Modelising the grain mass aeration process using the Thorpe Model with the Finite Volume Method

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Abstract. By the technological advancements in agriculture, rural production is searching for ways to improve grain storage. Rigorous control of temperature and moisture is essential as they are the main factors contributing to product deterioration and plague proliferation. One of the most effective ways of achieving this is by aeration, a process widely applied to maintaining grain quality in silos and warehouses. This work aimed to develop a control system for the aeration of stored grains based on experimental data from literature and process simulations. The control strategy employed in the aeration aims to maintain temperatures uniform inside the silo and cool down the grain mass whenever possible. During this process, the grain mass is split into multiple thin layers according to the flow of air (upwards). The mathematical model used was proposed by Thorpe and associates psychometric properties of the air with mass and energy balance equations. In this sense, the system of equations resulting from the mass and energy balances was solved iteratively for each time increment and each layer. Additionally, the model equations were discretized using the Finite Volume Method combined with the Upwind Differencing Scheme for the spatial approximations as well as explicit, implicit, and Crank-Nicolson temporal formulations. Moreover, *a posteriori* analysis of the discretization error orders was carried out. The proposed model in this study has proved satisfactory, with some variations depending on the combination between the method and the spatial and temporal approximations employed.

Keywords: Discretization Error, Effective Order, UDS, Aeration Model.

1 Introduction

With technological advancements in agriculture and the high global demand for food, rural production must seek ways to improve grain storage. In this sense, aeration is the most widely employed control process, which consists of the forced passage of air through the stored grain mass using ventilation and exhaust fans coupled to a ventilation system installed at the bottom of silos and warehouses. The aeration modifies the microclimate of the grain mass, inhibiting the development of organisms that are harmful to the grains, Pereira [1].

There are several reasons aeration is employed. The main ones are cooling and maintenance of the grain mass at low temperatures to ensure adequate storage. Additionally, aeration helps in the drying, prevents heating and dampening of the grain mass, removes odors, and inhibits insect activity and the development of microflora, avoiding the appearance of fungi that spoil the product, Lopes et al. [2].

It is possible to find various papers in the literature that discuss the numerical simulation of the aeration process, such as Lopes et al. [2, 3], Kwiatkowski Jr [4] and Oliveira et al. [5]. In all of these studies, the Finite Difference Method with the Upwind Difference Scheme (UDS) formulation in space and explicit in time is used to solve numerically the mathematical model proposed by Thorpe [6]. However, in Rigoni et al. [7], several other spatial and temporal discretization techniques were introduced.

This work aims to go deeper into the study of numerical simulations of the aeration process of a soybean grain mass, according to the Thorpe model [6], to help control the factors that might bring damage to it. To achieve this, we provide a comparison of two discretization methods, the Finite Volume Method (FVM) and the Finite Difference Method (FDM).

2 Mathematical Model

The proposed model is given by Eqs 1 and 2, which represent the equations of temperature (T) and moisture content (U) of the grain mass, respectively

$$\left\{\rho_\sigma(1-\varepsilon)\left[c_\sigma + c_W U + \frac{\partial H_W}{\partial T}\right] + \varepsilon\rho_a\left[c_a + R\left(c_W + \frac{\partial h_v}{\partial T}\right)\right]\right\}\frac{\partial T}{\partial t} = \rho_\sigma(1-\varepsilon)h_s\frac{\partial U}{\partial t} + \\ -u_a p_a\left[c_\sigma + R\left(c_W + \frac{\partial h_v}{\partial T}\right)\right]\frac{\partial T}{\partial y} + k_{eff}\frac{\partial^2 T}{\partial y^2} + (1-\varepsilon)\rho_\sigma\frac{dm}{dt}(Q_R - 0.6h_v) \tag{1}$$

and

$$(1-\varepsilon)\rho_\sigma\frac{\partial U}{\partial t} = -u_a p_a\frac{\partial R}{\partial y} + \frac{dm}{dt}(0.6+U), \tag{2}$$

where: t - time (s), y - axis in the vertical diretion (oriented from bottom to top) (m), U - grain moisture content (decimal), u_a - Darcy's velocity of dry air (ms^{-1}), c_σ - specific heat of grain $(Jkg^{-1}\ ^\circ C)$, c_W - specific heat of moisture content $(Jkg^{-1}\ ^\circ C)$, c_a - specific heat of air $(Jkg^{-1}\ ^\circ C)$, R - mixing ratio, ρ_a - density of dry air (kgm^{-3}), ρ_σ - grain density (kgm^{-3}), h_v - specific heat of water vapor (Jkg^{-1}), h_s - heat of sorption (Jkg^{-1}), T - grain temperature $(^\circ C)$, ϵ - grain mass porosity (decimal), dm - loss of dry matter to time (kgs^{-1}) and Q_R - grain heat of oxidation $(Js^{-1}m^{-3})$. Moreover, we will disregard the thermal conductivity (k_{eff}) and the term $\frac{\partial H_W}{\partial T}$, following the simplifications presented by Lopes et al. [2].

