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## Use of Multi-Diffusion Model to Study the Release of Urea from Urea Fertilizer Coated with Polyurethane-Like Coating (PULC)

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### Abstract

Controlled release fertilizer (CRF) play an important role in nutrient loss prevention and plant's uptake efficiency. This study uses a multi-diffusion model to simulate urea release from urea fertilizers coated with polyurethane-like coating (PULC). In this model, finite element method (FEM) and 2D geometry are applied for three sizes of urea granule using COMSOL Multiphysics software. Modeling results are in agreement with the experimental data for the "constant release" stage. Standard error of estimate (SEE) ranges from 0.00417 to 0.02084 in these simulations. Besides, relationship of coating thickness with release time and percent of urea released at the end of "constant release" stage has also been established.

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### 1. Introduction

Controlled release fertilizer (CRF) is meant to control the release of nutrients over the time instead of quickly dissolving in the moist soil after fertilizer application. Nutrient concentration is kept at appropriate level so that it helps to prevent nutrient loss and enhance nutrient utilization efficiency by plants [1]. The amount of fertilizers received by plant when applied in conventional forms is only 30-50%. However, CRFs

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resulted in minimum losses of the fertilizer which may be caused by volatilization or leaching, thus preventing the seedling damage. CRFs also provide good protection to ecosystem if the carrier/coating material is biodegradable [2]. Urea was selected as the material to be coated because of its high nitrogen content, low cost, and commercial availability [3].

First study on the application of controlled release technology to fertilizers was conducted in 1962 by Ortil et al. [4]. Nutrient released from CRFs are usually controlled by the diffusion through the coating layer. One of the major factors controlling the release of CRFs is the rupture of the coating membrane found in sulphur coated urea (SCU). Glaser et al. studied the release of polymer-coated granule and applied one-dimensional coordinate diffusion system in 1987 [4]. Gambash et al. used semi-empirical model in their study, and the effect of geometry and size was ignored. Besides these assumptions, the lag period, during which no release is observed, was not included [5]. Lu and Lee applied the Fick's law in spherical coordinate for the release of latex coated urea (LCU) [6]. Al-Zahrani modeled unsteady state release from polymeric membrane particle and assumed a well-mixed condition inside sphere particle [2]. Most of these modeling efforts were based on the assumption that the release of nutrients from coated fertilizer is controlled by simple solute diffusion. Based on Raban's experiments, it is proved that the release from a single granule of a polymer coated CRF consists of three stages: an initial stage during which no release is observed (lag period), a stage of constant release, and finally a stage of gradual decay of the release rate [4]. In 2007, Lu proposed a mathematical model for the release of a scoop of polymer coated urea which also took into account the effect of population of granules. This model was based on mass balance equation of pseudo-steady state of Fick's law. However, the first stage of release process was neglected [7].

Most of the studies in this area only concentrate on the simple diffusion of urea through coating layer without considering the diffusion through multilayer (coating and environment). To have a deeper insight into the "constant release" process of urea, this study investigates the release of urea from urea fertilizer coated with polyurethane-like coating (PULC).

## 2. Model Development

Fig. 1a illustrates the dissolution model of a spherical urea granule. In this model, coated urea granule is surrounded by water environment (fluid zone). Urea granule consists of two parts: urea core and coating layer outside the urea core. Model assumes that coating layer is saturated with water at the time when the release begins. Water at the surface of urea core will start dissolving solid urea. This urea solution is kept at saturated level; as long as solid urea exists in the core. Urea starts releasing through the coating layer by means of diffusion. Based on mass transport equation in porous medium, a transient stage for urea diffusion through the coating layer can be written as in Eq. 1 [7]

$$D_e \left[ \frac{\partial^2 C}{\partial r^2} + \frac{2}{r} \frac{\partial C}{\partial r} \right] = \varepsilon \frac{\partial C}{\partial t} \quad (1)$$

Since the urea pellet is motionless, it is assumed that urea flux from the coating interface to the liquid is controlled by the diffusion of urea in liquid. Hence, it is calculated on the basis of mass transport equation of urea in water as follows Eq. 2 and Eq. 3:

### Nomenclature

$C$  is concentration of urea, mol/m<sup>3</sup>  
 $D_e$  is effective diffusivity of urea in porous medium (coating), m<sup>2</sup>/s  
 $D_{urea}$  is diffusivity of urea in liquid, m<sup>2</sup>/s  
 $\varepsilon$  is porosity of the coating, %  
 $J_{Urea}$  is the diffusive flux at outer shell of urea granule in mol/(m<sup>2</sup>.s)  
 $l$  is coating thickness, mm  
 $m_{core}$  is mass of urea in core, g  
 $m_{sat}$  is mass of urea in core when solid core is totally dissolved, g  
 $R_0$  is urea core radius, mm

$$D_{urea} \frac{\partial^2 C}{\partial r^2} + \frac{2D_{urea}}{r} \frac{\partial C}{\partial r} = \frac{\partial C}{\partial t} \tag{2}$$

$$D_{urea} = (1.380 - 0.0782C + 0.00464C^2) 10^{-5} \text{ cm}^2/\text{s} \tag{3}$$

