MATHEMATICAL MODELLING OF MOMENTUM, HEAT AND
MASS TRANSFER IN GRAINS STORED IN SILOS. PART II:
MODEL APPLICATION

A. ARIAS BARRETO†, R. ABALONE‡‡ and A. GASTÓN†§

abarreto@fceia.unr.edu.ar
‡Instituto de Física Rosario (CONICET-UNRosario), 27 de Febrero 210 bis, 2000 Rosario, Argentina
rabalone@fceia.unr.edu.ar
§CIC-UNR, FCEyA, Universidad Nacional de Rosario, Av. Pellegrini 250, 2000 Rosario, Argentina
analiag@fceia.unr.edu.ar

Abstract — A 2D finite element momentum, heat and mass transfer model was applied to predict natural convection flows, temperature distribution and moisture migration in soybean stored in a cylindrical bin without aeration from autumn to spring for the weather conditions of Rosario, Argentina. The effect of the initial moisture content and temperature of the grain (13%w.b and 25, 20 and 15°C) on storability conditions was evaluated. During winter, stronger natural convection flows developed for 25°C, promoting an average moisture migration of 0.4%w.b and average grain temperature decrease of 5°C at the bin bottom. For 20°C, these values reduced to 0.15%w.b and 3°C. For 15°C, safe conditions remained and moisture migration was negligible during winter, but in spring, solar radiation and natural convection increased the temperature of a boundary layer of 1.5 m width above 18°C. Interstitial equilibrium relative humidity remained below the threshold for mold development (ERH > 75%). During spring, natural convection increased as the initial grain storage temperature decreased. Permeability has the strongest effect on natural convection and a five fold increase of this parameter resulted in the development of spoilage areas in the upper part of the bin. Soybean and corn showed comparable moisture migration while for wheat was not significant.

Keywords — grain storage, numerical modelling, natural convection, heat and mass transfer.

I. INTRODUCTION

Numerical simulation models based on transport principles are useful and inexpensive tools to predict the potential spoilage of stored grain. They can play a major role in the design and evaluation of methods for reducing temperature and moisture gradients in stored grains, which are the two main factors that affect grain quality during storage. Numerous models have been developed for conventional storage systems and applied to analyze the heat and mass transfer process in different grains. A revision of published results can be found in Navarro and Noyes (2002). These authors’ remark that the major advantage of validated models is the possibility to conduct “what-if” studies and thus predict storage conditions based on different climatic regions of the world. For the climatic conditions of South America, most of the published work refers to Brazil, addressing the analysis of heat and mass transfer of grains without aeration (Andrade et al., 2002) or the performance of aeration strategies for typical agricultural locations (Sinicio and Muir, 1996, 1998; Martins et al., 2001; Lopes et al., 2006, 2008a, 2008b; Khatchatourian and Oliveira, 2006). No references were found in the international literature regarding the simulation of heat and mass transfer, for the climatic conditions of Argentina. Studies on transport phenomena for wheat, from summer to winter were presented in Balzi et al. (2008) and Abalone et al. (2006).

The aim of this work was to analyze storability of soybean from autumn to summer, for the weather conditions of Rosario (Lat. 32°57’S, Long. 60°38’W), located on one of the most productive agricultural region of Argentina. The effect of initial grain temperature and permeability on the development of natural convection flows, temperature distribution and moisture migration was examined. A comparative analysis of moisture migration for soybean, corn and wheat, the three most important grains cultivated in Argentina, is also provided.

II. HEAT TRANSFER MODEL

A. Mathematical Model

The momentum, heat and mass transfer model described in Part I of present study (Arias Barreto et al.,
2013) was applied to predict natural convection flows, temperature distribution and moisture migration. The main model assumptions were local thermodynamic equilibrium between the grain and interstitial air, negligible accumulation of moisture in the interstitial air and moisture diffusion by grain to grain contact, ideal gas behavior of the air-vapor mixture and Darcy’s flow.

To accurately predict grain spoilage during storage, temperature and moisture distribution must be correctly estimated. They respond to seasonal variation of climatic conditions. Thus, realistic boundary conditions must include the effect of solar radiation and wind speed as discussed by Montross et al. (2002), who also analyzed the differences arising when daily or hourly weather data are inputs of the simulation.

