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INVESTIGATION OF COMPACT FINITE DIFFERENCE SOLUTIONS OF STEFAN PROBLEM WITH DIFFERENT BOUNDARY CONDITIONS

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ABSTRACT. In this work, two soybean hydration models are investigated as Stefan problem. Both models have variable diffusivity coefficient but have distinct surface boundary conditions. These models solved by Variable Space Grid (VSG) method with sixth order compact finite difference scheme (CFD6) and examined effect of method on the models and compared solutions between the models.

1. INTRODUCTION

Many physical problems which include volume variation or movement of system boundaries are modeled as Stefan problem which is a particular kind of boundary value problems, adapted the case the one of the boundary is moving and its motion is depend on time. One of the applications of Stefan problem is soybean hydration process. In this process, when the water enters the system the increase in size of the grain occurs. The models which take into account soybean hydration process can be dealt with two categories. These categories can be classified as having constant diffusivity and having variable diffusivity which varies exponentially with moisture content of soybean. In addition, these models are investigated with distinct surface boundary condition and as a result one obtains different model for soybean hydration process. In this study two models which have variable diffusivity are investigated as Stefan problem. In the first model the boundary condition reaches equilibrium moisture content at the beginning of the soaking and in the second model the boundary condition represents that diffusive flux is equal to convective flux at the surface.

Many authors have dedicated to the model has the boundary condition that reaches equilibrium moisture content at the beginning of soaking [1, 2, 3].

Yüzgeç et al. [4] solved the model has boundary condition that equality of diffusive and convective fluxes at the surface of drying of granular baker's yeast.

Engels et al. [5] proposed a diffusion model for rice hydration and solved the system with three different boundary conditions at the surface.

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The authors are mentioned above did not take into account the model as Stefan Problem. On the other hand Barry and Caunce [6], Davet et al. [7], McGuinness et al. [8], Nicolin et al. [9] and Nicolin et al. [10] consider the swelling problems as a Stefan problem.

Nicolin et al. [9] solved the model have variable diffusivity and the boundary condition that equilibrium moisture is instantly reached at the surface. They solved problem two type of soybean by using Variable Space Grid (VSG) method with finite difference scheme and compared solutions with experimental data. Again Nicolin et al. [10] solved the model with boundary condition that diffusive flux is equal to convective flux at the surface by the same method in Nicolin et al. [9].

In this work, we improved VSG by using sixth order compact finite difference scheme for two models and investigate effect of the method on the models and compared solutions between the models.

2. Mathematical Models

The model was obtained by transient mass balance on differential volume element of soybean grains. Since the geometry of soybeans are assumed spherical and equation (2.1) represents water absorbtion by soybean is developed in spherical coordinates based on Fick's law of diffusion. It is assumed that diffusion takes place only in radial direction,

$$\frac{\partial X}{\partial t} = D\left(\frac{2}{r}\frac{\partial X}{\partial r} + \frac{\partial^2 X}{\partial r^2}\right) \tag{2.1}$$

where X is the moisture content of the grain, r is the radial coordinate, D is the diffusion coefficient and t is the time coordinate.

Equation (2.1) is second order partial differential equation. For solving the model one initial condition and two boundary conditions which are adopted for the center and the surface are required. Equation (2.2) gives the initial condition which is uniform throughout the dry solid at time $t = 0$,

$$X(r,t) = X_0, \qquad t = 0 \tag{2.2}$$

and equation (2.3) defines symmetry of the problem in the center of the grain in any instant of time,

$$\frac{\partial X}{\partial r} = 0, \quad r = 0, \qquad t > 0\,. \tag{2.3}$$

In this study, two cases are investigated for surface boundary conditions. For the first model, equation (2.4) represents moisture content on the solid-fluid ($r = R(t)$) and it reaches equilibrium moisture content at the beginning of the soaking,

$$X = X_{eq}, \quad r = R(t), \quad t > 0 \tag{2.4}$$

where, X_{eq} is equilibrium moisture content which is obtained by experimental data.

