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Three-Dimensional Transient Heat, Mass, Momentum, and Species Transfer in the Stored Grain Ecosystem: Part II. Model Validation

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THREE-DIMENSIONAL TRANSIENT HEAT, MASS, MOMENTUM, AND SPECIES TRANSFER IN THE STORED GRAIN ECOSYSTEM: PART II. MODEL VALIDATION

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ABSTRACT. *The 3D heat, mass, momentum, and species transfer model for the stored grain ecosystem was validated using data collected from bins filled with corn at West Lafayette, Indiana, and wheat at Stillwater, Oklahoma. Linear and quadratic elements were used in the validation of the finite element model. Input to the model was hourly weather data such as total solar radiation, wind speed, ambient temperature, and relative humidity. The predicted grain temperatures were in accordance with the observed data. The conduction plus natural convection model predictions had a lower standard error than the conduction model. For the two locations, the standard error of prediction of grain temperatures for the conduction plus convection model was in the range of 0.9°C to 3.6°C for wheat and 1.0°C to 3.1°C for corn. The linear heat transfer model predicted reasonably well compared to the quadratic model for wheat, whereas the quadratic model was more accurate for corn. The predicted moisture content followed the trends of observed data with a standard error in the range of 0.1 to 1.28 percentage points. The absolute difference between the predicted and observed species concentrations was in the range of 0 to 0.3 mg* L^{-1}*. The 3D stored grain ecosystem model validated in this study can therefore be used to predict with confidence grain temperature, moisture content, natural convection, and species concentration changes in a stored mass of any type of grain in a cylindrical corrugated steel structure of any size at any geographical location.*

Keywords. *3D model, Finite element method, Heat, Mass, Momentum, Species, Stored grain ecosystem.*

Temperature, moisture, and CO_2 concentration vary during grain storage as a result of physical, chemical, and biological activities inside the grain mass. The temperature and moisture content of grain inside a bin change due to solar radiation, natural convection, forced convection by aeration, and insect and mold activity. The factors influencing grain deterioration during storage are grain temperature and moisture; the concentrations of insects, mites, and mold; geographical location; and bin structural orientation (Jayas, 1995). The best management practices for storage in a particular structure under specific grain and environmental conditions can be evaluated using a comprehensive stored grain ecosystem model (Montross et al., 2002a, 2002b). The factors that most affect grain storage are grain temperature and moisture. Computer simulation models can predict grain temperature and moisture over a period of time. Based on these predictions, grain storage managers can make management decisions based on factors other than just past experiences.

Validation is an integral component of the model development process. Different techniques have been used to validate heat, mass, and momentum transfer models for the grain storage ecosystem. Comparison of predicted and measured temperatures and moistures using graphical representations is a common method of validation (Khankari et al., 1995; Jia et al., 2000). Some validation methods involve quantification of the error or difference between measured and predicted values by calculating the standard error of prediction and the average absolute difference (Alagusundaram et al., 1990; Montross et al., 2002b; Jian et al., 2005). Alagusundaram et al. (1990) used standard error to validate their 3D heat conduction model. They reported an average standard error of 3.3°C with linear elements and 3.2°C with quadratic elements for stored rapeseed. Jian et al. (2005) validated their 3D heat transfer model based on linear elements by using the mean, standard error, and maximum of the absolute difference between the observed and predicted values, which were 2.1°C, 0.3°C, and 6.3°C, respectively.

The objective of this study was the validation of a developed 3D stored grain ecosystem model (Lawrence et al., 2013). The standard error of prediction was used to validate the model. The model was validated in two separate parts using grain storage systems with and without aeration. In the validation of non-aerated grain, it was assumed that heat, mass, and momentum transfer occurred by natural convection and diffusion of heat and moisture inside the grain mass. In the validation of aerated grain, it was as-

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sumed that forced convection and diffusion heat and moisture transfer occurred in the grain mass. Both corn and wheat were used for temperature data validation. The measured temperatures and moisture contents of grain were collected over time from experimental bins and used to validate the predicted results obtained using local site-specific weather data.

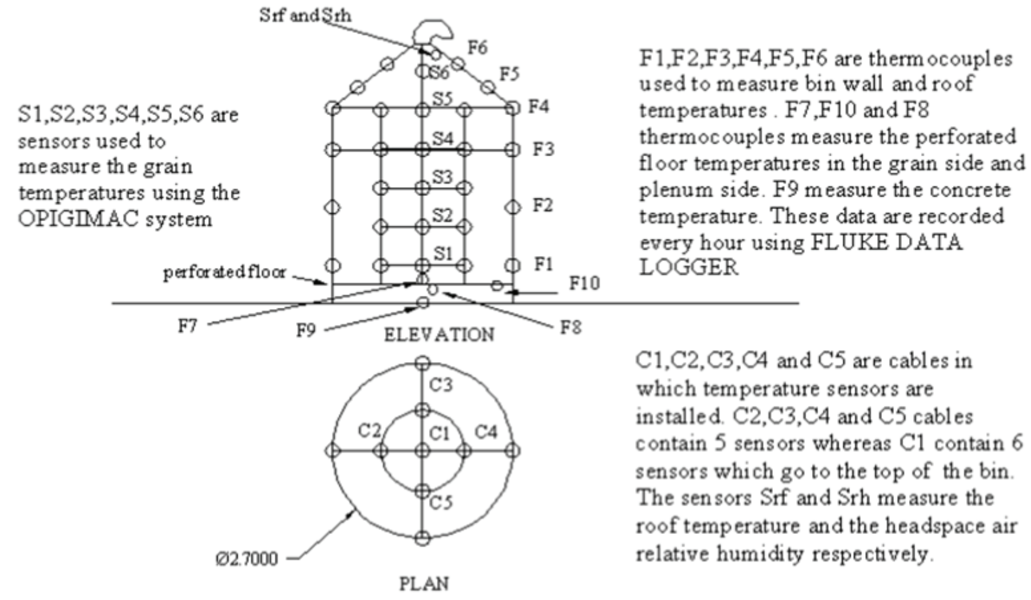
METHODOLOGY

DATA COLLECTION

Data collection for validation of the 3D stored grain ecosystem model was carried out in 12.5 MT pilot-scale bins at two locations using wheat and corn. The corn location was Purdue University's Post-Harvest Education and Research Center (PHERC), West Lafayette, Indiana and the wheat location was Oklahoma State University's Stored Products Research and Education Center (SPREC), Stillwater, Oklahoma. The PHERC pilot bin (Bin 12) was specially equipped for comprehensive data collection in order to validate the 3D PHAST-FEM stored grain ecosystem model. Bin 12 contained 26 thermistors installed on five cables that monitored hourly grain temperature. In addition, one thermistor monitored the roof surface temperature near the roof peak (S_{rf}), and one relative humidity sensor monitored the headspace air relative humidity (S_{rh}). An OPIGIMAC monitoring and aeration control system (fig. 1) (OPI Systems, Inc., Calgary, Alberta, Canada) was used to gather data from the sensors. Bin 12 also contained 28 thermocouples installed on the inside wall, roof, and floor surfaces for monitoring hourly temperatures using a data logger (Fluke Corp., Everett, Wash.). Environmental data including wind speed and direction, ambient air temperature and relative humidity, solar radiation, and rain events were recorded hourly by Purdue's ACRE weather station, located less than 0.8 km (0.5 mi) from the site (http://climate.agry.purdue.edu/climate/index.asp). The OPIGIMAC system also recorded ambient air temperature and relative humidity at the pilot bin facility, which was used to control grain temperatures and moistures using aeration fans.