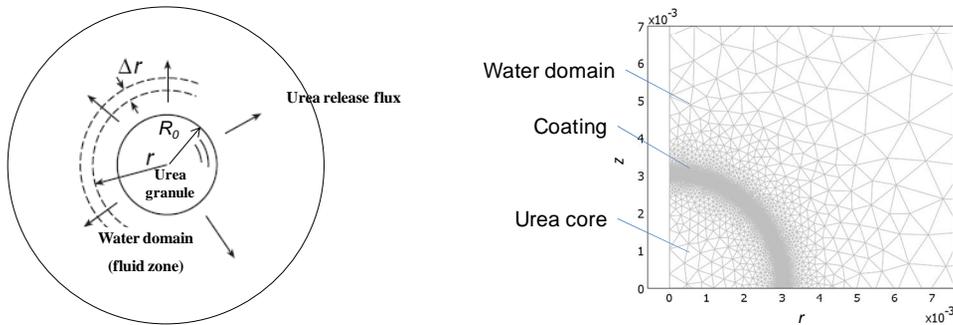


Fig. 1. (a) Dissolution model of a spherical urea; (b) Mesh generation for urea dissolution models for coated urea.

Finite element method (FEM) and 2D geometry are proposed for solving urea release model. Model is specified for single CRF granule coated with polyurethane-like coating (PULC) material. These data are based on previous publication of Shaviv et al. [4]. Geometry and meshing are done for single urea granule as in Fig. 1b. Fluid zone diameter i.e. the distance from center of urea granule to water boundary, is set to 22 times of core radius ( $R_0$ ) [8]. Initial values and boundary conditions are specified for the model. At the time  $t_0$  (obtained from experiment), urea solution at the surface of urea core is saturated, and concentration is zero at the outer layer of fluid field. In these simulations, urea release time depends on the amount of urea (size and shape) and coating material properties (thickness, diffusivity, porosity). A stop condition is specified for the constant release whenever solid urea core is totally dissolved. At this time, the whole urea core is liquid and equivalent to saturated urea concentration ( $m_{core} = m_{sat}$ ).

### 3. Simulation Results and Model Validation

Validation process uses experimental results of Shaviv [4]. Experiments were performed with spherical and non-damaged single granules which were coated with polyurethane-like coating (PULC) material. The coating thicknesses of these granules were 0.1167, 0.1500, 0.2000 mm. In the current study, they are designated as PULC 1, PULC 2, PULC 3 respectively in the simulations. Effective diffusivity, in all three simulations, is  $2.5 \times 10^{-5} \text{ cm}^2/\text{day}$ . Experimental release data is extracted using Engauge Digitizer 4.1, and all simulation results are compared with the extracted data.

Table 1. Summary of simulation data and results

No.	Code	Core Radius $R_0$ (mm)	Coating Thickness $l$ (mm)	Lag time $t_0$ (days)	Release time (day)	Urea Release (%)	SEE
1	PULC 1	1.2	0.1167	2	18.90	44.83%	0.02084
2	PULC 2	1.2	0.1500	2	22.72	42.97%	0.01145
3	PULC 3	1.2	0.2000	3	28.46	39.65%	0.00417

Simulation results are presented in Table 1 and Fig. 2. The difference between simulation and experimental

data can be explained by the difference in shape of urea granule. In the model, urea granule is a sphere while real urea granule is not exactly spherical in shape. Secondly, experimental observations are obtained for a population of granules instead of single granule as in simulations. Therefore, the variation in amount of urea and coating characteristics in population is not included in simulation results.

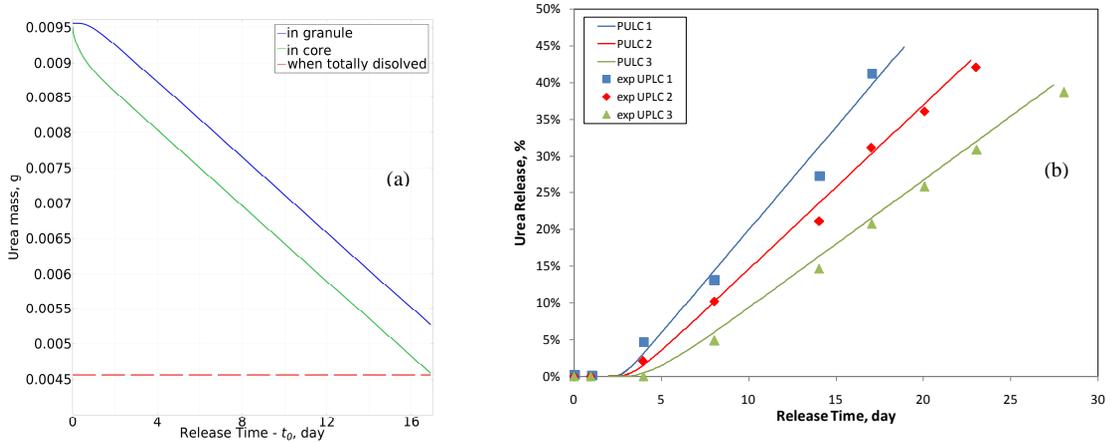


Fig. 2. (a) Urea mass profile in granule and core;

