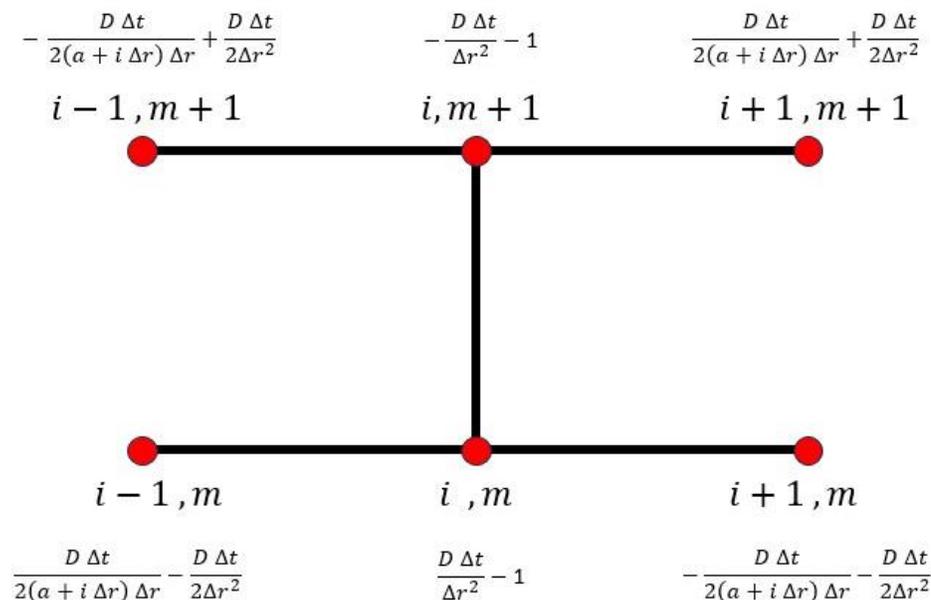


Fig. 4. The Molecule of the system based on the Crank-Nicolson method

With the obtained equations, the matrix of coefficients (A) and the matrix B, which includes the known values of the equations at present, are obtained (Figure 4). To determine the concentration of the nutrient C^{m+1} at present, it is necessary to multiply the inverse of the matrix of coefficients in matrix B (Equation 16).

$$C^{m+1} = A^{-1} \times B \quad (16)$$

In the next step, the calculated concentrations are placed in the time counter m , and the above steps are repeated for the next time with an interval of Δt from this time. By solving these equations, the concentration diagram for different times is obtained.

Also, by knowing the concentration of two final nodes (N and $N+1$) and determining the concentration gradient at $r=b$, M_t can be calculated (Equation 17). It should be noted that the dimension of concentration is g/L .

$$M_t = \int_0^t -4\pi b^2 D \frac{\partial C}{\partial r_{r=b}} dt \quad (17)$$

According to this article, the nitrogen concentration profile inside the membrane at any moment has been determined numerically; Therefore, equation 17 should be solved numerically. In this article, the above integral (Equation 17) is solved with the help of Simpson's 1/3 rule. Therefore, the value of the function inside the integral must be calculated first. For this purpose, the backward finite difference is used for the location derivative term to calculate the M_t value by having the concentration profile at each t (Equation 18). The time step of the integral is calculated from equation 19. The condition of using

Simpson's 1/3 rule is that the number of divisions (P) must be even.

$$f = -4\pi b^2 D \frac{C_{N+1}^m - C_N^m}{\Delta r} \quad (18)$$

$$\Delta t = \frac{t-0}{P} \quad (19)$$

Therefore, the value of M_t is calculated using MATLAB software and equation 20, which is Simpson's 1/3 rule according to equation 18.

$$\text{simpson}_{\frac{1}{3}} = \frac{\Delta t}{3} (f(a) + 4f(a+h) + 2f(a+2h) + \dots + 2f(a+(P-2)h) + 4f(a+(P-1)h) + f(b)) \quad (20)$$