The OPIGIMAC system consisted of five cables (C1, C2, C3, C4, C5) in which thermistor-type sensors were installed. Cable C1 at the center had six sensors. Cables C2, C3, C4, and C5 had five sensors, each of which passed through the grain mass at the four cardinal directions (N, S, E, W) and at a distance of 0.6 m from the center. The first sensor (S1) in the cable was placed at 0.3 m above the perforated floor, and the remaining sensors (S2, S3, S4, S5, and S6) were placed at 0.6 m intervals. Sensors S_{rf} and S_{rh} measured the steel roof temperature and headspace air relative humidity inside the bin, respectively. All sensors were connected to a computer and recorded data every hour using the OPIGIMAC software. The bin wall, roof, and floor temperatures were measured with thermocouples (F1-F4, F5, F6) installed at the four cardinal directions (N, S, E, W) on the inside bin wall surfaces. The perforated floor temperatures were measured with thermocouples F7 and F8 installed at the center of the perforated floor, one on top of the floor in contact with the grain mass and the other on the underside of the perforated floor exposed to the plenum. The concrete plenum floor temperature was measured with thermocouple F9. Thermocouples F1, F2, F3, and F4 were placed 0.43 m (1 ft 5 in.), 1.25 m (4 ft 1 in.), 2.2 m (7 ft 3 in.), and 2.7 m (9 ft) above the floor, respectively, and F5 and F6 were placed 0.3 m (1 ft) and 0.9 m (3 ft) above the eave, respectively in each direction. The readings were recorded hourly throughout the year. The bin wall and roof temperature readings gave an indication of how the heat flux (from both radiation and wind-induced convection) into the bin varied as a function of environmental conditions. The PHERC bin data were collected from 1998 to 1999.

A similar array of sensors was installed in a pilot bin of same size (12.5 MT) filled with wheat and located at



S1,S2,S3,S4,S5,S6 are sensors used to measure the grain temperatures using the OPIGIMAC system

F1,F2,F3,F4,F5,F6 are thermocouples used to measure bin wall and roof temperatures . F7,F10 and F8 thermocouples measure the perforated floor temperatures in the grain side and plenum side. F9 measure the concrete temperature. These data are recorded every hour using FLUKE DATA LOGGER

C1,C2,C3,C4 and C5 are cables in which temperature sensors are installed. C2,C3,C4 and C5 cables contain 5 sensors whereas C1 contain 6 sensors which go to the top of the bin. The sensors Srf and Srh measure the roof temperature and the headspace air relative humidity respectively.

Figure 1. Temperature sensor arrangement in PHERC Bin 12.

SPREC in Stillwater, Oklahoma. The data were logged every hour. Weather data for the SPREC location were collected from the Mesonet website (http://agweather.mesonet.ou.edu). The SPREC bin data were collected from January to August 2008.

SIMULATION MODELING SETUP

The 3D PHAST-FEM computer simulation model was used to predict grain temperature and moisture content using realistic boundary conditions calculated based on ambient temperature and relative humidity as well as solar radiation and wind speed. The control volume was the volume of grain mass surrounded by wall, headspace, and plenum, and it was used as the computational domain. The boundary conditions for the energy equations were calculated from the energy balance equations formulated for the wall, headspace, and plenum to predict temperatures. The boundary conditions for the moisture equations were calculated from the mass balance equations formulated for the headspace and plenum to predict relative humidities. These formulated transient first-order differential systems of equations were solved using the fourth-order Runge-Kutta method. The predicted temperature and relative humidities were used to find the equilibrium moisture content of the headspace and plenum. The simulated boundary temperature and moisture values were used as prescribed boundary conditions for the 3D model. The grain temperature and moisture values predicted by the 3D model were compared with the actual data collected from the PHERC and SPREC pilot bin facilities.

HEAT, MASS, AND MOMENTUM TRANSFER

Models with linear and quadratic elements were developed to study the heat, mass, and momentum transfer in the grain storage ecosystem. For non-aerated conditions, data collected in 1998 and 1999 at PHERC Bin 12 containing corn and data collected in 2008 at SPREC from a bin containing wheat were used to validate the model. For the pilot bins, the computational domain for PHERC Bin 12 had a grain depth of 2.1 m and bin diameter of 2.7 m, whereas the computational domain for the SPREC bin had a grain depth of 2.7 m and bin diameter of 2.7 m. The domains were meshed using Gambit 2.2.30 (ANSYS, 2009). The meshes that used linear models had 354 nodes and 235 linear hexahedron elements (eight nodes per element) for the PHERC bin (corn) and 472 nodes and 329 linear hexahedron elements (eight nodes per element) for the SPREC bin (wheat). More nodes were used for the SPREC bin to accommodate the extra 0.6 m grain depth. The meshes that used quadratic models had 415 nodes and 36 hexahedron elements (27 nodes per element) for the PHERC bin (corn) and 581 nodes and 54 hexahedron elements (27 nodes per element) for the SPREC bin (wheat). The initial conditions for the PHERC and SPREC bins simulations for each node were calculated using the temperature sensor information recorded on the first day and first hour of simulation. A separate Fortran code was written that inserted the sensor measurements as initial grain temperatures to the appropriate nodes. The geometry data, material properties, fan control information, initial conditions, and weather data were given as input into the 3D model through three separate text files. The parameter values for the shelled corn and hard red winter wheat used to run the 3D PHAST-FEM model are given in table 1. The executive program of the 3D stored grain ecosystem model was run, and the outputs were written in four separate output text files.

The simulations for the non-aeration mode were carried out using three different combinations of component models, i.e., conduction, natural convection (air infiltration), and internal heat generation. Initially, the 3D model was run with the conduction model, followed by conduction plus internal heat generation, and then conduction plus natural convection. It was noted from the preliminary runs that the internal heat generation term in the model did not improve the accuracy of the 3D model. Thus, the results due to internal heat generation term were neglected in the validation process.

The natural convection due to temperature differences in the pilot bin did not have a significant influence on temperature prediction, while air infiltration into the plenum and headspace of the bin did have a significant influence. This was due to the low resistance to airflow for small bins with 2.1 to 2.7 m grain depth. In addition, the effect of thermal buoyancy, which creates a pressure difference in the headspace, is higher in smaller bins compared to larger bins. The pressure difference formed inside the bin led to air infiltration into the plenum. This caused a natural convection air velocity through the grain mass that was previously approximated as 0.0008 m s^{-1} by Montross et al. (2002b). This value was used in this study for modeling and validating corn stored in PHERC Bin 12. For wheat stored in the SPREC pilot bin, the infiltration velocity of 0.0008 m s^{-1} did not predict the observed conditions accurately when the conduction and natural convection models were used. The quality of wheat stored in the SPREC pilot bin was poor, with much dust, fines, and foreign matter that presumably reduced its porosity and increased its resistance to airflow. Natural convection air velocities in wheat storage bins were experimentally measured by Gough et al. (1987, 1990) and ranged from 0.0002 to 0.0006 m s^{-1} depending on the tem-

Table 1. Parameter values for shelled corn and hard red winter wheat used to run the 3D PHAST-FEM model.

	Corn	Wheat
Grain properties		
Initial grain MC (d.b.)	16.28% (14% w.b.)	13.63% (12% w.b.)
Permeability of corn[a]	3.5e-9 m^2 s^{-1}	0.596e-8 m^2 s^{-1}
Density of corn[b]	721 kg m^{-3}	772 kg m^{-3}
Thermal conductivity[b]	0.1409+0.00112[c] W m^{-1} K^{-1}	0.117+0.0011[c] W m^{-1} K^{-1}
Specific heat[b]	1465+35.6[c] J kg^{-1} K^{-1}	1240+36.2[c] J kg^{-1} K^{-1}
Location	Lafayette, Indiana	Stillwater, Oklahoma
Latitude	40.42° N	36.13° N
Longitude	-86.85° W	97.08° W
Elevation	213 m	271.2 m
Radiation properties of the GI sheet[d]		
Longwave emissivity	0.26	0.26
Shortwave absorptivity	0.66	0.66
Re-radiation on roof	60.0 W	60.0 W
Re-radiation on wall	0.0 W	0.0 W

[a] Khankari et al. (1995).

[b] *ASABE Standards* (2008).

[c] Moisture content (% w.b.).

[d] Montross et al. (2002b).

perature gradient. Preliminary trial-and-error simulations indicated that a lower infiltration velocity of 0.0001 m s^{-1} resulted in reasonable predictions and was subsequently used for modeling and validating wheat stored in the SPREC pilot bin.

For validating the aeration scenario for corn, data collected from PHERC Bin 5 during 2009 were used. Experimental data were collected for four days by operating the aeration fan continuously. The design airflow rate for this pilot bin is 2.22 m^3 min^{-1} t^{-1} (2 cfm bu^{-1}). This resulted in a calculated air velocity of 0.3 m s^{-1} for corn with the shutter fully open, assuming 40% porosity in the grain mass. However, during the experiment, the shutter was kept half-open to reduce the airflow. Corn stored in the PHERC pilot bin was of poor quality with many fine particles. Therefore, three additional air velocities of 0.05, 0.1, and 0.2 m s^{-1} were evaluated in addition to the air velocity calculated with the shutter fully open. The simulations were run for four days using weather data collected at a weather station situated about 200 m away from PHERC Bin 5. The accuracy of the model predictions were evaluated by comparing the predicted data with the observed data.

