Comparison among numerical approximations in the simulation of the grain mass aeration process

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Abstract. In technological development and in the high scale of agricultural production, in the specific case of grains, efficient structures and ways are required to store the product. One widespread form is aeration, which consists of the forced passage of air through a mass of stored grains. The high cost of acquisition and maintenance of this technology is a factor that may inhibit its dissemination and acceptance, especially to a large number of small grain producers. There are several mathematical and numerical models in order to solve this type of problem. This work aims to solve numerically the model proposed by Thorpe of the aeration of the grain mass, using the finite difference technique and employing the spatial approximations UDS, CDS and UDS with deferred correction. Additionally, the explicit, implicit and Crank-Nicolson time formulations are used. The results obtained numerically were compared with experimental data taken from the literature, so the difference between the experimental data and the numerical solution for each approximation used can be observed. Thus, it was found that using the spatial approximation UDS with deferred correction and the Crank-Nicolson time approximation obtained the smallest difference to the experimental data.

Keywords: Finite Difference, Aeration, Simulation.

1 Introduction

The use of information and communication technologies has grown in various agricultural tasks. In effect, it has revolutionized the way of thinking and acting of the producer who aims to establish himself in an increasingly competitive market. The proper storage of grains is the main responsible for maintaining the quality of the product. According to Antunes et al. [1], the most used and widespread control method for the preservation of stored grains is aeration, which consists of the forced passage of air through the stored grain mass.

Even with the large scale of agricultural production and the use of techniques to improve the quality of the grain mass, investments in technology are still modest, especially for small grain producers. Therefore, making technology accessible to these producers, through low-cost solutions, is strategic to improve productivity, Ferrasa et al. [2]. In this sense, studies involving mathematical models and computational resolutions are relevant.

Many papers can be found in the literature involving the numerical simulation of the aeration process, among them, Lopes et al. [3, 4, 5], Rigoni and Kwiatkowski Jr [6], Kwiatkowski Jr [7], where the Finite Difference Method (FDM) with the explicit temporal formulation was used to numerically solve the model proposed by Thorpe [8].

Thus, the goal of this paper is to numerically solve the model proposed by Thorpe [8] using the FDM and employing the spatial approximations Upwind Difference Scheme (UDS), Central Difference Scheme (CDS) and UDS with deferred correction (UDS-C) and the explicit, implicit and Crank-Nicolson temporal formulations. The results obtained numerically were compared with experimental data obtained by Oliveira et al. [9], in order to observe the difference between the experimental data and the numerical solution for each approximation used.

The rest of the paper is organized as follows. In Section 2, the mathematical model proposed by Thorpe [8] is presented along with the boundary and initial conditions. In Section 3 the numerical resolution of the mathematical model is presented. In Section 4 the results obtained are shown. Finally, in Section 5 the conclusions are drawn.

2 Mathematical Model

The model that describes the temperature (T) and moisture (U) of the grains used in this work was proposed by Thorpe [10] and presented in detail in Thorpe [8]. According to Lopes et al. [3], some simplifications can be made in the original model, without loss of accuracy. Thus, the simplified model, which will be adopted here, is given by

$$\frac{\partial T}{\partial t}\left\{\rho_\sigma[c_g + c_W U] + \epsilon\rho_a[c_a + R(c_W + \frac{\partial h_v}{\partial T})]\right\} =$$

$$\rho_\sigma h_s \frac{\partial U}{\partial t} - u_a\rho_a\left[c_a + R(c_W + \frac{\partial h_v}{\partial T})\right]\frac{\partial T}{\partial y} + \rho_\sigma\frac{dm}{dt}(Q_r - 0,6h_v), \quad (1)$$

$$\rho_\sigma\frac{\partial U}{\partial t} = -u_a\rho_a\frac{\partial R}{\partial y} + \frac{dm}{dt}(0,6+U), \quad (2)$$

where: t - time (s), y - axis in the vertical direction (oriented from bottom to top) (m), U - grain moisture ($\%$), u_a - aeration air velocity (ms^{-1}), c_g - grain specific heat ($JKg^{-1}C$), c_W - specific heat of water ($JKg^{-1}C$), c_a - specific heat of air ($JKg^{-1}C$), R - humidity ratio of air ($KgKg^{-1}$), ρ_a - density of intergranular air (Kgm^{-3}), ρ_σ - bulk density of the grain (Kgm^{-3}), h_v - latent heat of vaporization of water (JKg^{-1}), h_s - differential heat of sorpion (JKg^{-1}), T - grain temperature (ºC), ϵ - grain porosity (decimal), $\frac{dm}{dt}$ - derivative of the grain dry matter loss in relation to time (kgs^{-1}), Q_r - heat of oxidation of the grain ($Js^{-1}m^{-3}$).

