Comparison and sensitivity analyses of models for simulating aeration of stored wheat

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Sinicio, R. and Muir, W.E. 1996. **Comparison and sensitivity analyses of models for simulating aeration of stored wheat.** Can. Agric. Eng. 38:183-193. The objectives were to compare equilibrium and non-equilibrium heat and mass balance models and to determine the relative importance of several parameters in a non-equilibrium model for simulating stored wheat aeration in Winnipeg, Canada with linear and non-linear airflow distributions. Predicted grain deterioration for each grain layer was compared after 3 months of storage for various input conditions. The relative importance of each parameter was determined by changing it within its expected range of variation and by calculating the effect of this change on the predicted grain deterioration, after 3 months of storage. The equilibrium and non-equilibrium models were not significantly different for most conditions analyzed when ventilating from 0000 to 0600 h. The most important parameter to simulate aeration of wheat stored for 3 months in Winnipeg, Canada was the parameter N in the thin-layer drying equation followed by the EMC desorption equation, fan temperature rise, and parameter K' in the thin-layer wetting equation, which were equally important. The deterioration model must be improved because the uncertainty in the calculation of wheat deterioration is much higher than the uncertainty generated by the equations used in the computer program for simulating aeration of stored wheat; wheat bulk density can be considered constant; the net heat of sorption can be neglected; and the ratio of bin diameter to bin height is not important in the mathematical model. Keywords: wheat, grain aeration, computer simulation, sensitivity analysis

Les objectifs étaient de comparer les bilans de chaleur et de masse, que suppose l'équilibre et le déséquilibre, et de déterminer l'importance relative des divers paramètres dans un modèle en déséquilibre pour faire la simulation de l'aération de blé en conservation à Winnipeg, Canada, avec une distribution linéaire et non linéaire d'air. La détérioration du grain a été calculée pour chaque couche et comparée après 3 mois de conservation dans différents conditions. L'importance relative de chaque paramètre a été déterminée on le changement dans des limites de variation antecipées et pour calculer l'effet du changement prévu au grain détérioré calculé, après 3 mois de conservation. Les modèles d'équilibre et de déséquilibre n'étaient pas significativerent différents pour la majorité des conditions analysées sous la ventilation de 00:00 a 06:00 h. Le paramètre le plus important pour la simulation d'aération de blé après 3 mois de conservation à Winnipeg, Canada était le paramètre N d'équation de séchage en couche mince suivi par l'equation de EMC de désorption, le chauffage de l'air en ventilateur, et le paramètre K' d'équation d'humidification en couche mince, laquelle était également était importante. Le modèle de détérioration a dû être amélioré à cause de l'incertitude des calcul de détérioration du blé que est plus élevé que l'incertitude crée pour les équations utilisées dans le programme des ordinateurs pour faire la simulation d'aération de blé en conservation; le poids spécifique apparent du blé peut être considéré constant; le chaleur liquide de sorption peut être négligée; et la proportion de diamètre et le hauteur du réservoir ne sont pas importants dans le modèle mathématique.

INTRODUCTION

Metzger and Muir (1983a) developed and validated a computer model to predict heat conduction and forced convection in stored grain. The model can be used to simulate grain temperature and moisture changes in cylindrical granaries aerated intermittently using hourly weather data. Metzger and Muir (1983a) simulated forced convection using the equilibrium model developed by Thompson (1972). Later, Metzger and Muir (1983b) used their model to determine the best airflow rates and fan control strategies for four Canadian Prairie locations using historical weather data for 15 or more harvest years.