The 3D mass (moisture) transfer in the grain mass was validated using the conduction plus natural convection model for the data from 1998 and 1999. Only a few data points were available to check for standard error. The sample moisture content data collected by Montross (1999) at a location 0.7 m from the plenum were used as the observed data for validation. The initial moisture content of the corn was 14% (w.b.) for both years.

SPECIES TRANSFER

Presently, few models are available to predict species transfer inside grain storage bins. In this study, we attempted to model the rate of evolution of the fumigant phosphine and its movement in the grain mass. The species (fumigant) transfer component in the 3D stored grain ecosystem model was validated using experimental data collected at different temperature and moisture levels by Reed and Pan (2000). They studied the loss of phosphine from unsealed experimental storage bins with hard red winter wheat at 11.1% to 13.5% moisture content and 20°C, 25°C, and 30°C initial grain temperatures. The grain was fumigated with tablets of aluminum phosphide. The phosphine concentration profile was recorded over a period of time at selected locations in the bin. Details about the sampling procedure are given by Reed and Pan (2000). The fumigation data for wheat at 11.1% moisture and 25°C initial temperature were used for this study.

The experimental setup used by Reed and Pan (2000) was simulated with the 3D stored grain ecosystem model. The computational domain consisted of a 1.83 m^3 capacity steel bin with a diameter of 1.4 m and a height of 1.2 m. The domain was meshed with 413 nodes and 282 linear hexahedron elements. Daglish and Pavic (2008) experimentally found that phosphine sorption by wheat was in the range of 1.7% to 9.8%, depending on the filling ratio and fumigant concentration, at 25°C and 55% RH. The sorption of phosphine by the wheat was not included in the model due to its complexity. A fumigant diffusion coefficient of 0.5×10^{-5} m^2 s^{-1} was used in the model (Singh et al., 1993). No equation was available to quantify the rate of evolution of phosphine based on grain temperature and moisture content. It typically takes 2 to 3 days for the pellets to disintegrate and for phosphine to stop evolving. It was assumed that one pellet liberates 1 g of phosphine in total (Reed and Pan, 2000). Therefore, five pellets would liberate 5 g of phosphine in 1.83 m^3 volume. Based on these data, and initially assuming three days as the disintegration period, a calculated constant phosphine generation rate of 2.53×10^{-7} kg m^{-3} s^{-1} was used in the simulation. However, the predicted phosphine concentrations obtained with this phosphine generation rate were 1/10 of the experimental values from Reed and Pan (2000). Using trial and error to match the results of Reed and Pan (2000) gave a phosphine generation rate of 2.5×10^{-6} kg m^{-3} s^{-1} with a disintegration time of two days. A time step of 100 s was found to be appropriate to use in this species transfer model in order to avoid oscillation in the numerical solutions.

RESULTS

NON-AERATION

The three-dimensional model was validated with two different combinations of heat transfer modes (i.e., conduction and natural convection) during the non-aeration period and with linear and quadratic elements.

Heat Transfer for Corn

The standard error of prediction between the observed and predicted grain temperatures for the conduction and conduction plus natural convection model simulations using linear and quadratic elements at PHERC Bin 12 during 1998 and 1999 are given in table 2. The 3D conduction model predicted the temperatures with standard errors of 2.1°C to 7.0°C. It predicted the center temperature at the

Table 2. Standard error of prediction (°C) between observed and predicted corn temperatures during the years 1998 and 1999 for PHERC Bin 12 using the 3D conduction and conduction + natural convection combination models with linear and quadratic elements.

Element Type	Distance above Plenum	Conduction						Conduction + Natural Convection					
		1998			1999			1998			1999		
		Center	South	North	Center	South	North	Center	South	North	Center	South	North
Linear	0.3 m	2.9	4.5	5.3	2.2	4.4	5.5	1.0	1.6	2.5	1.9	1.8	2.4
	0.9 m	4.7	5.5	6.3	4.6	5.5	6.8	1.0	2.4	3.0	1.7	2.4	3.7
	1.5 m	5.5	5.2	6.6	6.4	5.5	7.0	1.3	2.9	3.9	2.3	3.0	5.4
Quadratic	0.3 m	2.4	2.4	3.6	1.9	2.8	4.0	1.0	1.2	2.1	1.9	1.8	2.4
	0.9 m	3.1	2.5	3.7	3.3	2.8	4.7	1.0	1.4	2.3	2.2	1.9	3.3
	1.5 m	2.8	2.1	3.5	4.1	2.6	5.0	1.0	1.6	2.3	2.8	2.1	4.0

0.3 m location with less standard error when compared to locations at 0.9 m and 1.5 m. The predicted grain temperatures did not follow the path of observed values at all locations above 0.3 m.

The predicted and observed grain temperatures at the center, south, and north locations during 1998 for the linear element conduction model are given in figures 2 and 3. The 3D conduction model overpredicted the grain temperatures in all locations for 1998 and 1999 by 2°C to 10°C. For both the center and south locations, the predicted grain temperatures followed the observed values more closely at 0.3 m than at 1.5 m above the plenum. The model predicted that the temperatures at the 1.5 m location increased from early July through the end of August, while the observed temperatures either leveled off or increased in comparison. The standard errors of prediction in several locations were above 4.0°C, which is slightly higher than the values reported in the literature (Alagusundaram et al., 1990; Montross et al., 2002b).

The quadratic element conduction model was better than the linear element conduction model in predicting the grain temperatures. The standard error of prediction was in the range of 1.9°C to 4.1°C at the center location and 2.1°C to 2.8°C at the south location, which was 0.5°C to 3.1°C lower than for the linear element model (table 2). The temperature variations at two locations (0.3 m above the plenum at the center and 1.5 m above the plenum at the south) during 1998 are given in figures 4 and 5. The predicted grain temperatures at the south locations followed the trend of observed grain temperatures more closely than did the center. At the center location, the predicted grain temperature followed a smoother line and did not show the variability shown by the observations. Similar results were observed for 1999.

The standard error of prediction for the validation of heat transfer using the conduction plus natural convection model with linear elements in the PHERC bin filled with corn is given in table 2. The conduction plus convection model reduced the standard error substantially compared to the conduction model in predicting the corn temperature in the PHERC bin. The standard errors were 1.9°C to 4.2°C lower at the center locations and 0.3°C to 4.1°C lower at the south locations versus the conduction-only model results (table 2). Presumably due to the effect of solar radiation, higher standard errors were observed in the south locations than at the center locations. The predicted grain temperatures followed the pattern of observed grain temperatures more accurately than for the conduction-only models (fig. 6). The variability in predicted temperatures, especially at the 0.3 m location in both the center and south locations, followed the observed temperatures much more closely. At 1.5 m above the plenum, the predicted grain temperatures deviated from the observed values by up to 2°C to 5°C at the south location.

The 3D conduction plus natural convection model was also validated for corn using quadratic elements. The standard errors of prediction between the observed and predicted values are given in table 2. For the simulation year 1998, the standard errors were 0.5°C to 1.8°C less than for 1999 for both the south and center locations. The temperature variations between the observed and predicted grain temperatures for 1998 are given in figure 7. The predicted

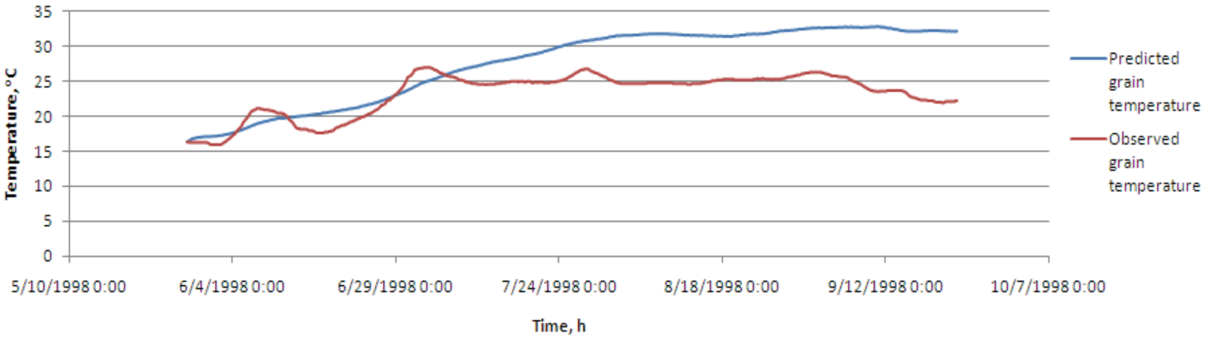


Figure 2. Predicted and observed corn temperatures at 1.5 m above the plenum at the center of PHERC Bin 12 during May-September 1998 for the conduction model simulation with linear elements.