The grain mass was considered in the vertical direction, that is: $y \in [0, L]$, where L represents the height of the grain mass storage location, according to Fig. 1. Therefore, a one-dimensional simplification of the model was considered. For the boundary condition at $y = 0$, it was assumed that the grains located at the base of the storage location come into equilibrium with the aeration air, thus: $T(0,t) = T_0$.

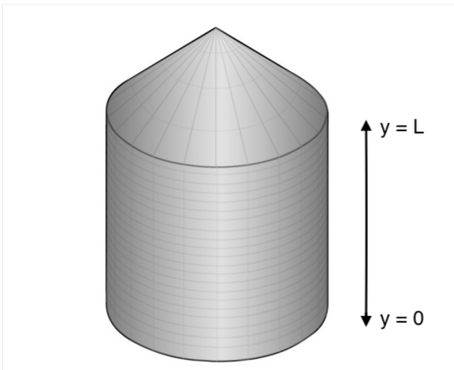


Figure 1. Calculation domain

According to Chung and Pfost [11], the moisture at $y = 0$ can be calculated by

$$U(0,t) = -\frac{1}{B}ln[ln(-\frac{\text{URA}}{100})(-\frac{T_0 + C}{A})], \quad (3)$$

where A, B and C vary according to the type of grain, URA represents the relative humidity of heating and can be calculated by

$$\text{URA} = 100\frac{\frac{Ur}{100}((6\times10^{25})/(1000(T_{amb}+273,15)^5))e^{-6800/(T_{amb}+273,15)}}{((6\times10^{25})/(1000(T_0+273,15)^5))e^{-6800/(T_0+273,15)}}, \quad (4)$$

where Ur is the relative humidity and T_{amb} represents the ambient temperature.

At $y = L$ there is a Neumann boundary condition, that is:

$$\frac{\partial T}{\partial y}|_{y=L} = \frac{\partial U}{\partial y}|_{y=L} = 0. \quad (5)$$

The grains before entering the storage location are preheated to an ideal temperature, so in all of the domain the initial condition is equal to this temperature, $T(y, 0) = T^0$.

The initial moisture can be obtained according to Thorpe [8], by

$$U(y, 0) = \frac{U_i}{100 - U_i}, \quad (6)$$

where U_i is the initial grain moisture.

3 Numerical Model

The differential equations that describe the temperature and moisture of the grains were solved numerically using the FDM, Cuminato and Meneguette [12].

3.1 Spatial approximation by UDS

Approximating the spatial derivatives of T and R by UDS and the temporal derivative of T using the θ formulation, and denoting Λ_i^{n+1} any variable Λ evaluated at the point i and at the current time $n+1$, the discretized form of eq. (1) is given by

$$T_i^{n+1} = \left[\frac{1}{\frac{\alpha_1}{\Delta t} - \frac{\alpha_3 \theta}{\Delta y}}\right] \left\{\frac{\alpha_1}{\Delta t} T_i^n + \alpha_2 + \frac{\alpha_3}{\Delta y}\left[T_i^n - \theta T_i^n - [T_{i-1}^n + \theta[T_{i-1}^{n+1} - T_{i-1}^n]]\right] + \alpha_4\right\}, \quad (7)$$

where α_1, α_2, α_3 and α_4 are constants in the time T_i^{n+1}, given by:

$$\alpha_1 = \rho_\sigma[c_g + c_W[U_i^n + \theta[U_i^{n+1} - U_i^n]] + \epsilon\rho_a[c_a + [R_i^n + \theta[R_i^{n+1} - R_i^n]](c_W + \frac{\partial h_v}{\partial T})], \quad (8)$$

$$\alpha_2 = h_s\left[-u_a\rho_a[\frac{[R_i^n + \theta[R_i^{n+1} - R_i^n]] - [R_{i-1}^n + \theta[R_{i-1}^{n+1} - R_{i-1}^n]]}{\Delta y}] + \frac{dm}{dt}(0,6 + [U_i^n + \theta[U_i^{n+1} - U_i^n]])\right], \quad (9)$$