The calculation domain is depicted in Fig. 1, with an upward airflow, that is, $y \in [0, L]$, where L is the silo height.

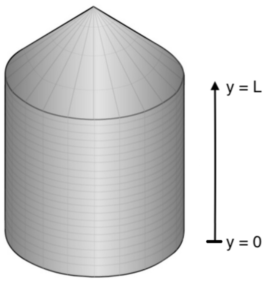


Figure 1. Calculation Domain [7].

As the grain mass goes through the drying process before being stored at the silo, the initial grain temperature across the whole domain is $T(y,0) = T_I$. The initial moisture content (U_I), according to Thorpe [6], and is given by

$$U(y,0) = \frac{U_P}{100 - U_P} = U_I, \tag{3}$$

where U_P corresponds to the initial moisture content, written as a percentage (%).

As for the moisture content in $y = 0$ (U_C), the equation is given by Chung and Pfost [8] as follows

$$U(0,t) = -\frac{1}{B}ln\left[ln\left(\frac{U_{RA}}{100}\right)\left(-\frac{T_B + C}{A}\right)\right] = U_B, \tag{4}$$

where, A, B and C depend on the type of stored grain, T_B is the temperature at the base of the silo, that is, the temperature of the aeration airflow, U_{RA} is the relative humidity of aeration air, given by

$$U_{RA} = 100\frac{\frac{U_r}{100}\left(\left(6\times10^{25}\right)/\left(1000\left(T_{amb}+273.15\right)^5\right)\right)e^{-6800/(T_{amb}+273.15)}}{\left(\left(6\times10^{25}\right)/\left(1000\left(T_{amb}+273.15\right)^5\right)\right)e^{-6800/(T_B+273.15)}}, \tag{5}$$

with T_{amb} - being the room temperature and U_r - the relative humidity of the ambient air.

The boundary conditions in $y = L$, follow Neumann conditions, such as

$$\left.\frac{\partial T}{\partial y}\right|_{y=L} = \left.\frac{\partial U}{\partial y}\right|_{y=L} = 0. \tag{6}$$

3 Numerical Model

The Finite Volume (FVM) is a method to discretize differential equations based on achieving the balance of certain physical properties in a control volume (CV), also called cell, of the domain. In this study, the physical properties are the temperature and moisture content.

There can be more than one property stored in a given cell of the grid. When all properties are stored at the center of the volume, there is what is called a co-localized arrangement (non-stagerred grid), and when this does not occur, there is a staggered arrangement (Maliska [9]). We chose to work with the co-localized arrangement as it is easier to implement and requires only one type of CV for all the integrations of the mathematical model equations.

The FVM uses the integral form of the continuity equation. The solution domain is divided into a finite number of contiguous CV, and the continuity equation is applied to each one of them (Fig. 2). At the center of each CV there is a computational node where the values of the variables are calculated. The values of the variables at the boundaries of the CV are obtained by interpolation of the node values, Maliska [9].

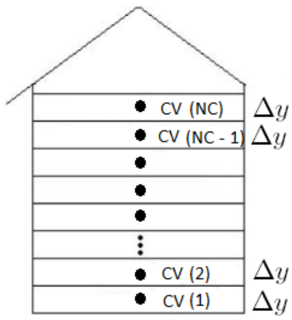


Figure 2. Discretized domain.

As we can see in Fig. 2, NC represents the boundary volume, $\Delta y = L/N_y$ is the distance between the centers of two contiguous cells and N_y is the number of volumes in the spatial direction. Since the problem is transient, there is also $\Delta t = t_f/N_t$, where t_f is the final time and N_t is the number of time steps. Thus, by discretizing the spatial approximation of T and R using the UDS, and the temporal approximation of T using the θ formulation in Eq. 1, and adding a source term F to fit the analytical solution proposed by Rigoni et al. [10], we achieve:

$$A_P^\theta T_P^{n+1} = A_P^\theta T_P^n - B_P^\theta \frac{\Delta t}{\Delta y} \left(T_P^n - T_S^n\right) + F_P^\theta \Delta t, \tag{7}$$