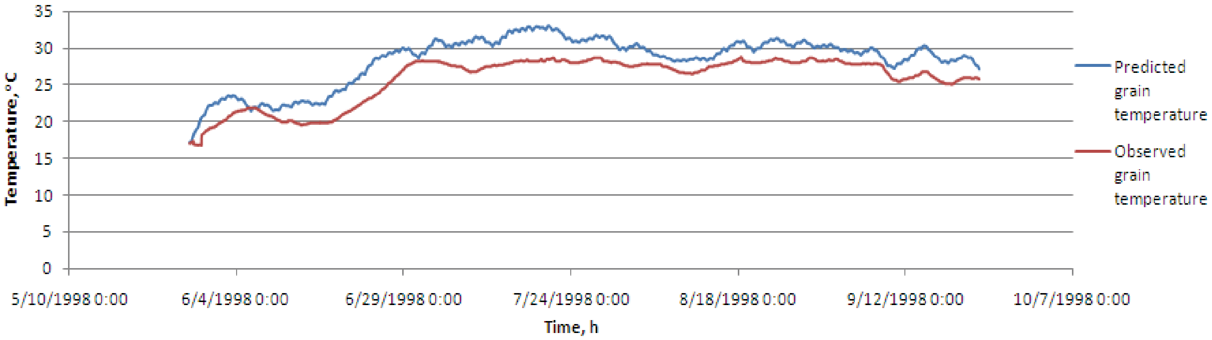


Figure 3. Predicted and observed corn temperatures at 1.5 m above the plenum at the south of PHERC Bin 12 during May-September 1998 for the conduction model simulation with linear elements.

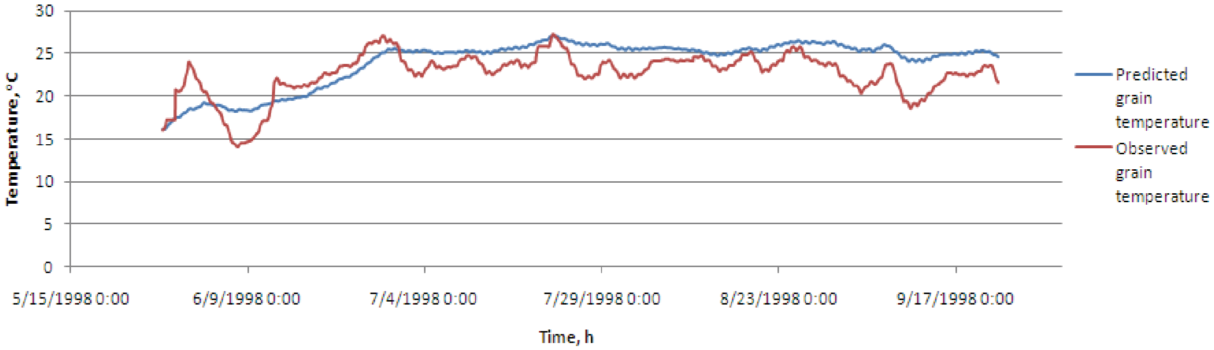


Figure 4. Predicted and observed corn temperatures at 0.3 m above the plenum at the center of PHERC Bin 12 during May-September 1998 for the conduction model simulations with quadratic elements.

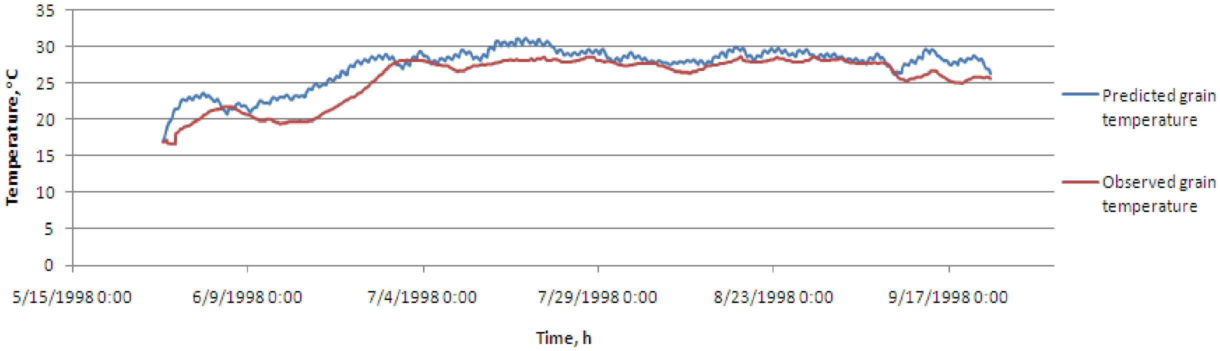


Figure 5. Predicted and observed corn temperatures at 1.5 m above the plenum at the south of PHERC Bin 12 during May-September 1998 for the conduction model simulations with quadratic elements.

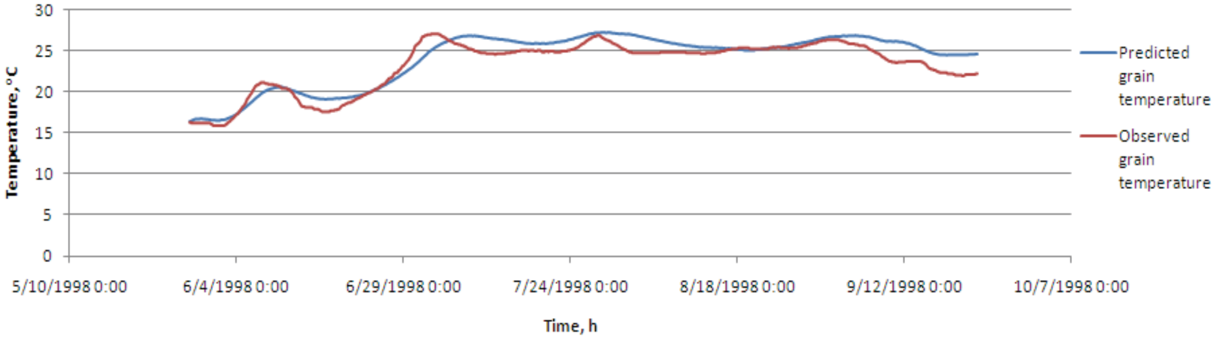


Figure 6. Predicted and observed corn temperatures at 1.5 m above the plenum at the center of PHERC Bin 12 during May-September 1998 for the conduction plus natural convection model simulation with linear elements.

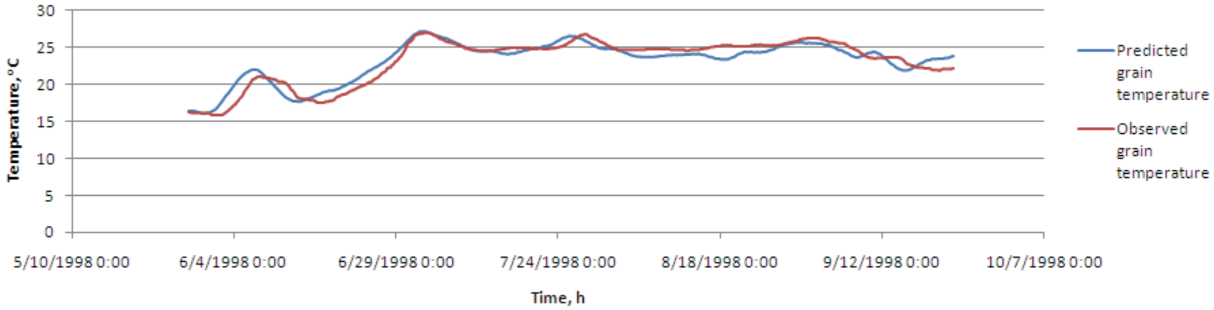


Figure 7. Predicted and observed corn temperatures at 1.5 m above the plenum at the center of PHERC Bin 12 during May-September 1998 for the conduction plus natural convection model simulation with quadratic elements.

grain temperatures closely followed the observed grain temperatures for 1998 in all locations. Similar results were found for 1999. The predicted results and the standard error of prediction values were similar to the literature values reported by Chang et al. (1993), which showed a standard error of prediction of 0.9°C to 1.8°C.