In present study, a 2D axisymmetric domain was considered as shown in Fig. 1. Boundary and initial conditions are expressed by Eqs. (1) to (8). To satisfy symmetry conditions on \( \Gamma_1 \), the stream function and normal gradient of water vapour pressure must vanish. The same condition must be applied on the rest of the boundaries to model an impermeable condition to moisture transfer. Both conditions are represented by Eqs. (1) and (2). Auxiliary expressions for model functions \( \eta \) and \( \omega \) were given in detail in Abalome et al. (2006) and Gastón et al. (2009). A symmetry temperature condition was applied on \( \Gamma_1 \) and thermal isolation on \( \Gamma_2 \) as expressed by Eq. (3).

\[
\Psi = 0 \quad \text{on} \quad \Gamma
\]

\[
\frac{\partial p_v}{\partial n} = 0 \quad \Rightarrow \eta D_{ef} \frac{\partial W_f}{\partial n} = -\omega D_{ef} \frac{\partial T}{\partial n} \quad \text{on} \quad \Gamma
\]

\[
\frac{\partial T}{\partial n} = 0 \quad \text{on} \quad \Gamma_1 + \Gamma_2
\]

\[-k_b \frac{\partial T}{\partial n} = h_{eq}(T - T_{amb}) + \alpha G - \xi \sigma (T^4 - T_s^4) \quad \text{on} \quad \Gamma_3
\]

\[-k_b \frac{\partial T}{\partial n} = h_{eq}(T - T_{hs}) \quad \text{on} \quad \Gamma_4
\]

\[
\Psi(r, z, t = 0) = 0
\]

\[
W_g(r, z, t = 0) = W_0(r, z)
\]

\[
T(r, z, t = 0) = T_0(r, z)
\]

On \( \Gamma_3 \), convection and radiation with the surroundings and solar radiation were taking into account (Eq. (4)). The equivalent heat transfer coefficient \( h_{eq} \) includes the effect of wind speed \( (h_{eq}) \) and conduction through the steel wall \( (h_{bin}) \). A simplified boundary condition was applied on \( \Gamma_4 \), assuming that the top grain surface exchanges energy with an “environment” which has a variable temperature \( T_{hs}(t) \), the temperature of the bin headspace (Alagusundaram et al., 1990). Definitions of headspace temperature \( T_{hs} \), sky temperature \( T_s \) as well as model parameters of boundary conditions are listed in Table 1.

To estimate solar radiation on the vertical wall, the cylindrical bin was approximated by a prism of 32 sides (Jiang and Jofriet, 1987). To account for seasonal variations and orientation, solar radiation \( G \) on each plane was estimated according to Duffie and Beckmann (1980) and the mean value over the 32 planes was applied on the bin wall. Horizontal global solar irradiance was calculated applying Model C (Iqbal, 1983). Model C is a well documented radiation model that evaluates solar radiation by considering the mechanisms of transmittance, reflectance and absorbance of the atmosphere.

### B. Numerical Solution. Finite Element Formulation

The model was implemented in COMSOL Multiphysics 4.2a and solved by the Finite Element Method. A refined mesh was generated at the boundaries were the highest temperature and moisture gradients were expected to occur. Quadratic Lagragian elements and a fourth order numerical quadrature were applied. UMFPACK solver was selected to solve the PDE system (unsymmetrical multifrontal method and direct sparse LU factorization).

Table 1: Mathematical model parameters

<table>
<thead>
<tr>
<th>Model parameters</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T_{hs}(t) = T_{amb}(t) + 5 )</td>
<td>Alagusundaram et al. (1990)</td>
</tr>
<tr>
<td>( \sigma T_s^4 = \xi \sigma T_{amb}^4 )</td>
<td>Mills (1995)</td>
</tr>
<tr>
<td>( h_{eq} = (h_{eq} + h_{bn})^{-1} )</td>
<td>Alagusundaram et al. (1990)</td>
</tr>
<tr>
<td>( h_{eq} = 1Wm^{-2K^{-1}} )</td>
<td>Alagusundaram et al. (1990)</td>
</tr>
<tr>
<td>( h_{bn} = 2x10^4Wm^{-2K^{-1}} )</td>
<td>Kreith (1973)</td>
</tr>
<tr>
<td>( \xi = 0.82 )</td>
<td>Kreith (1973)</td>
</tr>
<tr>
<td>( \xi = 0.28 )</td>
<td>Kreith (1973)</td>
</tr>
<tr>
<td>( \alpha = 0.89 )</td>
<td>Kreith (1973)</td>
</tr>
<tr>
<td>Bin height = 13 m</td>
<td></td>
</tr>
<tr>
<td>Bin ratio = 5.4 m</td>
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</tbody>
</table>

Figure 1: Schematic diagram of the domain
III. APPLICATION EXAMPLES

A. Storage of soybean from autumn to summer. Effect of initial storage temperature

The numerical model was applied to study the storage of soybean during seven months (210 days), from 15th May to 15th December (autumn-winter-spring) for the climatic conditions of Rosario (Lat. 32°15'08'0" Long. 60°38'30") in the south of Santa Fe province, Argentina. Averaged daily weather data (ambient temperature, relative humidity, wind speed and solar radiation) from 1981 to 1990 were used as input data.