$$\alpha_3 = -u_a\rho_a\left[c_a + [R_i^n + \theta[R_i^{n+1} - R_i^n]](c_W + \frac{\partial h_v}{\partial T})\right], \quad (10)$$

$$\alpha_4 = \rho_\sigma\frac{dm}{dt}(Q_r - 0,6h_v). \quad (11)$$

Now, approximating the spatial derivative of R by UDS and the temporal derivative of U using the θ formulation, the discretized form of eq. (2) is given by

$$U_i^{n+1} = \frac{1}{(\frac{\rho_\sigma}{\Delta t} - \theta\frac{dm}{dt})}\left\{\frac{\rho_\sigma}{\Delta t}U_i^n - u_a\rho_a\alpha_5 + \frac{dm}{dt}(0,6 + U_i^n - \theta U_i^n)\right\}, \quad (12)$$

where, α_5 can be written as:

$$\alpha_5 = \frac{R_i^n + \theta[R_i^{n+1} - R_i^n] - [R_{i-1}^n + \theta[R_{i-1}^{n+1} - R_{i-1}^n]]}{\Delta y}, \quad (13)$$

where: i and n, respectively, are the spatial and temporal locations being used in the calculations; $\Delta t = \frac{t_f}{N_t}$, where t_f is the simulation time and N_t is the number of time steps; $\Delta y = \frac{L}{N_y - 1}$, where N_y is the number of nodes; θ is the identifier of the time formulation (for θ = 0 explicit formulation, θ = 1 implicit formulation and $\theta = \frac{1}{2}$ Crank-Nicolson formulation, Cuminato and Meneguette [12]).

As mentioned, at $y = L$ there is a Neumann boundary condition. Approximating by UDS, the temperature and the moisture at $y = L$ are given by:

$$T_{NC}^{n} = T_{NC-1}^{n}, \tag{14}$$

$$U_{NC}^{n} = U_{NC-1}^{n}, \tag{15}$$

where NC represents the node located at the boundary, as in Fig. 2.

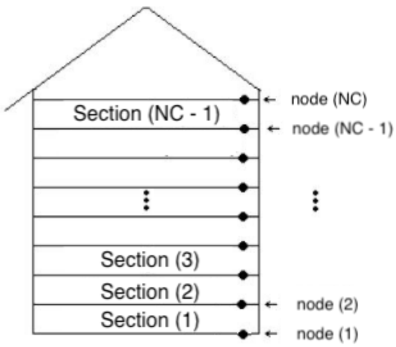


Figure 2. Discretized domain

3.2 Spatial approximation by CDS

Approximating the spatial derivatives of T and R by CDS and the temporal derivative of T using the θ formulation, the discretized form of eq. (1) is given by

$$T_i^{n+1} = \left[\frac{\Delta t}{\alpha_1}\right]\left\{\frac{\alpha_1}{\Delta t}T_i^n + \alpha_2' + \frac{\alpha_3}{2\Delta y}\left[T_{i+1}^n + \theta[T_{i+1}^{n+1} - T_{i+1}^n] - [T_{i-1}^n + \theta[T_{i-1}^{n+1} - T_{i-1}^n]]\right] + \alpha_4\right\}, \tag{16}$$

where α_1, α_3 and α_4 are the same as in the previous section and α_2' is given by:

$$\alpha_2' = h_s\left[-u_a\rho_a\alpha_5' + \frac{dm}{dt}(0,6 + [U_i^n + \theta[U_i^{n+1} - U_i^n]])\right]. \tag{17}$$

Now, approximating the spatial derivative of R by CDS and the temporal derivative of U using the θ formulation, the discretized form of eq. (2) is given by:

$$U_i^{n+1} = \frac{1}{(\frac{\rho_\sigma}{\Delta t} - \theta\frac{dm}{dt})}\left\{\frac{\rho_\sigma}{\Delta t}U_i^n - u_a\rho_a\alpha_5' + \frac{dm}{dt}(0,6 + U_i^n - \theta U_i^n)\right\}, \tag{18}$$

where α_5' can be written as:

$$\alpha_5' = \frac{R_{i+1}^n + \theta[R_{i+1}^{n+1} - R_{i+1}^n] - [R_{i-1}^n + \theta[R_{i-1}^{n+1} - R_{i-1}^n]]}{2\Delta y}. \tag{19}$$