Sinicio and Muir (1996) compared the equilibrium model of Metzger and Muir (1983a) with a non-equilibrium model for simulating aeration of wheat stored in Brazil using both linear and non-linear airflow distributions. The non-equilibrium model was developed by Thompson et al. (1968) and modified by Sinicio and Muir (1996) to include thin-layer drying and wetting equations and EMC adsorption and desorption equations developed by Sinicio et al. (1995). The rates of grain deterioration, predicted by the equilibrium and non-equilibrium mathematical models for each grain layer, were compared after one year of storage for various input conditions such as airflow, fan temperature rise, location, and ventilation time. Sinicio and Muir (1996) determined significant differences between the equilibrium and non-equilibrium models. The differences between the equilibrium and non-equilibrium models, however, were affected by parameters such as geographical location, grain layer thickness, grain depth, ventilation time, or assuming a 5% offset in the equilibrium relative humidity in moisture adsorption.

Sinicio et al. (1996) used sensitivity analysis to determine the relative importance of different parameters in the non-equilibrium model of Sinicio and Muir (1996) to simulate aeration of stored wheat in Curitiba, Brazil, using uniform and non-uniform airflow distributions. The model's sensitivity, however, was affected by parameters such as geographical location, grain depth, grain layer thickness, and initial moisture content of the grain.

The objectives were to compare equilibrium and non-equilibrium heat and mass balance models and to determine the relative importance of several parameters for simulating aeration of wheat stored in Winnipeg, Canada for both linear and non-linear airflow distributions. Heat and mass balance models, such as the models being compared, are recommended for operational research studies because they are reasonably accurate and computationally efficient (Sharp 1982).

METHODOLOGY

Allowable safe storage time elapsed (ASTE)

The mathematical model of grain deterioration (Eq. 1) presented by Fraser and Muir (1981) was used to predict the allowable safe storage times for wheat as a function of grain moisture content and temperature:

$$\theta_{\max} = 10^{(a + bM_w + cT_c)} \qquad (1)$$

where:

$\theta_{\max}$ = maximum allowed storage times before seed germination drops by 5% or visible mould appears (d),
M_w = grain moisture content (% wet mass basis-wb),
T_c = grain temperature (°C),
a = 6.2347; b = -0.21175; c = -0.05267 for $12 \leq M_w \leq 19\%$ wb, and
a = 4.1286; b = -0.09972; c = -0.05762 for $19 \leq M_w \leq 24\%$ wb.

This model (Eq. 1) predicts maximum storage times for wheat before germination drops by 5% or visible mould appears. A numerical procedure to calculate the allowable storage time elapsed for each time interval was used by Sanderson et al. (1989). In that procedure, the deterioration model was used to calculate the allowable storage time at each time interval based on the predicted temperature and moisture content of each spatial element. The proportion of allowable storage time elapsed during the time interval is the length of the time interval divided by the allowable storage time. These decimal fractions for all preceding time increments were added to obtain an estimate of the total proportion of allowable storage time elapsed (*ASTE*).

Comparison of equilibrium and non-equilibrium models

The grain deterioration (ASTE), calculated as a function of moisture contents and temperatures, predicted by the equilibrium (Metzger and Muir 1983a) and non-equilibrium mathematical (Sinicio and Muir 1996) models for each grain layer, was compared for 3 months of storage starting from 1 September for various sets of input conditions using the method presented by Sinicio and Muir (1996). The deviation in *ASTE* between equilibrium and non-equilibrium models for each grain layer at any time was calculated as:

$$DC_{ASTE} = 100\left(1 - \frac{ASTE_{neg}}{ASTE_{eq}}\right) \qquad (2)$$

where:

DC_{ASTE} = deviation of allowable storage time elapsed (ASTE) predicted by equilibrium and non-equilibrium models in the comparison of models (%),
$ASTEneq$ = ASTE predicted by the non-equilibrium model (fraction), and
$ASTE_{eq}$ = ASTE predicted by the equilibrium model (fraction).