Heat Transfer for Wheat

The data collected in 2008 at the SPREC bin during non-aeration were used to validate the 3D heat transfer model for wheat using both linear and quadratic elements.

Table 3. Standard error of prediction (°C) between observed and predicted wheat temperatures from January to May 2008 for the SPREC bin using the 3D conduction and conduction + natural convection combination models with linear and quadratic elements.

Element Type	Distance above Plenum	Conduction					Conduction + Natural Convection				
		Center	South	North	East	West	Center	South	North	East	West
Linear	0.3 m	1.5	2	2.5	2.8	2.7	1.9	2.1	2.4	2.6	2.8
	0.9 m	0.8	2.7	3.2	3.3	2.6	1.2	2.7	3	3.1	2.6
	1.5 m	1.2	3.1	3.6	3.5	2.6	0.9	3	3.4	3.3	2.5
Quadratic	0.3 m	1.4	3.2	3.8	3.7	3.2	1.8	2.9	3.5	3.4	3.1
	0.9 m	2.4	4.6	5.2	4.7	4	2.1	4.3	4.9	4.4	3.8
	1.5 m	3.4	5.3	5.8	5.1	4.7	2.8	5.1	5.6	4.8	4.5

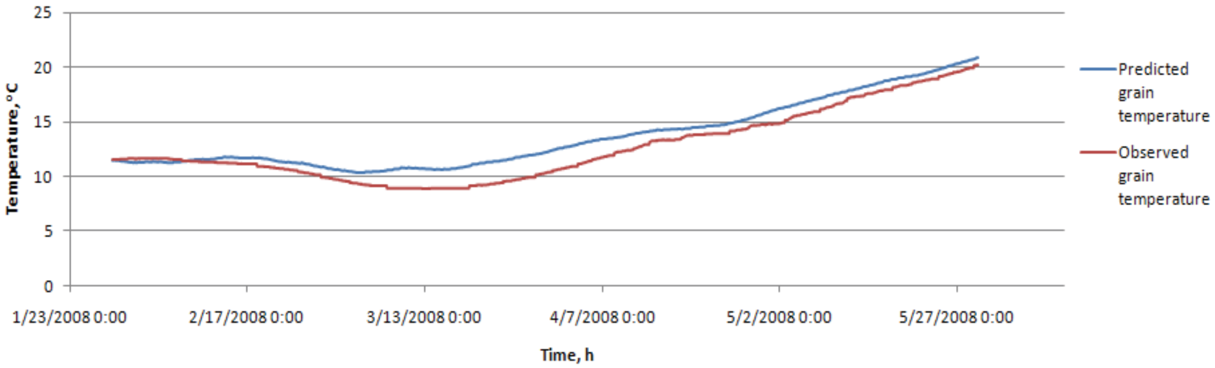


Figure 8. Predicted and observed wheat temperatures at 1.5 m above the plenum at the center of the SPREC bin during January-May 2008 for the conduction model simulation with linear elements.

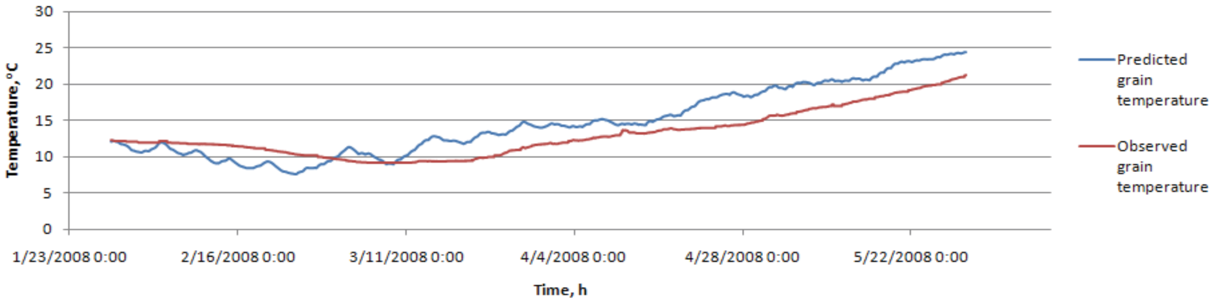


Figure 9. Predicted and observed wheat temperatures at 0.9 m above the plenum at the south of the SPREC bin during January-May 2008 for the conduction model simulation with linear elements.

The standard error of prediction between observed and predicted temperatures from January to May 2008 using the conduction and conduction plus natural convection models are given in table 3. The standard error of prediction was 1°C to 2°C higher for the sides (N, S, E, W) than for the center. The 3D conduction and conduction plus natural convection models predicted temperatures with almost same standard error of prediction. This showed that influence of natural convection was less in predicting these wheat temperatures.

The predicted and observed grain temperatures for the center location (1.5 m above the plenum) in the SPREC bin during 2008 is given in figure 8. The predicted grain temperature followed the trends of the observed values in all locations quite well. Unlike the data observed in the PHERC bin, there was no fluctuation of grain temperatures, especially at 0.3 m above plenum, observed in the SPREC bin. This indicated that the ambient air infiltration into the bin was low and did not cause grain temperature changes. However, the predicted temperatures showed more variation, especially at the 0.3 m center location and the three south locations (fig. 9). This might be due to the assumed air infiltration rate used in the simulation model despite the lower porosity of wheat versus corn. The center location grain temperatures were predicted more closely than at the south location. The 3D conduction model overpredicted temperature by 1°C to 2°C at the 0.3 m location at the center and by 2°C to 5°C at the 0.9 m and 1.5 m locations at the side. Overall, the 3D conduction model predictions were better for wheat grain stored in the SPREC bin than for corn in the PHERC bin.

The standard errors of prediction between observed and predicted wheat temperatures from January to May 2008 using the 3D conduction model with quadratic elements are given in table 3. The use of quadratic elements in the 3D model did not improve the standard error of prediction compared to the model with linear elements. As a matter of fact, the standard error increased by 0.5°C to 2.2°C except at the 0.3 m location at the center, where the standard error decreased by 0.1°C. The temperature variations between the predicted and observed values are shown in figure 10. As was observed for the linear elements, the predicted grain temperatures followed the trends in the observed values similarly well at the 0.3 m center and south locations.

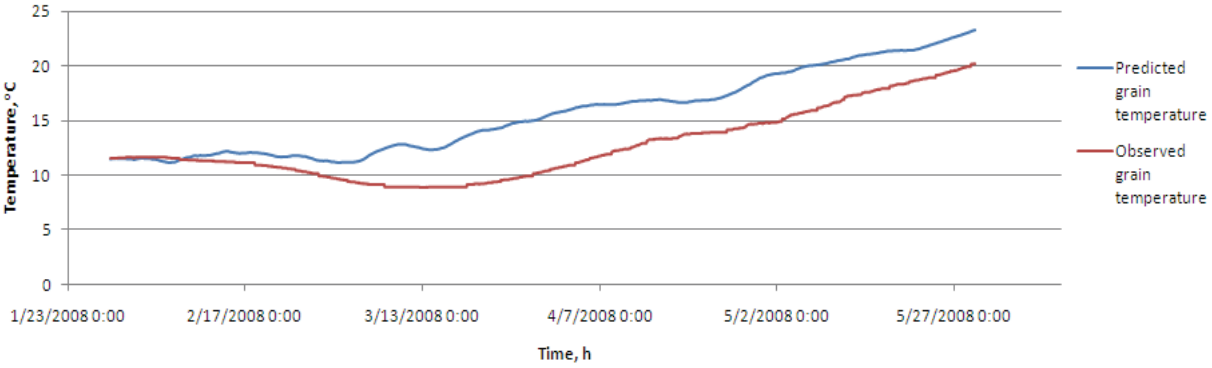


Figure 10. Predicted and observed wheat temperatures at 1.5 m above the plenum at the center of the SPREC bin during January-May 2008 for the conduction model simulation with quadratic elements.