3. Results and Discussion

The results of the release rate from slow-release urea fertilizer are presented in Figure 5. In Figure 5, the time lag method leads to a small error according to the linear trend of the release up to about 40000 seconds. In the time lag method, using the best transmissive line of the total mass exiting the membrane determined in the laboratory per time, two values of D and k of nitrogen can be obtained between the solution and the membrane. Considering that the release time is known for each sample, the total mass of nitrogen transferred to the environment is determined at a specific time by measuring the released nitrogen concentration. Since the driving force on both sides of the membrane is almost constant during the release time and the constant path of the fluid entering and leaving the membrane at all times, except for the initial release times, the intensity of mass transfer can be considered constant.

Therefore, the value of M_t increases linearly with increasing time. According to Figure 5, the linear equation was obtained with the help of linear fitting for the experimental data. According to the equations mentioned in section 2.2, having the fertilizer's radius, the coating's thickness, and the urea's solubility in water at the test

temperature, the value of k is calculated first from the intercept. Then, knowing k and using the slope of the line, the D can be calculated. According to the slope value of the line, 1.744×10^{-6} , and the intercept -1.769×10^{-3} , the k was calculated as 1.709528 and the D as $5.931639 \times 10^{-8} \text{ cm}^2/\text{s}$.

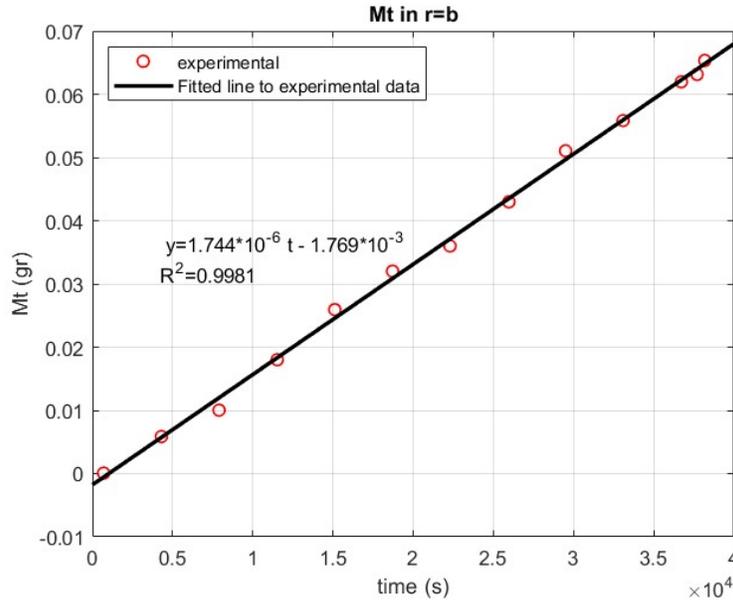


Fig. 5. M_t changes over time and best line fit.

Also, based on Figure 6, by drawing the best line of experimental M_t in terms of time, the maximum time when M_t was not released from the membrane to the aqueous environment is 1014 seconds. This time is called lag time.

Based on the time lag method, it is expected that up to 1014 seconds, nitrogen will not be transferred from the modified lignin-sulfonate coating to the aqueous environment.