where

$$A_P^\theta = \rho_\sigma \left[c_\sigma + c_W U_P^\theta\right] + \epsilon \rho_a \left[c_a + R_P^\theta \left(c_W + \frac{\partial h_v}{\partial T}\right)\right], \tag{8}$$

$$B_P^\theta = u_a \rho_a \left[c_a + R_P^\theta \left(c_W + \frac{\partial h_v}{\partial T}\right)\right], \tag{9}$$

$$F_P^\theta = \left\{ A_P^\theta \left[-\frac{2exp\left[\frac{-125000\left(y-2.2\times10^4 t\right)^2}{t}\right]\left(-\frac{176.777\left(y-2.2\times10^{-4}t\right)}{\sqrt{t^3}}-\frac{0.0777817}{\sqrt{t}}\right)}{\sqrt{\pi}} + \right.\right.$$
$$\left. -\frac{2exp\left[27.5y-\frac{125000\left(y+2.2\times10^4 t\right)^2}{t}\right]\left(\frac{0.0777817}{\sqrt{t}}-\frac{176.777\left(y+2.2\times10^{-4}t\right)}{\sqrt{t^3}}\right)}{\sqrt{\pi}} \right] +$$
$$+B_P^\theta \left[27.5exp\left(27.5y\right)erfc\left(\frac{353.553\left(y+2.2\times10^{-4}t\right)}{\sqrt{t}}\right) - \left(\frac{exp\left[\frac{-125000\left(y-2.2\times10^{-4}t\right)^2}{t}\right]}{\sqrt{t}} + \right.\right.$$
$$\left.\left.\left. + \frac{exp\left[27.5y-\frac{125000\left(y+2.2\times10^{-4}t\right)^2}{t}\right]}{\sqrt{t}} \right) 398.942 \right] \right\} \frac{1}{2}\left(T_B - T_I\right). \tag{10}$$

In every equation, θ represents the explicit ($\theta = 0$), implicit ($\theta = 1$) or Crank-Nicolson ($\theta = 0.5$) formulations, Maliska [9].

Approximating the spatial derivative of R by UDS and the temporal derivative concerning the variable U in Eq. 2, we have that:

$$U_P^{n+1} = U_P^n - \frac{u_a \rho_a \Delta t}{\rho_\sigma \Delta y}\left(R_P^\theta - R_S^\theta\right) + \frac{\Delta t \frac{dm}{dt}}{\rho_\sigma}\left(0.6 + U_P^\theta\right). \tag{11}$$

The equations presented correspond to inner volumes, that is, it is necessary to obtain the equations at the boundaries of the domain to have complete algebraic equations. There are several techniques for this in the literature and in this study, we will use the ghost volume one.

The ghost volume technique consists of adding control volumes outside the physical domain so that the balance between the properties in the ghost volumes and their neighbors satisfies the problem's original boundary conditions. Thus, for the boundary conditions, in $y = L$, for the temperature T, and the water content U, respectively, we have:

$$T_{NC}^{n+1} = T_{NC-1}^n \tag{12}$$

and

$$U_{NC}^{n+1} = U_{NC-1}^n. \tag{13}$$

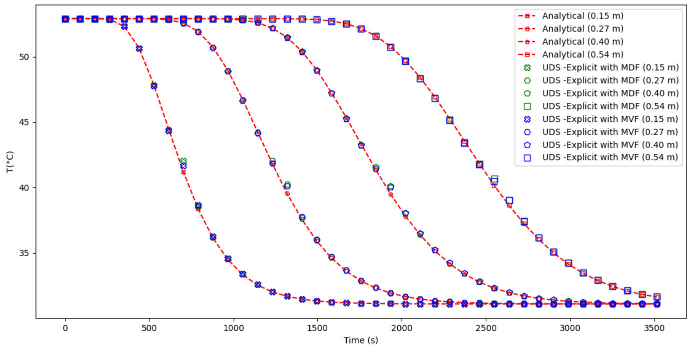
4 Results

The codes were written in Fortran 95, with quadruple precision. A comparison of the analytical and numerical solutions, solved with both the FDM and FVM, widely used in the literature for such model, is presented.