Simulations were carried out for 13 % w.b initial moisture content (MC) and 25, 20 and 15°C initial grain temperature. Moisture dependent thermal properties for soybean were taken from ASAE Standard D241.4 (2003) and Navarro and Noyes (2002); permeability and coefficients of the Modified Henderson Thompson isotherm from Brooker et al. (1992).

Predicted streamlines, temperature and MC distributions for 25°C are presented for several selected months (July, October, December) in Figs. 2a through 2c. This rather high initial temperature was selected as it represents the worst initial storage condition.

Isotherm distributions are shown in Fig. 2a. Ambient temperature and solar radiation decreased from May to July. In response, temperature gradients developed near the top surface and vertical wall promoting natural convection flows flowing clockwise. During the first month, as convection transport was weak, isotherms remained parallel to the boundaries, typical of a conductive transport phenomenon. By the end of July the circulation displaced the isotherms towards the top and upper corner wall, while at the bottom bended them towards the center of the bin. Convection flows contributed to cooling the grain layer at the outer bottom corner to near 17°C by end of September, temperature level which arrests insect development, but unfavorable storage conditions remained in most regions of the bin. By December the effect of solar radiation was strong, being the temperature at the outer boundary about 10°C higher than at the center of the bin.

Streamlines are illustrated in Fig. 2b. A positive value of the stream function $\psi$ means a clockwise circulation. Convection flows reached their maximum value $\psi_{\text{max}}$ of 77 m$^3$ d$^{-1}$ in July. By the end of September and during October the flow reversed and reached in December similar values to those of July.

Moisture content redistribution is presented in Fig. 2c. As result of temperature gradients moisture migrated by diffusion below the top surface and along the side wall in a narrow boundary layer ($\sim 0.15$ m). Counter-clockwise circulation from May to September transported moisture from the bottom to the top layer and outer corner. In July, a very small wet spot at 14 %w.b (not visible in Fig. 2c) developed close to the side wall. By the end of September, on average, MC increased 0.3 % at the top corner and decreased in the same proportion at the bottom one. After the flow reversal in October, the spot of higher MC accumulated at the top outer corner started to be redistributed towards the interior. In this region, radial inward temperature gradients and counterclockwise convection flows contributed to transport moisture form outside to inside.

ERH was calculated by use of the sorption isotherm. On average, ERH increased from 72 to 75 % (low risk for mold development) in the layers of higher MC while decreased below 70 % at the bottom of the bin.

For 20°C initial temperature, similar streamline patterns were obtained (not shown). The effect of natural convection flows was lower during winter ($\psi_{\text{max}} \sim 47$ m$^3$ d$^{-1}$); the flow reversal started earlier (end of August) and continued during September. By December $\psi_{\text{max}}$ increased to 100 m$^3$ d$^{-1}$. The lower initial temperature and the effect of solar radiation warming the bin side wall minimized the radial temperature gradient (driving force for natural convection flows) during autumn and winter, while maximized it during spring. The isotherm distribution showed that by September the central region of the bin (r < 3 m; 3 m < z < 12 m) remained nearly at 19 - 20°C. MC redistribution at the top surface decreased to 0.1 - 0.2 % w.b from June to August and the zone of lower MC at the bottom became very small.

For 15°C initial temperature, safe conditions remained during winter. From May to August convection flows were low ($\psi_{\text{max}} \sim 16$ m$^3$ d$^{-1}$) and migration was practically suppressed. In spring, solar radiation increased the temperature of a boundary layer of about 1.5 m width above 18°C and stronger natural convection developed ($\psi_{\text{max}} \sim 126$ m$^3$ d$^{-1}$).

Numerical results obtained for soybean were in accordance with published results for wheat and corn (Khankari et al., 1995; Montross and Maier, 2001; Casada et al., 2002). In present study, the inclusion of solar radiation and less severe ambient conditions during winter reduced the magnitude of natural convection flows for comparable values of grain permeability and bin size. In general, patterns of temperatures, moisture content, and streamline distribution were compatible with those obtained by other researches. (Montross, 1999; Jia et al., 2000; 2001; Carrera-Rodríguez et al., 2011).