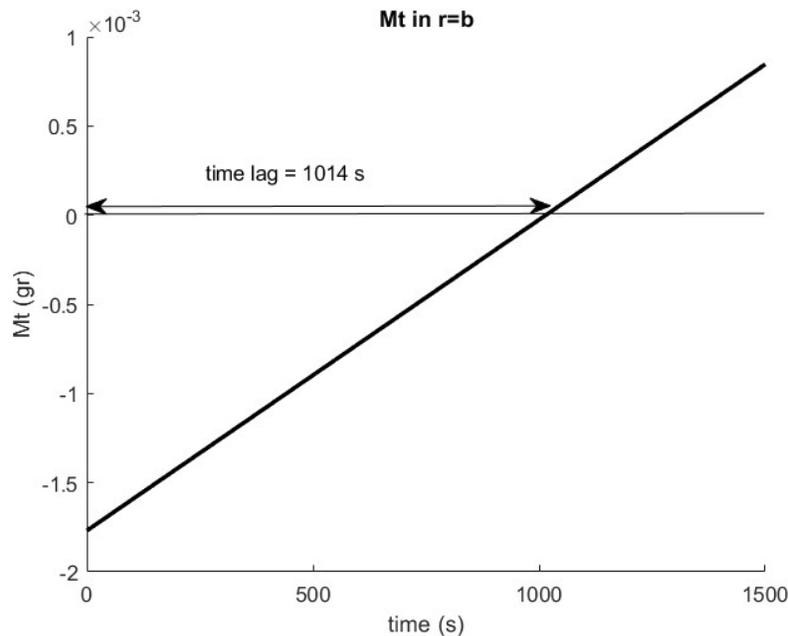


Fig. 6. Determining the lag time of modified lignin-sulfonate coating

Now, with the values of k and D , equation 6 can be solved numerically to obtain the concentration profile inside the membrane. As mentioned in section 2.3, the Crank-Nicolson method solved the PDE governing the modified lignin sulfonate membrane. Considering that the Crank-Nicolson method creates a good balance between past and present time, it is expected to have less error than the excellent Fully Implicit method. Also, in this method, because it always leads to a convergent solution, the solution can be reached faster by choosing larger time steps. This causes this method to achieve a solution with a higher convergence speed than the Explicit Method. Also, the Crank-Nicolson method uses 6 points to obtain the unknown concentration, while the implicit method uses the previous 3 points. Therefore, Crank Nicholson uses more data, which is more powerful than the implicit method. This article divided the number of spatial steps in the distance from a to b into $N=100$ equal parts ($\Delta r=0.00019$ cm). Also, the time step was considered $\Delta t=1$ sec. To solve spatial nodes in $m+1$ time, 99 equations must be written to determine 99 unknown nodes. The matrix of coefficients is obtained from equations 13-15. Then, the concentration of

unknown nodes is determined by solving 99×99 linear equations in each time step.

Figure 7 shows the concentration changes over time. It should be noted that the calculated concentrations are needed as initial concentrations for the next step. For example, to determine the concentration after 12000 seconds, considering that the time step is equal to 1 second, 12000-time steps must be solved, and 99 equations should be solved each time (1188000 equations) to obtain the concentration profile at 12000 seconds according to Figure 7. Among the other interesting points obtained from Figure 7, we can refer to the graph presented at 12000 seconds, which is linear ($R^2=1$). In other words, it indicates that the concentration is no longer a function of time. Also, by observing the concentration profile at 2000 seconds, it can be seen that the concentration profile is very close to the profile at 12000 seconds. Investigations show that in about 3000 seconds, the concentration profile becomes completely linear and consistent with the concentration profile in 12000 seconds. Also, at a time higher than 3000 seconds, due to the stability of the concentration profile per time, the concentration profile is independent of time, and the system is steady-state.