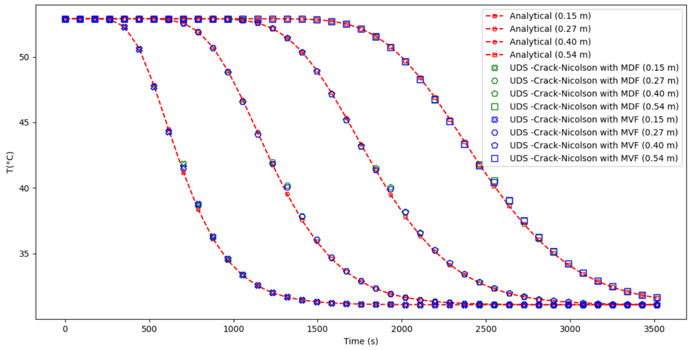
We analyzed the temperature according to time (final time, $t_f = 3600s$) of the grain mass at different heights of, 0.15*m*, 0.27*m*, 0.40*m* and 0.54*m*, in an experimental silo of $L = 1m$ height and 100*mm* diameter, with $T_I = 52.9^0C$ and T_B varying about 31^0C due to the aeration process, Oliveira [5].

Figure 3 presents the behavior of the temperature *versus* time in a spatial grid of $N_y = 2048$ volumes and a temporal grid of $N_t = 4096$ time steps. The numerical solutions of the grain mass tend to the analytical solutions when discretized by the FVM, which is similar to the behavior when using the FDM, for all explicit, implicit and Crank-Nicolson formulations at different heights.

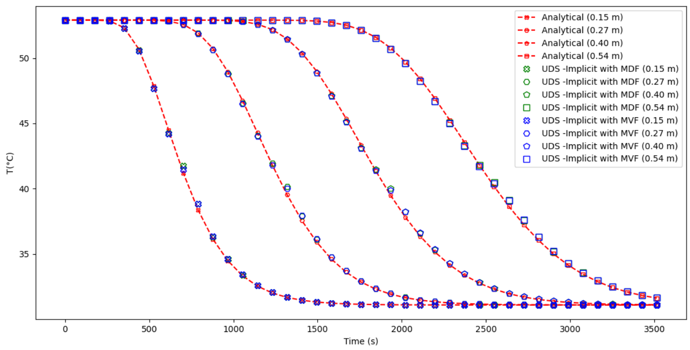
It is important to highlight that the FDM is serving as a base of comparison since the subject of this study is the performance of the FVM. As it is possible to see below, the method describes well the behavior of the grain mass temperature, regardless of each temporal discretization used.



(a) Explicit



(b) Crank-Nicolson



(c) Implicit

Figure 3. Comparison between the analytical and numerical solutions with the use of the FVM and the FDM for $N_y = 2048$ and $N_t = 4096$.

To evaluate the numerical models, we compared their solutions using an error analysis to monitor their effective order error (p_E) (Marchi [11]), and the error decay following the refinement of the grid. The equation for the effective order error is given as

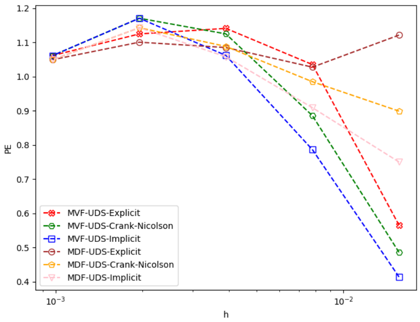
$$p_E = \frac{log\left(\dfrac{\Phi - \phi_2}{\Phi - \phi_1}\right)}{log(q)}, \tag{14}$$

where Φ is the exact analytical solution, ϕ_1, ϕ_2 are numerical solutions and $q = h_2/h_1$ which is the grid refinement ratio, where h_1 and h_2, represent a fine and coarse grid, respectively.

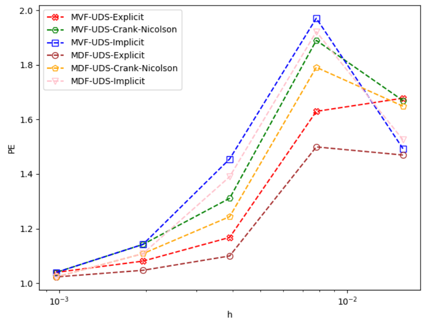
According to Marchi [11], the effective order (p_E) tends to the asymptotic order (p_L) as the grid is refined.

Given the combinations of the spatial discretization method $p_L = 1$ (UDS), with the temporal discretization methods $p_L = 1$ (Explicit and Implicit) and $p_L = 2$ (Crank-Nicolson), the asymptotic orders for all approximations analyzed tend to $p_L = 1$ (Ferziger e Peric [12]).