In the second model, equation (2.5) is surface boundary condition where the diffusive flux is equal to the convective flux, which is represented by the driving force given by the difference between surface and equilibrium moisture content.

$$-\rho_{DS} D\frac{\partial X}{\partial r} = K_C(X_S - X_{eq}), \quad r = R(t), \quad t > 0 \tag{2.5}$$

where X_s is the moisture at the surface of the grain, K_C is the coefficient of convective mass transfer and ρ_{DS} density of the dry solid.

The position of moving boundary, radius, is given mass balance equation known as Stefan condition,

$$\frac{dR(t)}{dt} = \alpha \frac{\partial X}{\partial r}, \quad r = R(t) \tag{2.6}$$

subject to initial condition, $R(0) = R_0$. For soybeaan hydration model, $\alpha = D\frac{\rho_{DS}}{\rho_{H_2O}}$ is obtained by Nicolin et al [9], where ρ_{DS} is the density of the dry solid, ρ_{H_2O} is the density of the water and R_0 is the initial radius.

The boundary condition is defined by equation (2.3) causes an indeterminacy in the equation (2.1) since the equation (2.1) is not defined at the center of the grain. Therefore, L' Hospital rule was applied to equation (2.1) to obtain the solution for the center [9].

$$\frac{\partial X}{\partial t} = 3D\frac{\partial^2 X}{\partial r^2}\,. \tag{2.7}$$

3. Compact Finite Difference Scheme

Compact finite difference schemes (CFD) can be dealt with two kind of categories. These are explicit compact finite differences which computes the numerical derivatives at each grid by using large stencils and implicit compact finite differences which evaluates the numerical derivatives through solving a system of linear equation by using smaller stencil [11, 12, 13].

Spatial derivatives are computed by the compact finite difference scheme. A uniform 1D mesh consisting of N points: $r_1 < r_2 < ... < r_N$. The mesh size $\Delta r = r_{i+1} - r_i$ is equal at any instant of time. The first derivatives are for all interior points (r_i, t^j), $2 \leq i \leq N-1$ is given by equation (3.1) [14].

$$\begin{aligned} \alpha X'(r_{i+1}, t^j) + X'(r_i, t^j) + \alpha X'(r_{i-1}, t^j) &= b\frac{X(r_{i+2}, t^j) - X(r_{i-2}, t^j)}{4\Delta r^j} \\ &\quad + a\frac{X(r_{i+1}, t^j) - X(r_{i+1, t^j})}{2\Delta r^j} \end{aligned} \tag{3.1}$$

which provides one parameter α-family of fourth order tridiagonal schemes with

$$a = \frac{2}{3}(\alpha + 2) \quad b = \frac{1}{3}(4\alpha - 1)\,.$$

In this study we use sixth order compact finite difference scheme. For $\alpha = \frac{1}{4}$ sixth order tridiagonal scheme as in the system (3.2)

$$\begin{aligned} X'_i + 5X'_{i+1} &= \frac{1}{\Delta r}\left(-\frac{197}{60}X_i - \frac{5}{12}X_{i+1} + 5X_{i+2} - \frac{5}{3}X_{i+3} \right. \\ &\quad \left. + \frac{5}{12}X_{i+4} - \frac{1}{20}X_{i+5}\right), i = 1\,; \end{aligned} \tag{3.2}$$

$$\begin{aligned}
\frac{2}{11}X'_{i-1} + X'_i + \frac{2}{11}X_{i-1} &= \frac{1}{\Delta r}\left(-\frac{20}{33}X_{i-1} - \frac{35}{132}X_i + \frac{34}{33}X_{i+1} - \frac{7}{33}X_{i+2}\right. \\
&\quad \left. + \frac{2}{33}X_{i+3} - \frac{1}{132}X_{i+4}\right), i = 2\,; \\
\frac{1}{3}X'_{i-1} + X'_i + \frac{1}{3}X'_{i+1} &= \frac{1}{4\Delta r}\left(\frac{1}{9}X_{i+2} - \frac{1}{9}X_{i-2}\right) \\
&\quad + \frac{1}{2\Delta r}\left(\frac{14}{9}X_{i+1} - \frac{14}{9}X_{i-1}\right), i = 3, 4, ..., N-2\,; \\
\frac{2}{11}X'_{i-1} + X'_i + \frac{2}{11}X_{i+1} &= \frac{1}{\Delta r}\left(\frac{20}{33}X_{i+1} + \frac{35}{132}X_i - \frac{34}{33}X_{i-1}\right. \\
&\quad \left. + \frac{7}{33}X_{i-2} - \frac{2}{33}X_{i-3} + \frac{1}{132}X_{i-4}\right), i = N-1\,; \\
5X'_{i-1} + X'_i &= \frac{1}{\Delta r}\left(\frac{197}{60}X_i + \frac{5}{12}X_{i-1} - 5X_{i-2}\right. \\
&\quad \left. + \frac{5}{3}X_{i-4} + \frac{1}{20}X_{i-5}\right), i = N\,.
\end{aligned}$$