The evolution of average grain temperature, average ambient temperature and horizontal solar irradiance are plotted in Fig. 3a and interstitial air equilibrium relative humidity (ERH) in Fig. 3b. On average, these results show that the feasibility of storing soybean without aeration is acceptable for 15°C initial storage temperature (temperatures < 17°C prevent insect infestation; ERH < 75 % mold development), though locally, risky areas were identified. In the other cases, the climatic conditions during winter were not as se-
Figure 2: Predicted variables for soybean stored at 25°C and 13 %w.b permeability $K_1=1.86 \times 10^{-8}$ m$^2$ (a) Isotherm distribution; (b) Streamline distribution; (c) Moisture content distribution

Figure 3: Average soybean temperature and interstitial air ERH from winter to spring as function on initial storage temperature

B. Effect of grain permeability

Relevant model parameters are listed in Table 2 for wheat, corn and soybean. It is observed that moisture dependent bulk thermal properties of grains (evaluated at 13 %w.b) are comparable while a large range in values of permeability was found in the literature.

Table 2: Grain properties evaluated at 13 %w.b.

<table>
<thead>
<tr>
<th></th>
<th>$c_b$ [J/kgK]</th>
<th>$k_h$ [W/mK]</th>
<th>$\rho_b$ [kg/m$^3$]</th>
<th>$\varepsilon$</th>
<th>$K$ [x10$^{-5}$ m$^2$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wheat</td>
<td>1934</td>
<td>0.15</td>
<td>756</td>
<td>0.38</td>
<td>0.26-4.59*</td>
</tr>
<tr>
<td>Corn</td>
<td>1931</td>
<td>0.16</td>
<td>763</td>
<td>0.40</td>
<td>0.35-1.61*</td>
</tr>
<tr>
<td>Soybean</td>
<td>1923</td>
<td>0.15</td>
<td>772</td>
<td>0.34</td>
<td>1.85-2.87</td>
</tr>
</tbody>
</table>

(*) (Khankari et al., 1995)

Moisture migration depends on the intensity of natural convection flows. The magnitude of these currents is governed by the Rayleigh number of the porous media $Ra$. Therefore, for a given temperature difference $\Delta T$ and bin ratio $R$, on average, the source of natural convection flows (Eq.(11), Part I of present study) is 2.5 times higher for soybean than for corn and 6 times higher than for wheat. To quantify the effect of permeability on grain cooling and moisture migration during winter, the standard case (soybean, 13 %w.b and 25°C initial conditions, $K = 1.85 \times 10^{-8}$ m$^2$) was run for the range shown in Table 1, $K_1=0.255 \times 10^{-8}$ m$^2$, $K_2 = K$, $K_3=2.87 \times 10^{-8}$ m$^2$, and $K_4=5K$. Table 2 compares maximum value of the stream function.
Figure 4: Predicted variables at the end of September for wheat, $K = 0.255 \times 10^{-8}$ m$^2$; corn, $K = 1.61 \times 10^{-8}$ m$^2$; soybean $K = 1.86 \times 10^{-8}$ m$^2$(a) Isotherm distribution; (b) Streamline distribution; (c) Moisture content distribution

($\psi_{\text{max}}$), temperatures at the center and boundary wall in the bin bottom layer ($z < 2.5$ m) and moisture accumulation at the corner area by end of August (before radiation starts to warm the outer boundaries and flow to reverse).

For the lowest permeability, migration was not significant. For the highest one, at the top corner MC increased to 15.8 %w.b and ERH to 79 %, creating conditions for potential grain spoilage.

As result of the 5 times increase in the intensity of natural convection flows, in the lower part of the bin ($z < 5$ m), the temperature at the center decreased from 25 to 19°C. Such a strong natural cooling effect in the central part of the bin is not consistent with general field observation.

C. Comparison of moisture migration in wheat, corn and soybean

Finally, simulations were run setting model parameters to those of wheat and corn. Predicted results at the end of September were compared with those obtained for soybean (standard case) in Fig. 4a through 4c. Temperature isotherms for wheat remain parallel to the boundaries, typical of conductive transfer, while those for corn and soybean showed the cooling effect at the bottom of the bin by natural convection flows 8 times higher than those for wheat. As expected, moisture migration for wheat was very low and redistribution concentrated by diffusion at the boundaries in response to temperature gradients (for both values of permeability shown in Table 1). When permeability