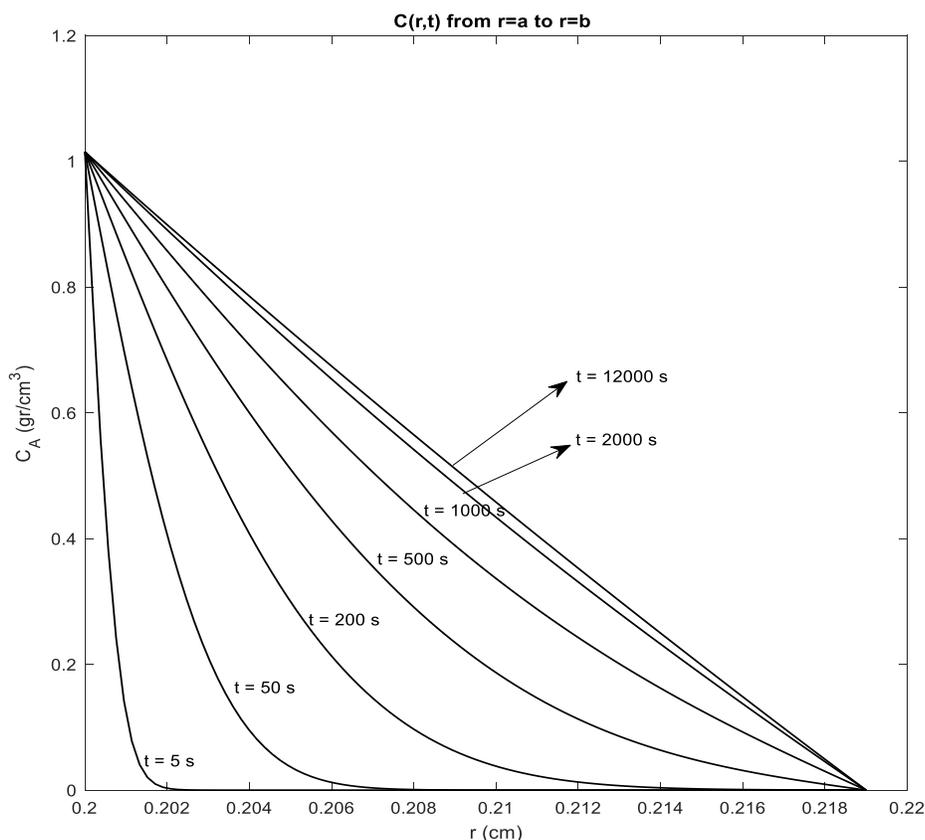


Fig. 7. Nitrogen concentration profile in the membrane at different times

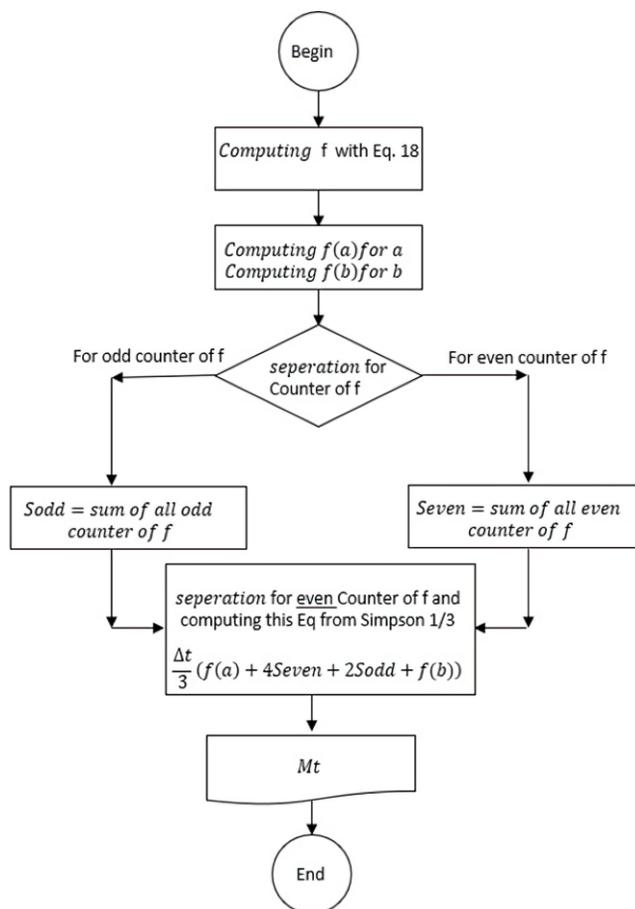


Fig. 8. Algorithm to determine M_t per time

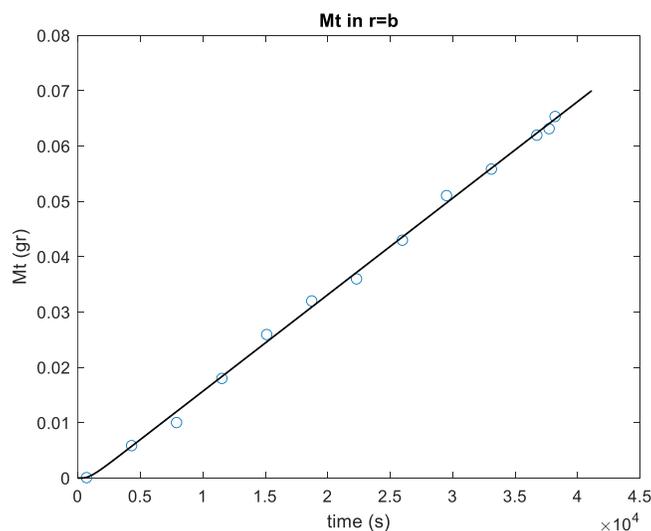


Fig. 9. Changes of M_t , total released nitrogen per time-based on numerical method and experimental data

Equations 17-20 are used to calculate M_t . Based on the algorithm presented in Figure 8; M_t can be determined as a function of time or independent of time.

Figure 9 shows M_t values obtained from the numerical method compared with the experimental data. The results show the numerical method's high accuracy. In other

words, the numerical method is highly able to predict the experimental data.

This paper presents the error of experimental and calculated M_t values in Table 1. Table 1 also presents the relative error of the prediction method compared to the experimental data. The results show that the maximum relative error was obtained in 7895 seconds after the release. This error is probably the error of the equipment or the tester.

Coated urea fertilizer releases nutrients more slowly and has a much slower release than uncoated urea fertilizer. This has led to a reduction in the frequency of fertilization and minimized fertilizer waste issues. Consequently, it helps prevent nitrates and nitrites from contaminating water sources, reducing environmental problems and the risk of irreparable diseases such as methemoglobinemia and cancer.

Table 1. Comparison of M_t obtained from numerical method and experimental data

Time	Numerical	Experimental	Error
4299	0.005736	0.00586	2.12
7895	0.012011	0.01003	19.75
11522	0.018343	0.018006	1.87
15112	0.02461	0.025936	5.11
18714	0.030898	0.032009	3.47
22297	0.037151	0.035997	3.21
25968	0.043559	0.042983	1.34
29501	0.049727	0.05105	2.59
33091	0.055994	0.05593	0.29
36724	0.062335	0.061964	0.60
37705	0.064048	0.063136	1.44