The system (3.2) can be expressed by vector-matrix form:

$$AX' = \frac{1}{\Delta r}BX\,,$$

where $X = (X_1, X_2, ..., X_N)^T$. The second order derivative terms are obtained by applying the first operator twice,

$$AX'' = \frac{1}{(\Delta r)^2}BX'\,,$$

where

$$A = \begin{bmatrix}
1 & 5 & & & & & \\
\frac{2}{11} & 1 & \frac{2}{11} & & & & \\
\frac{1}{3} & 1 & \frac{1}{3} & & & & \\
 & \ddots & \ddots & \ddots & & & \\
 & & & \frac{1}{3} & 1 & \frac{1}{3} & \\
 & & & & \frac{2}{11} & 1 & \frac{2}{11} \\
 & & & & & 5 & 1
\end{bmatrix}$$

$$B = \begin{bmatrix}
-\frac{197}{60} & -\frac{5}{12} & 5 & -\frac{5}{3} & \frac{5}{12} & -\frac{1}{20} & \\
-\frac{20}{33} & -\frac{35}{132} & \frac{34}{33} & -\frac{7}{33} & \frac{2}{33} & -\frac{1}{132} & \\
\frac{-1}{36} & -\frac{7}{9} & 0 & \frac{7}{9} & \frac{1}{36} & & \\
 & \ddots & \ddots & \ddots & & & \\
 & & -\frac{1}{36} & -\frac{7}{9} & 0 & \frac{7}{9} & \frac{1}{36} \\
 & \frac{1}{132} & -\frac{2}{33} & \frac{7}{33} & -\frac{34}{33} & \frac{35}{132} & \frac{20}{33} \\
 & \frac{1}{20} & -\frac{5}{12} & \frac{5}{3} & -5 & \frac{5}{12} & \frac{197}{60}
\end{bmatrix}.$$

4. Numerical solution

In numerical solution of the soybean hydration model, three-point sixth order compact finite difference scheme and explicit finite difference scheme are used for derivatives of radial coordinate where the interval $[0, R(t)]$. The time derivatives are discretized by forward finite difference scheme.

To solve the model the radial coordinate was divided into N points $(i = 1, 2, .., N)$. The number of time intervals is determined by amount of absorbation water. When the whole grain reaches 99% of the equilibrium moisture content, the process is cut off.

Discretization of equation (2.2), equation (2.3) and equation (2.7) as below,

$$X_i^1 = X_0, \quad \forall r, \quad t > 0, \quad i = 1, 2, ..., N\,;$$

$$X_2^j = X_0^j, \quad r = 0, \quad t > 0\,;$$

$$X_1^{j+1} = X_1^j + \frac{6D\Delta t}{(\Delta r^j)^2}(X_2^j - X_1^j), \quad at \quad r = 0\,.$$

For interior points $(i = 2, ..., N-1)$,

$$X_i^{j+1} = X_i^j + \left(\frac{\Delta t r_i^j v^j}{R^j \Delta r^j} + \frac{2D\Delta t}{r_i^j}\right) X_{ri}^j + \frac{D\Delta t}{(\Delta r^j)^2} X_{rri}^j \tag{4.1}$$

is obtained. The term v^j which appears in equation (4.1) represents motion of the boundary, is radius. The velocity of motion of the radius is represented by equation (2.6) and discretization of it is given by equation (4.2).