The Neumann boundary condition can be approximated by CDS, using the ghost point technique, Maliska [13]. With this, the temperature and moisture at $y = L$ are given by:

$$T_{NC}^{n+1} = \left[\frac{\Delta t}{\alpha_1}\right]\left\{\frac{\alpha_1}{\Delta t}T_{NC}^n + h_s\left[\frac{dm}{dt}(0,6 + [U_{NC}^n + \theta[U_{NC}^{n+1} - U_{NC}^n]])\right] + \alpha_4\right\}, \tag{20}$$

$$U_{NC}^{n+1} = \frac{1}{(\frac{\rho_\sigma}{\Delta t} - \theta\frac{dm}{dt})}\left\{\frac{\rho_\sigma}{\Delta t}U_{NC}^n + \frac{dm}{dt}(0,6 + U_{NC}^n - \theta U_{NC}^n)\right\}. \tag{21}$$

3.3 Spatial approximation using the deferred correction method (UDS-C)

According to Patankar [14], the deferred correction method (UDS-C) is a hybrid scheme developed by Spalding [15]. The scheme consists in mixing the UDS and CDS approximations, so the method is given by

$$T_P = T_{P,UDS} + \beta(T^*_{P,CDS} - T^*_{P,UDS}), \tag{22}$$

where, $T^*_{P,CDS}$ and $T^*_{P,UDS}$, are known values from the previous time, and are applied according to the scheme given by

$$\beta = \begin{cases} 0, & UDS \\ 1, & CDS \\ 0 \leq \beta \leq 1, & Mixture \end{cases}. \tag{23}$$

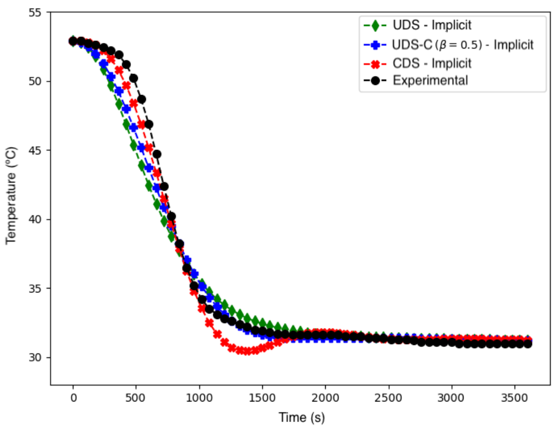
4 Results

In order to validate the computational simulation, data obtained by Oliveira et al. [9] were considered. These data were obtained in the laboratory of physical measurements and mathematical modeling at the Regional University of the Northwest of Rio Grande do Sul (UNIJUI), in a small "silo" composed of a PVC tube with thermal insulation on the sides, height of 1.0 m (L = 1 m) and 0.15 m of diameter.

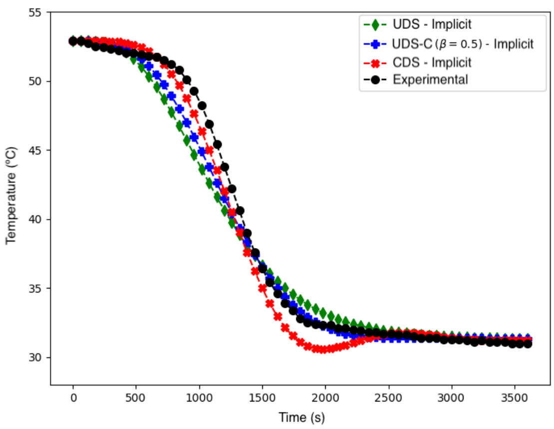
To perform the experiments, soybeans with an average water content of 12% were previously selected, cleaned and heated to a temperature of approximately 52.9ºC. That is, at the beginning of the experiment, the initial temperature was 52.9ºC. The grain temperature was measured by thermocouples inserted inside the grain mass, along the tube, at the following sections of the grain column: y = 0.15 m; y = 0.27 m; y = 0.40 m and y = 0.54 m for one hour.

The codes were programmed in Fortran language, using quadruple precision and initial data equal to those used in the experiment, so the numerical and experimental solutions were compared in the heights of 0.15 m, 0.27 m, 0.40 m and 0.54 m in relation to time.