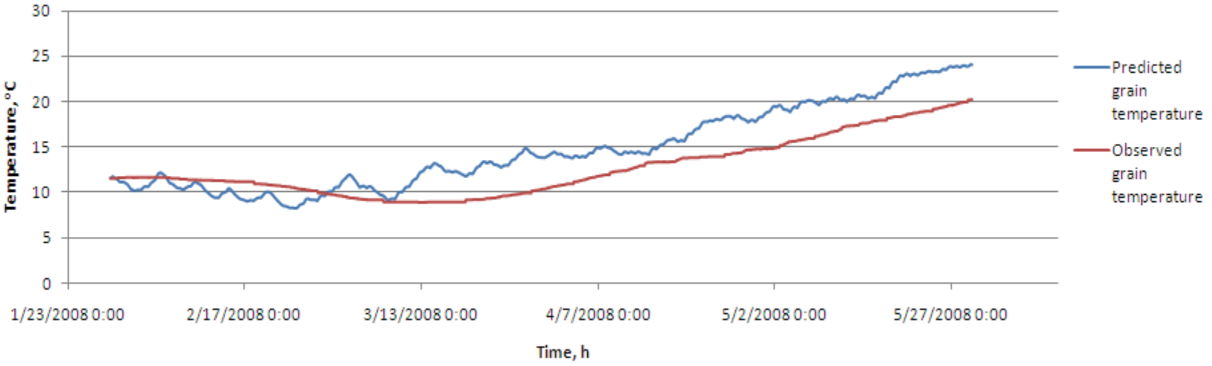


Figure 11. Predicted and observed wheat temperature at 1.5 m above the plenum at the south side of the SPREC bin during February-May, 2008 for the conduction plus convection model with linear elements.

However, higher deviations from observed values were found at the 1.5 m location (fig. 10).

Validation of the 3D heat transfer conduction plus natural convection model using linear elements was carried out using the data collected for the SPREC bin with wheat. The standard errors of prediction between the observed and predicted grain temperatures are given in table 3. In comparison to the conduction model, standard errors were -0.2°C to 0.4°C different. The predicted results were very much in accordance with the conduction model when the natural convection velocity of 0.0001 m s^{-1} was used, i.e., difference in the standard error between conduction and conduction plus natural convection were in the range of -0.3°C to 0.4°C at the center and -0.1°C to 0.1°C at the south locations. The temperature variations at south side location (1.5 m above the plenum) for the 0.0001 m s^{-1} case are given in figure 11. There were no fluctuations in the observed grain temperatures over a short period of time. This indicates that the air infiltration rate must have been low. In general, the predicted grain temperatures mostly followed the trends of the observed values. For the south locations, the deviations in the predicted grain temperatures from the observed values were 2°C to 5°C.

The validation of the 3D heat transfer conduction plus natural convection model with quadratic elements was conducted with the presumed infiltration rate of 0.0001 m s^{-1} using data collected in the SPREC bin during 2008. The standard errors of prediction between the observed and predicted grain temperatures are given in table 3. The center locations predicted the grain temperatures with standard error of 1.1°C to 2.3°C lower than the south locations. As was true for the linear model, the predicted values followed the trend of the observed values similar to the linear model (data not shown). Comparing the table 3 values, the standard errors of prediction were 0.9°C to 1.9°C higher at the center, except at the 0.3 m location, and 0.8°C to 2.1°C higher at the south than the linear element results.

Mass Transfer

The mass transfer component of the 3D stored grain ecosystem model with linear conduction plus convection (0.0008 m s^{-1}) finite elements was validated with data collected from PHERC Bin 12 during 1998 and 1999. There were only a few dates on which grain samples were collected and analyzed for moisture content. Thus, comparison and therefore validation using observed data was limited. The predicted and observed moisture content of corn in the PHERC bin are given in figures 12 and 13. The predicted moisture content followed the trend of observed moisture content with an error of 0.1% to 0.41% for 1998. For 1999, the predicted moisture had an error of 0.34% to 1.28%. The predicted moisture content variation between the measured and observed values might be due to the assumption of constant natural convection used in the model. It is acknowledged that the moisture content data collected in the PHERC and SPREC bins were not sufficient to allow for a rigorous validation of the 3D model.

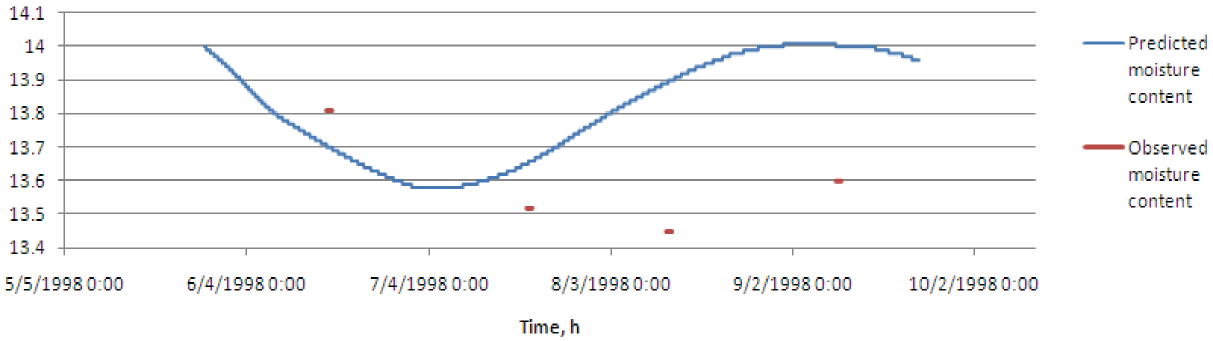


Figure 12. Observed and predicted corn moisture contents at 0.9 m above the plenum at the center of PHERC Bin 12 during May 28-September 22, 1998 for the conduction plus convection (0.0008 m s^{-1}) model.

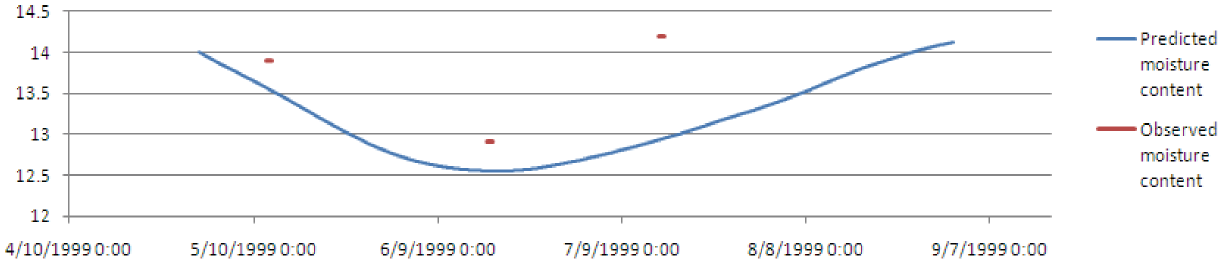


Figure 13. Observed and predicted corn moisture contents at 0.9 m above the plenum at the center of PHERC Bin 12 during May 1- August 31, 1999 for the conduction plus convection (0.0008 m s^{-1}) model.