$$v^j = \left(\frac{dR}{dt}\right)^j = \frac{\rho_{DS}}{\rho_{water}} D X_{rri}^j, \quad r = R(t)\,. \tag{4.2}$$

The position of radius at the next time step is calculated by the following approximation:

$$R^{j+1} = R^j + \Delta t v^j\,.$$

Discretization of surface conditions, for the first model is given by equation (4.3):

$$X_N^{j+1} = X_{eq}, \quad r = R(t)\,, \tag{4.3}$$

and for the second model is given by equation (4.4):

$$X_N^{j+1} = \frac{-\rho_{DS} D X_{ri}^j + \Delta r^j K_c X_{eq}}{\rho_{DS} D X_{ri}^j + \Delta r^j K_c}, \quad r = R(t)\,. \tag{4.4}$$

To compare our numerical results with available experimental data (from [15]), the averaging over the volume of the grain as below [9],

$$X_m = \frac{\int_0^R X.r^2 dr}{\int_0^R r^2 dr}\,. \tag{4.5}$$

5. Results

The soybean hydration models are solved by sixth order compact finite difference scheme in radial coordinate and forward finite difference in time coordinate.

The computations are performed using the software MATLAB R2012a on ASUS machine with Intel Core i7 2.4 GHz and 6 GB memory.

Different numbers of uniform mesh point are used for numerical calculations. Constants in the models at 10^o C are given as below [15],

$X_0 = 0.126(kg_{water}/kg_{DS})$
$X_{eq} = 1.651(kg_{water}/kg_{DS})$
$D = 3.277.10^{-11}(m^2/sn)$ Model 1
$D = 3.514.10^{-11}(m^2/sn)$ Model 2
$\rho_{DS} = 1.057(kg_{DS}/m^3)$
$\rho_{water} = 1.000(kg_{water}/m^3)$
$K_c = 1.286.10^{-3}(kg/m^2 s)$
$R_0 = 0.003m$

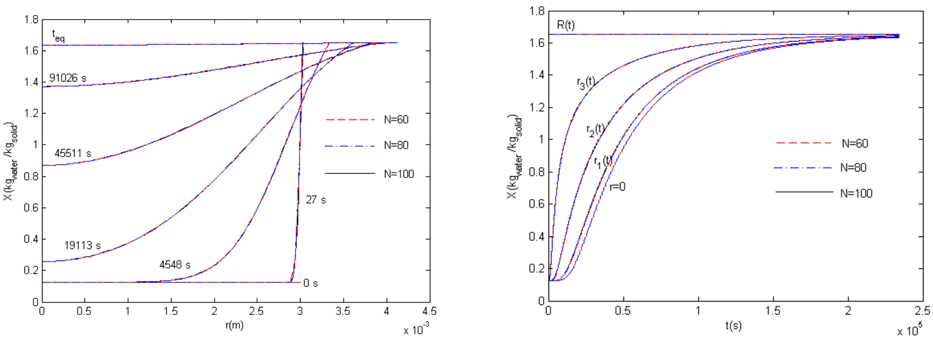

Figure 1. Moisture profiles as a function of variable radius for various values of time (left) and moisture profiles as a function of time for various radial positions (right)

5.1. Solution of the First Model.

The number of divisions of the radius is performed for $N = 60, 80$ and 100. As it seen in figure 1 (left and right), there is no significant difference among the profiles obtained for $60 \leq N \leq 100$.

Figure 1 (right) represents moisture profiles as a function of time for different N values. Moisture profiles are close each other for these N values. As time increases, moisture content inside the soybean increase and reaches the equilibrium moisture value.

It is seen that in figure 2 average moisture content profiles which is calculated by equation (4.5) and available experimental data (from [15]) are in good agrement.

In figure 3 the increase of size of the grain calculated by CFD6 for $N = 60, 80, 100$ is shown. Nicolin et al. [9] demonstrated experimentally R_{max} has the 40.6% increase and numerically R_{max} has the 37.4% increase. We obtain 37.46% increase by the present method.

5.2. Solution of the Second Model.

Similar procedures apply to the first model are applied to the second model.