38183	0.064882	0.065343	0.70

4. Conclusion

Acetylated lignin sulfonate was prepared to produce a slow-release fertilizer. The system's behavior is predicted by modeling the nitrogen diffusion process in the fertilizer coating, and the effect of different parameters, such as D , is obtained. The concentration profile was calculated numerically using the Crank-Nicolson method. For this purpose, the D was first calculated using the time lag method equal to 5.931639×10^{-8} cm²/s. The backward difference method and Simpson's 1/3 rule were used to calculate M_t numerically. During the release process, the concentration inside and outside the membrane remains almost constant, and a constant flow of water containing nitrogen enters and exits the membrane. As a result, the value of M_t remains constant most of the time. When urea fertilizer is finished in solid form, the concentration profile decreases. Observing the concentration profile shows that the profile at 2000 seconds is very similar to the profile at 12000 seconds. Therefore, it can be considered linear with a small error. Also, after 3000 seconds, the system will be in a steady state. Considering the linear trend of the release up to about 40000 seconds, using the time lag method leads to a small error. The data obtained from the numerical method and the experimental data were compared. The results showed that the numerical method (Crank-Nicolson) has high accuracy and will have a very low

relative error. The most significant error was related to the time of 7895 seconds, which is 19.75%. Also, the lowest error was for 33091 seconds, with a 0.29% error. According to the physics and the second boundary condition of equation 7, this paper was investigated for infinite volume. In future works, this case will be investigated in finite volume and even in perfectly mixed conditions.

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