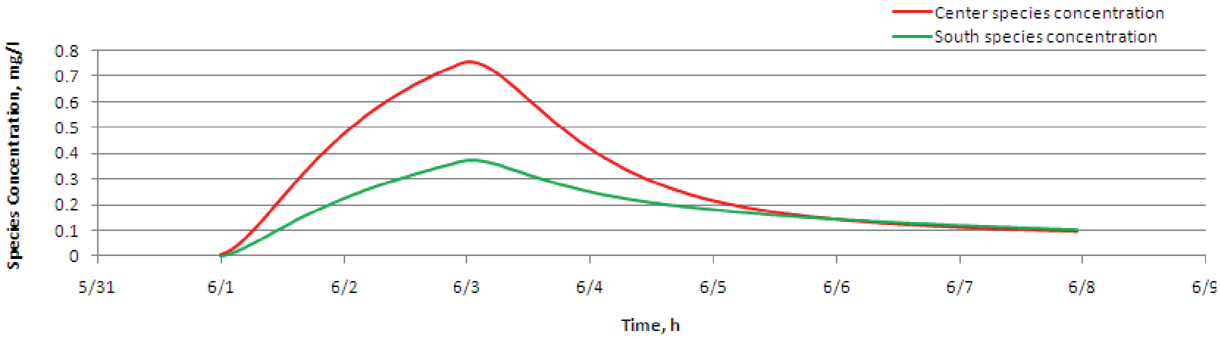


Figure 14. Predicted fumigant (species) concentrations at the center and south locations of the Reed and Pan (2000) experimental bin over a seven-day period for a phosphine generation rate of 2.5 × 10^{-6} kg m^{-3} s^{-1}.

Gas (Fumigant) Transfer

The phosphine concentrations predicted for the experimental grain bin of Reed and Pan (2000) for a fumigant (species) generation rate of 2.5 × 10^{-6} kg m^{-3} s^{-1} is given in figure 14. The predicted and observed fumigant (species) concentrations over a period of seven days are given in figure 15. At the center, where the phosphine pellets were placed, predicted species concentration was about 50% higher than at the south side during maximum peak. After one day, the species concentration inside the bin increased to 0.46 mg L^{-1} at the center, which was similar to the value of 0.42 mg L^{-1} observed by Reed and Pan (2000) at a temperature of 25°C. On the second and third days, the predicted species concentrations were 0.76 and 0.43 mg L^{-1}, respectively, at the center, whereas measured mean concentrations of 0.79 and 0.62 mg L^{-1} were reported by Reed and Pan (2000) at a temperature of 25°C. The predicted concentration value after the third day was 26% less than the observed mean concentration value. After the phosphine pellets were spent and the maximum was reached at both locations, the species concentrations were predicted to decrease sharply over the next two days to about 0.2 mg L^{-1}, after which point the concentrations at the two locations overlapped and followed the same pattern of decrease for the remainder of the fumigation. The absolute differences between the predicted and observed species concentrations were in the range of 0 to 0.3 mg L^{-1}. Based on these results, the species transfer component of the 3D stored grain ecosystem model was assumed to have attained an acceptable accuracy.

AERATION

Heat Transfer

The standard error for predicted grain temperatures at the south and center locations during aeration with four different air velocities in PHERC Bin 5 are given in table 4. For the lower air velocity of 0.05 m s^{-1}, the grain temperatures were predicted more accurately than for the higher air velocities. The standard error of prediction between the

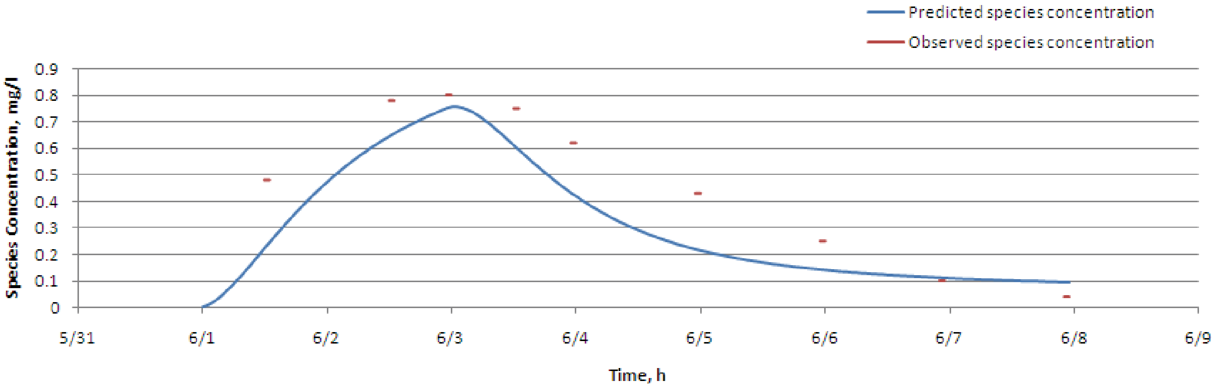


Figure 15. Predicted and observed species concentrations at the center locations over a seven-day period for a phosphine generation rate of 2.5 × 10^{-6} kg m^{-3} s^{-1}.

Table 4. Standard error of prediction (°C) between predicted and observed center grain temperatures at three depths above plenum floor and in the center and south side of the grain mass in PHERC Bin 5 during aeration during 10 to 14 October 2009.

Air Velocity	Center (distance above plenum)			South (distance above plenum)		
($m\ s^{-1}$)	0.3 m	0.9 m	1.5 m	0.3 m	0.9 m	1.9 m
0.05	2.0	1.9	1.7	1.9	2.2	2.1
0.1	2.0	2.3	2.0	2.0	2.9	2.9
0.2	2.1	2.5	2.5	2.2	3.3	3.6
0.3	2.2	2.6	2.6	2.3	3.4	3.8

predicted and observed grain temperatures was in the range of 2.0°C to 2.9°C for an air velocity of 0.1 m s^{-1}. Higher standard errors were observed for higher air velocities (0.2 and 0.3 m s^{-1}). The predictions at the center locations were better than at the south locations by 0.0°C to 1.2°C, except at location 0.3 m above plenum for air velocity 0.05 m s^{-1}.

The predicted and observed temperatures in PHERC Bin 5 at the center and south locations for an aeration air velocity of 0.1 m s^{-1} at 1.5 m above the plenum are given in figures 16 and 17. The predicted grain temperatures followed the pattern of the observed grain temperatures but differed by about 1°C to 2°C. The predictions from the 3D model developed in this study were in accordance with results reported in the literature. Chang et al. (1993) reported a standard error of 2°C to 3°C in temperature predictions for wheat stored in a 6.6 m diameter bin with aeration. Their results suggest that a standard error of 2°C to 4°C during aeration is acceptable. This would make the validation of the 3D ecosystem model acceptable.

DISCUSSION

A number of parameters that were assumed during model development influenced the variation between predicted and observed grain temperatures. The coefficient of thermal

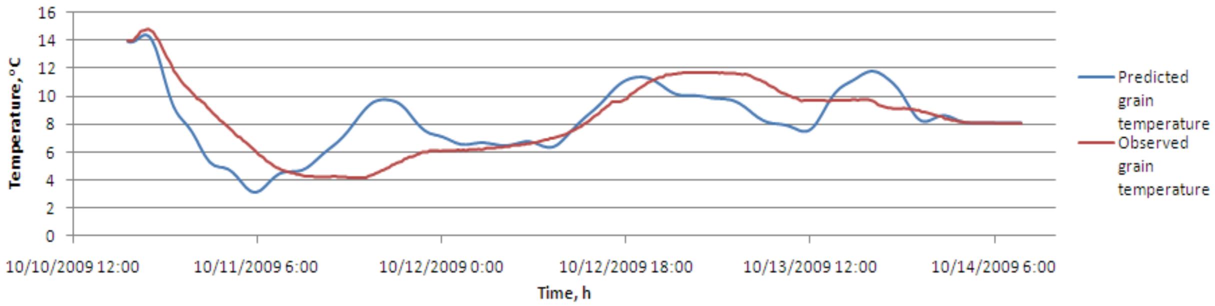


Figure 16. Predicted versus observed corn temperatures at 1.5 m above the plenum in the center of PHERC Bin 5 during 10 to 14 October 2009 for aeration at 0.1 m s^{-1} air velocity.