<table>
<thead>
<tr>
<th>$\psi_{\text{max}}$</th>
<th>$T_{\text{center}}$ ($^\circ$C)</th>
<th>$T_{\text{wall}}$ ($^\circ$C)</th>
<th>$M_{\text{top}}$ % w.b</th>
<th>$M_{\text{bottom}}$ % w.b</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_1$ 9</td>
<td>24.0</td>
<td>15.0</td>
<td>13.0</td>
<td>12.9</td>
</tr>
<tr>
<td>$K_2$ 77</td>
<td>24.0</td>
<td>15.0</td>
<td>13.3</td>
<td>12.7</td>
</tr>
<tr>
<td>$K_3$ 148</td>
<td>23.0</td>
<td>15.0</td>
<td>13.5</td>
<td>12.6</td>
</tr>
<tr>
<td>$K_4$ 300</td>
<td>19.0</td>
<td>14.5</td>
<td>15.8</td>
<td>12.8</td>
</tr>
</tbody>
</table>
of soybean and corn was similar \((K = 1.85 \times 10^{-8} \text{ m}^2\) and \(K = 1.61 \times 10^{-8} \text{ m}^2\), respectively) moisture migration was about 0.3 %w.b for both grains. A close inspection of the wet spot at the top corner showed that accumulation was higher for soybean than for corn, with stepper moisture gradients as discussed in Part I of this study.

**IV. CONCLUSIONS**

In this work, a 2D momentum, heat and mass transfer model was applied to predict natural convection flows, temperature distribution and moisture migration in soybean stored in a cylindrical bin without aeration for the weather conditions of Rosario, Argentina.

For soybean stored at 25°C and 13 % w.b convection flows and temperature gradients during autumn and winter promoted moisture migration of about 0.3 % w.b near the top grain surface and side wall. At the bin bottom moisture content decreased in the same proportion. The upper layers of grains remained almost at the initial temperature while the temperature of the bottom layers ranged from 23 to 17°C. As the initial grain temperature decreased convection flows decreased during winter and moisture migration reduced. At 15°C safe conditions remained during winter but during spring the temperature of a boundary layer 1.5 m width increased above 18°C. Permeability has the strongest effect on natural convection and as result of moisture migration areas of potential spoilage may develop at the upper corner of the bin. A comparative study showed that moisture migration during autumn and winter was very small for wheat and comparable for corn and soybean.

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**NOTATION**

- \(c_b\): specific heat capacity of grain bulk, \(\text{JK}^{-1} \text{g}^{-1} \text{K}^{-1}\)
- \(D_{ef}\): effective diffusivity of water vapour in intergranular air, \(\text{m}^2 \text{s}^{-1}\)
- \(G\): incident solar radiation, \(\text{Wm}^{-2}\)
- \(h_c\): convective heat transfer coefficient, \(\text{Wm}^{-2} \text{K}^{-1}\)
- \(k_b\): bulk thermal conductivity, \(\text{Wm}^{-1} \text{K}^{-1}\)
- \(K\): grain permeability, \(\text{m}^2\)
- \(L\): bin height, \(\text{m}\)
- \(n\): normal direction
- \(p_v\): partial pressure of water vapour, \(\text{Pa}\)
- \(Ra\): Rayleigh number of porous media, \(\frac{K\rho_b\Delta TR}{\mu_\alpha}\)
- \(r, z\): cylindrical coordinates, \(\text{m}\)
- \(t\): time, \(\text{s}\)
- \(T\): temperature, \(\circ\text{C}, \text{K}\)
- \(V\): wind speed, \(\text{ms}^{-1}\)
- \(W_g\): grain moisture content, d.b

**Greek Symbols**

- \(\alpha\): solar surface absorptivity
- \(\alpha_{ef}\): effective thermal diffusivity of porous media (\(\text{m}^2 \text{s}^{-1}\))
- \(\xi\): emissivity
- \(\Gamma\): boundary domain
- \(\eta\): change in the partial pressure due to change in the moisture content at constant \(T\), \(\text{Pa}\)
- \(\rho_b\): grain bulk density, \(\text{kgm}^{-3}\)
- \(\omega\): change in the partial pressure due to change in the temperature at constant \(W\), \(\text{PaK}^{-1}\)
- \(\psi\): stream function (\(\text{m}^3 \text{s}^{-1}\))
- \(\Omega\): domain
- \(\mu\): viscosity of air (\(\text{kgms}^{-1}\))
- \(\sigma\): Stefan-Boltzmann’s constant, \(\text{Wm}^{-2} \text{K}^{-4}\)

**Subscripts**

- \(b\): grain bulk
- \(hs\): headspace
- \(amb\): ambient
- \(s\): sky
- \(0\): initial or reference value

**REFERENCES**