(b) Comparison of simulated and experimental urea release profile [4]

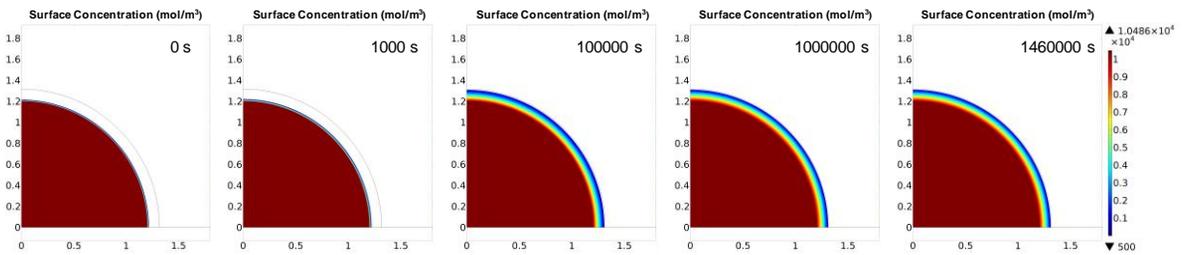


Fig. 3. Concentration profile of urea in coating layer during "constant release" stage ( $\tau = \text{release time} - t_0$ )

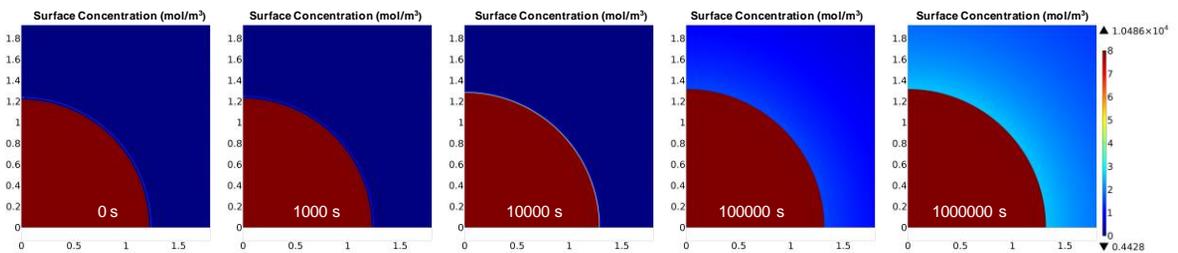


Fig. 4. Release profile of urea in water zone during "constant release" stage ( $\tau = \text{release time} - t_0$ )

The change of urea mass in core and in overall coated granule is shown as a function of release time in the simulation is shown in Fig. 2a. At time  $t_0$ , urea core is dissolved by water in the coating layer and urea concentration in urea core is kept at saturated level. As in Fig. 2a, granule mass remains constant, while core mass quickly decreases at the beginning of the release. The delay in urea release can be explained by looking into the urea concentration profile (Fig. 3). Urea is not present in coating layer at time  $t_0$ . After the urea is dissolved, it still has to pass through the coating layer before releasing to the environment (Fig. 3,  $\tau = 0$ ; 1000s). As urea reaches interface between coating and environment, the release begins and its rate increases until reaching constant. During constant release stage, amount of urea gone into the coating equals to the

amount of urea released to the environment. This is demonstrated by the zone where curves for urea mass in core and granule are parallel to each other as shown in Fig. 2a. It also shows in Fig. 3 ( $\tau = 10000; 100000; 1460000$ ) that there is no change in urea concentration in the coating layer. The constant release stage will end when solid urea is totally dissolved. At this moment, urea mass is equivalent to saturated urea concentration.

A study on the released urea in water is shown in Fig. 4. First, there is no urea in water zone, and hence the urea concentration in water zone does not change during the time 0, 1000 and  $10^4$  s. From  $10^4$  to  $10^6$  s, urea concentration in water zone keeps increasing during constant release because of urea accumulation.

Simulations also show a linear relationship between coating thickness and release time (Eq. 4), percent of urea at the end of “constant release” stage (Eq. 5). These equations are:

$$\text{Release time (day)} = 102.19 l + 7.1285 \quad (4)$$

$$\text{Urea released (\%)} = -0.6246 l + 0.522 \quad (5)$$

#### 4. Conclusion

By applying FEM to the urea diffusion process, a model for the release from PULC urea granule has been formed for “constant-release” stage. The granule shows no release at the beginning of the simulation due to the time taken by the urea solution to reach the coating-environment interface. After reaching the interface, the release rate keeps increasing for some time and finally becomes constant till the end of the ‘constant release’ period. Simulation results are in good agreement with the experimental data. The minor discrepancies are attributed to imperfection of granular shape and the effect of granular population. A better understanding on release process is obtained based on 2D-FEM model. However, this model focuses mainly on the “constant release” stage. It needs to enhance to suit with three stage of the release.

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