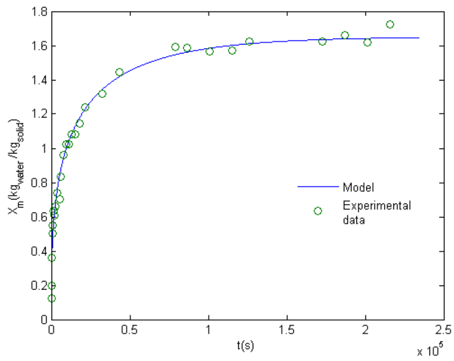

FIGURE 2. Average moisture content profiles and experimental data

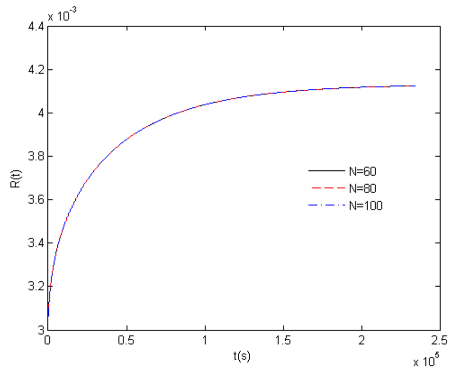

FIGURE 3. Grain radius as a function of time

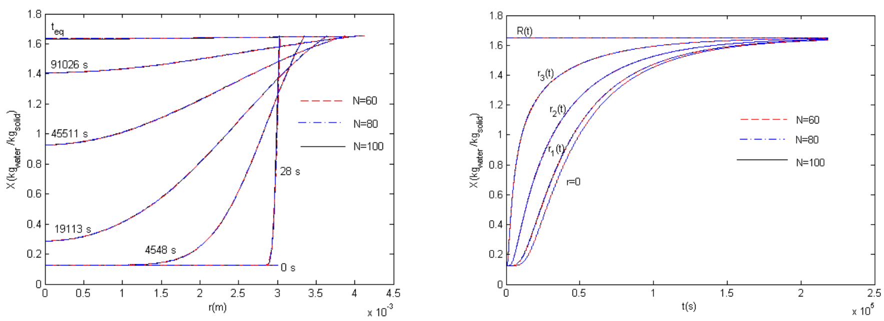

FIGURE 4. Moisture profiles as a function of variable radius for various values of time (left) and Moisture profiles as a function of time for various radial positions (right)

5.3. **Comparison of the first model and the second model.** In figure 7, at the beginning of hydration the two models show similar prediction of the moisture content behavior as a function of radius, especially at the center and at the surface of the grain.

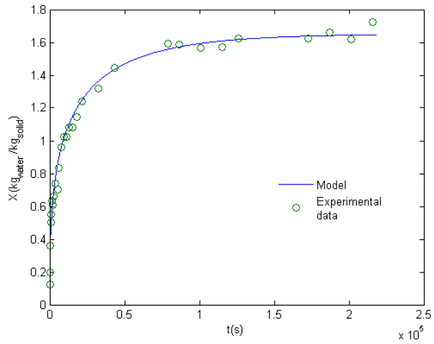

FIGURE 5. Average moisture content profiles and experimental data

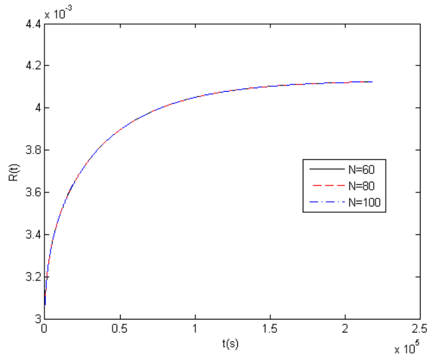

FIGURE 6. Grain radius as a function of time

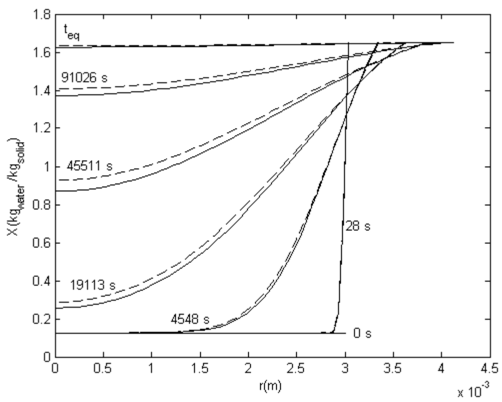

FIGURE 7. Moisture profiles as a function of variable radius for various values of time

After approximatelly 19000 s the description of the moisture content variation with the radius given by the first model varied greatly the other model.