Sensitivity analysis

The method presented by Sinicio et al. (1996) was used in the sensitivity analysis for simulating aeration of stored wheat. The non-equilibrium model of Sinicio and Muir (1996) was used in the sensitivity analysis to predict the moisture content and temperature for grain layers under forced convection. The relative importance of each parameter in the non-equilibrium model was determined by adding or subtracting fixed increments from that parameter and by calculating the effect of these changes on the predicted grain deterioration. These fixed increments correspond to the uncertainties to measure or calculate each parameter (Table II).

The effect of changing different parameters on the predicted grain moisture contents and temperatures is not needed in the sensitivity analysis because grain deterioration, unlike grain moisture content and temperature, is a continuously increasing cumulative parameter. Grain moisture content and temperature might change significantly depending on the aeration conditions (weather conditions, aeration system, and fan control method) but these variables do not provide an indication of grain quality.

The sensitivity of the non-linear equilibrium model relative to different parameters was determined by the maximum deviations in *ASTE* for all grain layers during 3 months of storage starting from 1 September. The percent deviation in *ASTE* for a given change in a parameter was calculated as:

$$DS_{ASTE} = 100\left(1 - \frac{ASTE_c}{ASTE}\right) \qquad (3)$$

where:

DS_{ASTE} = deviation in *ASTE* caused by adding or subtracting an increment from one or more parameters in the mathematical model (%),
$ASTE_c$ = *ASTE* predicted by the mathematical model after adding or subtracting an increment from one or more parameters (fraction), and
$ASTE$ = *ASTE* predicted by the mathematical model with standard values of parameters (fraction).

Sensitivity analyses were also conducted with several parameters changed simultaneously with random variation for the increments within their range of uncertainty according to the method presented by Sinicio et al. (1996).

Weather data, year of simulation, and total grain depth

Weather database from 1953 to 1992 for Winnipeg, MB, Canada consisting of hourly data of dry-bulb temperatures and relative humidities, obtained from Environment Canada, was used for the simulations. The weather data that prevailed in the median year (1979) and the worst year (1963) for grain storage were selected on the basis of the maximum *ASTE* simulated for any grain layer when ventilating from 0000 to 0600 h during the period 1 September to 30 November. The

Table I: Average weather conditions during the worst (1963) and median (1979) years to aerate stored wheat in Winnipeg, Canada

Year	Month	Temperature (°C)			Relative humidity (%)	
		Mean[1]	Minimum[2]	Maximum[2]	Minimum[2]	Maximum[2]
1963	9	15	7	22	51	86
	10	13	6	20	50	78
	11	-2	-7	4	68	80
1979	9	13	7	19	49	90
	10	4	-1	10	51	90
	11	-5	-9	-1	70	90

[1] Daily mean temperature for 24 h.
[2] Daily minimum and maximum temperatures and relative humidities.

fall season was chosen for the simulation to compare the mathematical models with the same cool-down period used by Metzger and Muir (1983b). The maximum ASTE for each year was determined by simulating aeration of stored wheat for 40 years with the weather data using the equilibrium model of Metzger and Muir (1983a), 15% wb initial moisture content, 30°C initial grain temperature, 1 $L\cdot s^{-1}\cdot m^{-3}$ airflow rate, 1°C fan temperature rise, and 5.7 m grain depth. The grain depth was divided into 20 layers: the first grain layers from the bottom were 50, 100, 150, 200, and 250 mm thick and the remaining 15 layers were 330 mm thick. In all the simulations to determine the median and the worst years, the maximum grain deterioration occurred in the top layers. Therefore, the grain depth for the comparison of models and the sensitivity analysis was 5.7 m for the linear airflow distribution.

Metzger and Muir (1983b) recommended the airflow rate of $1.0\ Ls^{-1}m^{-3}$ for continuous aeration and the aeration time from 0000 - 0600 h for four Canadian Prairie locations including Winnipeg. They also compared this ventilation time with 0600 - 1200, 1200 - 1800, or 1800 -2400 h and concluded that this aeration period provided effective grain quality control, reduced energy use, and minimized moisture content reductions.