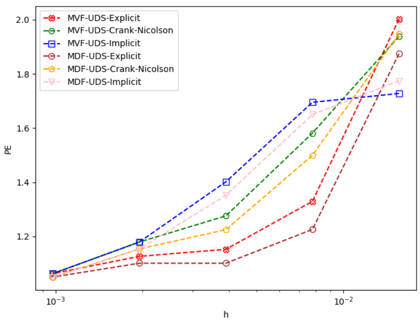
Figure 4 shows the effective orders for the different heights of grain mass studied (y=0.15m, 0.27m, 0.40m and 0.54m), at different time increments, $450s$, $675s$, $1125s$ and $1575s$, using the FVM and FDM. Moreover, a simulation of the whole process, $3600s$ is presented.



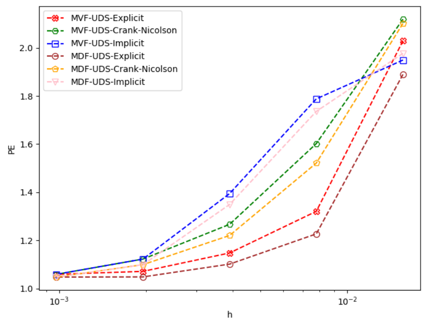
(a) For $y = 0.15m$ and $t = 450s$



(b) For $y = 0.27m$ and $t = 675s$



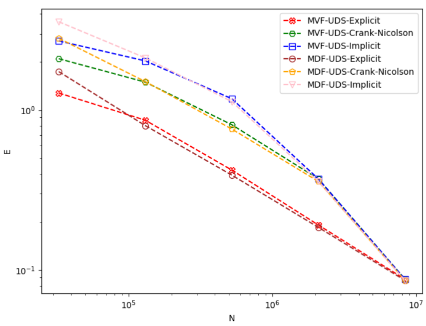
(c) For $y = 0.40m$ and $t = 1125s$



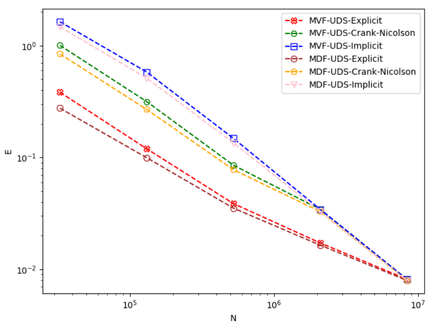
(d) For $y = 0.54m$ and $t = 1575s$

Figure 4. Effective discretization error orders according to the refinement of the grid.

We note, one can note that regardless of the height or time, the effective order tends to the asymptotic order $(p_E \Rightarrow p_L = 1)$, corroborating the theory with the data from the numerical simulation for the FVM as well as the FDM. In Figs. 5 and 6, we fixed the time at $t = 3600s$ and observe the decay of the discretization error when the grid is refined. The more refined the grid, the smaller the discretization error. In this sense, we have, for the model studied, an efficient discretization using the FVM when compared to the FDM.

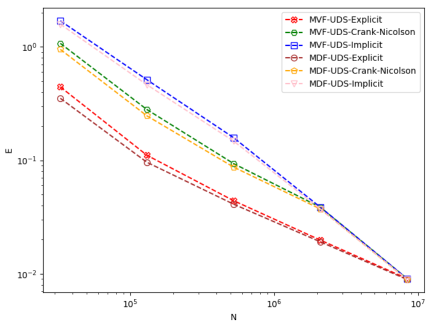


(a) For $y = 0.15m$

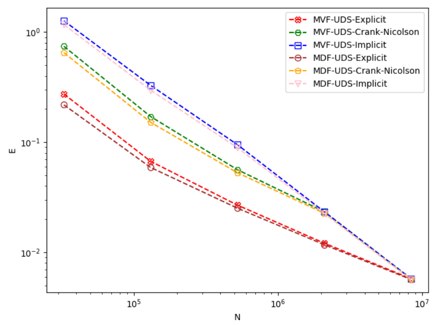


(b) For $y = 0.27m$

Figure 5. Discretization error *versus* the grid refinement for $y = 0.15m$ and $y = 0.27m$.



(a) For $y = 0.40m$



(b) For $y = 0.54m$

Figure 6. Discretization error *versus* the grid refinement for $y = 0.40m$ and $y = 0.54m$.

5 Conclusions

We performed an error analysis and compared the effective order of the discretization error and the error decay with the refinement of the grid in the simulation of the aeration process of a grain mass using the finite volume and finite difference methods. We observe that the FVM represents well the decay of discretization error with the refinement of the grid and reaches the expected effective order for different heights, such as the FDM, widely used in the literature, does. Thus, we can consider using the FVM in the simulation of the Thorpe model for the aeration of a grain mass, using the UDS for spatial discretization and the explicit, implicit, and Crank-Nicolson for temporal discretizations.

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