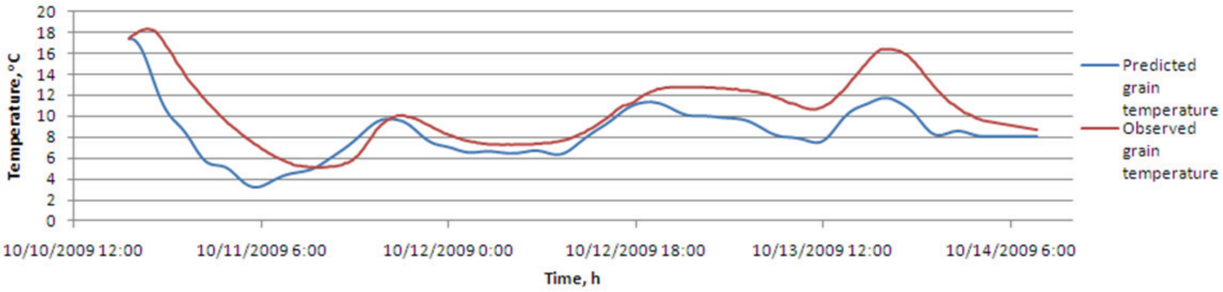


Figure 17. Predicted versus observed corn temperatures at 1.5 m above the plenum in the south of PHERC Bin 5 during 10 to 14 October 2009 for aeration at 0.1 m s^{-1} air velocity.

conductivity of grain is one of the important parameters that affect the accuracy of grain temperature prediction. The experimentally determined constants in the thermal conductivity coefficient equation for some grain types published in ASABE Standard D243.4 (*ASABE Standards*, 2008) were not sufficiently accurate for different varieties of the same grain type. The variety of corn or wheat used in the experiments was unknown. Therefore, the coefficients of thermal conductivity of corn and wheat calculated using these constants influence the accuracy of prediction. In addition, the presence of fines and foreign particles in the grain bulk affect the thermal conductivity property of grain, which is not well documented in the literature. The presence of fines and foreign particles also influences the variation in porosity and bulk density, which could affect the prediction of grain temperature during aeration and non-aeration periods.

The other parameter that affects the grain temperature prediction is the airflow distribution. During the aeration period, airflow is the main driving factor for heat transfer. During the non-aeration period, natural convection airflow drives the heat transfer in addition to conduction. Bartosik and Maier (2006) reported that the presence of fine material at the center core increased airflow resistance in the grain mass, which led to non-uniform airflow distribution. Uniform airflow distribution, which was assumed in the simulation during aeration, resulted in a higher than expected standard error of prediction. During aeration, the variation in the predicted temperatures in the PHERC bin was probably caused by non-uniform airflow. The center grain temperature did not follow the observed values as well when compared to the south side grain temperature. Given that the bin contained much broken corn and fine material, there was a high probability of non-uniform airflow, with less airflow at the center and more at the side (Bartosik and Maier, 2006). Four different airflow rates were used to predict grain temperature to represent these variations, and the lower airflow of 0.05 m s^{-1} produced more accurate results than the higher airflow. The design air velocity was 0.3 m s^{-1}, which was equivalent to an airflow rate of 2.22 m^3 min^{-1} t^{-1} (2 cfm bu^{-1}). The self-closing fan shutter was half-closed during fan operation, which would have reduced the airflow.

Accurate prediction of momentum transfer in the grain mass during the non-aeration period is highly complex. It depends on the accuracy of the temperature gradient prediction and permeability values used in the model. A wide range of permeability values (from 1.61×10^{-8} to 5.96×10^{-9} m^2 s^{-1}) for corn has been published in the literature, as reported by Montross et al. (2002b), who used a value of 3.5×10^{-9} m^2 s^{-1}. They also found that adjusting the permeability values did not improve the prediction accuracy. In addition, predicting the development of a boundary layer during natural convection and a time step of one hour was difficult, if not impossible, considering that there were relatively few elements on the boundary. Usually, a greater temperature gradient exists near the wall than at the inner core, which causes a higher natural convection current to develop near the wall versus the inner core. The natural convection current values developed by the temperature gradients used in the simulation during non-aeration did not predict as well as expected. However, for the PHERC bin, a uniform and constant natural convection air velocity of 0.0008 m s^{-1} used in the model predicted temperature changes with reasonable accuracy. This showed that the influence of wind velocity was higher for these small bins compared to the natural convection developed due to the temperature gradient. These results were in accordance with the results of Montross et al. (2002b).

In the PHERC bin, the fluctuation of grain temperature over short periods of time was observed during the non-aeration period. This may have been due to the fact that the grain bin was small, with a grain depth of only 2.1 m. It is possible that air infiltration into the plenum had a greater effect in these bins due to the low static pressure required for fluid flow, taking into consideration the grain mass porosity of 38% to 40%; the greater the grain depth, the higher the static pressure required to achieve the desired airflow (Shedd, 1953).

There was no fluctuation pattern of grain temperatures observed for wheat in the SPREC bin. The following are possible explanations: (1) The wheat in the bin was of poor quality with many damaged kernels, dust (fines), and foreign material that may have reduced the porosity of the wheat. This would increase the airflow resistance, thereby lowering the infiltrated air velocity. (2) The fan shutter was effective enough to stop air infiltration into the plenum. (3) The airflow resistance of wheat was 2.7 times higher than that of corn, which ensured low airflow in the grain mass. Therefore, using a natural convection velocity of 0.0008 m s^{-1} (as in the PHERC bin), the model did not predict temperature changes well for the SPREC bin. However, with a 0.0001 m s^{-1} natural convection velocity, the model predicted with reasonable accuracy. This proved that the wheat was apparently of poor quality, which resulted in low porosity of the stored wheat.

The conduction-only model for corn and wheat did not predict well compared to the conduction plus convection model during the non-aeration period. This implies that the influence of natural convection was greater in these small bins. The temperature predictions for wheat using linear elements were better than those that used quadratic elements; the predictions of the two types of elements were reversed for corn. For wheat, the quadratic elements gave much higher heat conduction (diffusion) rates than the linear elements. There could be the possibility that the element size and one-hour time step used in the quadratic model for wheat were not appropriate for the parameters used in the 3D model.

The variations between the observed and predicted moisture contents might have been caused by several factors. One probable reason is that the calculated diffusion and convection coefficients for moisture transfer in the grain mass were not sufficiently accurate, causing the moisture redistribution component of the model to be ineffective. Lack of available literature limited the comparison of the moisture equation and the results from this study. This warrants further investigation as part of future work. It was observed that the moisture variation was very sensitive to the temperature gradient. There could be a possibility that the moisture transfer due to the temperature changes was not as well captured by the model, as reported by Khankari et al. (1994).

The species transfer model predicted fumigant movement with respect to time in a sealed bin reasonably well. It was assumed that the pellets disintegrated completely after two days. The fumigant concentration inside the bin started decreasing after the second day. The concentration difference between the south and center locations decreased with time and became equal after the sixth day of fumigation. The variations in species concentration prediction were due to several factors. One of the factors was the assumed disintegration rate of phosphine pellets. No data were available in the literature about the disintegration rate of phosphine pellets and tablets. The second factor was the phosphine sorption by wheat. The rate of sorption depends on the phosphine concentration and the temperature and moisture content of the grain. This was not included in the model due to its complexity. The third factor is the diffusion coefficient of phosphine used in the model. There was no literature available that showed how this was determined; however, a value of 0.5×10^{-5} was used by Singh et al. (1993).

CONCLUSIONS

The 3D heat, mass, momentum, and species transfer model for the stored grain ecosystem was validated using data collected from PHERC (West Lafayette, Indiana) for corn and SPREC (Stillwater, Oklahoma) for wheat. The following conclusions were drawn from the validation results:

- The predicted grain temperatures most closely followed the observed grain temperatures during aeration and non-aeration periods for the conduction plus natural convection model. The standard error of prediction was in the range of 0.9°C to 3.4°C for wheat and 1.0°C to 4.0°C for corn during the non-aeration period.
- The linear element model gave the best predictions for wheat, while the quadratic element model gave the best predictions for corn. The standard errors of prediction were 0.9°C to 1.9°C at the center and 2.1°C to 3.0°C at the south for wheat, and 1.9°C to 2.8°C at the center and 1.8°C to 2.1°C at the south for corn.
- The difference between the observed and predicted moisture values was within the acceptable limits. The absolute difference between the predicted and observed corn moisture content was in the range of 0.1 to 0.41 percentage points for 1998.
- The species transfer model predicted evolution of and change in phosphine fumigant concentration in accordance with observed fumigant concentrations available in the literature. The absolute difference between the predicted and observed species concentrations was in the range of 0 to 0.3 mg L^{-1}.

The observations summarized above indicate that the 3D heat, mass, momentum, and species transfer model for stored grain ecosystems developed in this study can therefore be used to predict with confidence grain temperature, moisture content, natural convection, and species concentration changes in a stored mass of any type of grain in a cylindrical corrugated steel structure of any size at any geographical location.

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