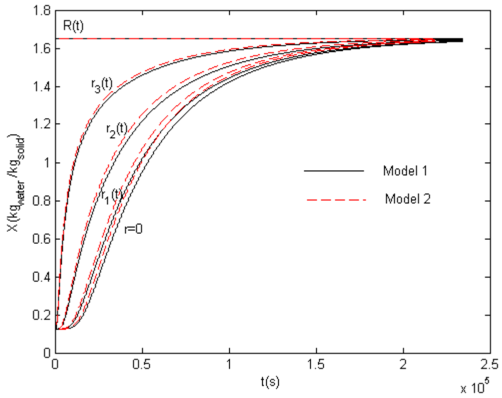

FIGURE 8. Moisture profiles as a function of time for various radial positions

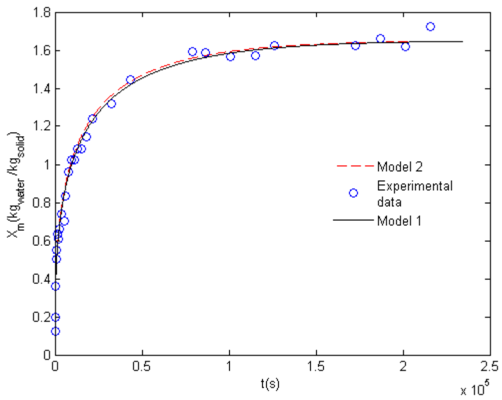

FIGURE 9. Average moisture contents and experimental data

Figure 8 represents moisture profiles as a function of time for various radial positions for the first model and seconf model and in figure 9, it is shown relation between obtained numerical solution and experimental data.

Figure 10 represents the second model reaches the equilibrium point faster than the first model.

TABLE 1. Equilibrium times and CPU times at different N values for the first model

	Nicolin et al.[15]		CFD6	
N	*teq*	CPU	*teq*	CPU
60	234662	293.124552	234148	10.052013
80	234507	329.169541	234145	18.794400
100	234423	368.56395	234144	22.644993

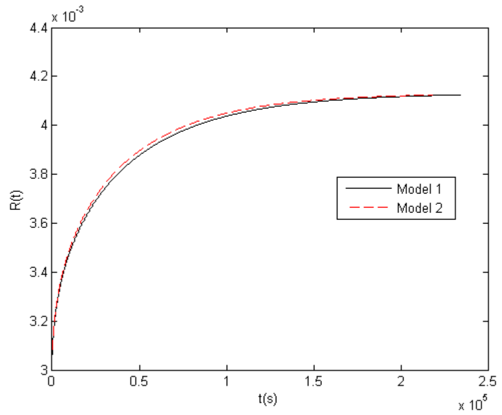

FIGURE 10. Grain radius as a function of time

Present method (CFD6) reaches equilibrium time faster with high accuracy and computational effort is less than compared method as seen in Table 1 and Table 2.

TABLE 2. Equilibrium times and CPU times at different N values for the second model

	Nicolin et al.[15]		CFD6	
N	teq	CPU	teq	CPU
60	218845	12.886249	218362	12.002812
80	218700	18.145747	218360	21.673539
100	218623	19.624960	218360	25.643130

TABLE 3. Grain radius for the first model and the second model

	First Model	Second Model
N	R	R
60	0.0041242019	0.0041242432
80	0.0041241798	0.0041242235
100	0.0041241688	0.0041242148

It is seen that the increase in size of the grain is much the same for two model.

6. CONCLUSION

In first model, sixth order compact finite difference (CFD6) solution has less computational time than explicit solution [9, 10, 15] and it reaches equilibrium time faster with same accuracy. For the second model sixth order compact finite difference solution and explicit solution [9, 10, 15] have about the same computational time but in this case equilibrium time is shorter than explicit solution.

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