Figures 3 and 4 shows the behavior of the UDS, CDS and UDS-C ($\beta = 0.5$) spatial approximations with the implicit temporal approximation using 30 nodes and 60 time steps ($N_y = 30$ and $N_t = 60$) at the heights of 0.15 m, 0.27 m, 0.40 m and 0.54 m.



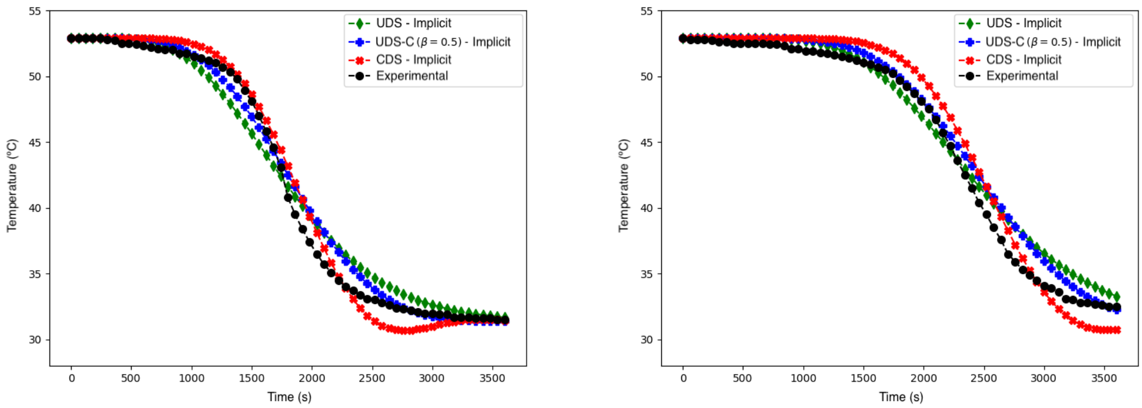
(a) y = 0.15 m



(b) y = 0.27 m

Figure 3. Comparison of the numerical simulations ($N_y = 30$ and $N_t = 60$) and the experimental data at the heights (a) 0.15 m and (b) 0.27 m.

Simulations were performed varying the number of nodes (N_y) and the number of time steps (N_t) for each approximation. It was used N_y equal to 30, 40, 50, 60, 70, 80, 90 and 100 nodes combined with N_t equal to 60, 120, 240 and 480 time steps.



(a) y = 0.40 m

(b) y = 0.54 m

Figure 4. Comparison of the numerical simulations ($N_y = 30$ and $N_t = 60$) and the experimental data at the heights (a) 0.40 m and (b) 0.54 m.

In order to calculate the error between numerical simulations and experimental data, it was used

$$L_\infty = \|T^n_{Num} - T^n_{Exp}\|_\infty, \tag{24}$$

where T_{Num} is the numerical temperature, T_{Exp} represents the experimentally obtained temperature.

Table 1 shows for each approximation the values of N_y and N_t corresponding to the smallest difference to the experimental data according to the L_∞ norm.

Table 1. Best parameters for each approximation used and the corresponding L_∞ norm.

Approximation	N_y	N_t	L_∞
UDS - Explicit	50	120	2.76 ºC
UDS - Implicit	70	240	2.65 °C
UDS - Crank-Nicolson	50	60	2.53 °C
CDS - Explicit	30	480	7.10 ºC
CDS - Implicit	30	60	2.41 °C
CDS - Crank-Nicolson	30	480	6.00 °C
UDS-C - Explicit	30	60	2.58 ºC
UDS-C - Implicit	80	60	2.71 °C
UDS-C - Crank-Nicolson	30	60	2.40 °C

As the analytical solution of the mathematical model is unknown, the numerical simulations were compared to experimental data. Therefore, not necessarily the numerical simulation with the largest number of nodes and the largest number of time steps presents the smallest difference to the experimental data.

It can be seen that using the CDS - Implicit approximation, the largest difference to the experimental data is 2.41°C. Using the UDS-C - Crank-Nicolson approximation (with $\beta = 0.5$), the largest difference to the experimental data is 2.40°C. That is, the method with the UDS-C - Crank-Nicolson combination obtained the smallest difference to the experimental data for the cases tested.

5 Conclusion

In this work, studies were performed on the behavior of several types of numerical approximations using the Finite Difference Method when applied to the model proposed by Thorpe [8]. It was verified with the simulations that using the deferred correction method and Crank-Nicolson temporal approximation, the numerical solution found presents a smaller difference to the experimental data than the simulations with other approximations.

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