The grain deterioration was highest during the worst year compared with the median year because 1963 was warmer than 1979 (Table I) and most deterioration occurred primarily due to the grain temperature. Usually the predicted grain moisture content of the first layer where the ventilation air enters the grain was the highest and the temperature was the lowest. For example, the grain moisture content, temperature, and *ASTE* for the first layer (50 mm thickness) were 17.3% wb, -8.4°C, and 0.27, while for the top layer (330 mm thickness) they were 14.1% wb, 0°C, and 0.61, respectively, after 3 months of ventilation starting from 1 September 1979. Therefore, the effect of grain temperature is more important than that of grain moisture content for aeration of stored wheat under Winnipeg weather conditions.

The same ventilation time, aeration period, total grain depth, and initial moisture content and temperature of the grain were used in the comparison of the models and the sensitivity analysis. The grain layer thickness was determined by dividing the grain depth into 20 layers of equal thicknesses.

Table II: Uncertainties (95% confidence level) in the measurement or calculation of the parameters used in the sensitivity analysis for aerating wheat at an average moisture content of 14.4% wb and temperature of 10.5°C during 1 September to 30 November 1979 in Winnipeg, Canada

Parameter	Uncertainty		References
	Estimated	Used	
Fan temperature rise	±0.5°C	±0.5°C	Benedict (1984); Omega (1986)
Wheat bulk density	±2.5%	±6%	Browne (1962); Muir and Sinha (1988); Nelson (1980); Jayas et al. (1992)
Wheat specific heat	±5.3%	±6%	Mohsenin (1980); Muir and Viravanichai (1972); Singh (1988)
EMC adsorption equation	±7.0%	±6%	ASAE (1993)
EMC desorption equation	±7.0%	±6%	ASAE (1993)
Thin-layer drying equation			Sinicio et al. (1995); Jayas and Sokhansanj (1986)
parameter *K*	±21%	±20%	
parameter *N*	±32%	±30%	
Thin-layer wetting equation			Sinicio et al. (1995); Misra and Brooker (1980)
parameter *K′*	±139%	±90%	
parameter *N′*	±12.9%	±10%	
Airflow	±15%	±6%	Metzger et al. (1981)

Parameters and uncertainty in the measurement or calculation of the parameters

The uncertainties of the parameters (Table II) used in the sensitivity analysis were estimated by Sinicio et al. (1996) except those for the thin-layer drying and wetting equations, which were estimated at the average grain moisture content of 14.4% wb and temperature of 10.5°C during the aeration period. The uncertainties for the parameters *K* and *N* of the thin-layer drying equation and *K′* and *N′* of the thin-layer wetting equation (Table II), which were developed based on the equation of Page (1949), were estimated using the same method presented by Sinicio et al. (1996).

Uncertainties in predicting ASTE

Sinicio and Muir (1996) estimated the minimum uncertainty in predicting *ASTE* to be 30% at the 95% confidence level through an error analysis of the deterioration model developed by Fraser and Muir (1981). Thus, any absolute deviation in ASTE that is less than 30% was considered to be not significant at the 95% confidence level in the comparison of models and the sensitivity analysis.

Input data

The temperature rise of the air as it passed through the fan and ducting was set at 1 to 5°C because axial fans add about 1 to 3°C and centrifugal fans operating at 1.24 - 3.73 kPa add about 3 to 5°C due to heat of compression (Noyes 1990). Air heating in the fan also can be caused by the friction between the air and the fan blades and by the energy lost by the motor. The airflow of 5.7 $L\bullet s^{-1}\bullet m^{-2}$, that was used for the standard conditions with linear airflow (Table III), corresponded to an airflow rate of 1 $L\bullet s^{-1}\bullet m^{-3}$ for a grain depth of 5.7 m. The grain depth for the non-linear airflow case was also set at 5.7 m. The air velocity gradients for non-linear airflow were determined at 1 and 5 $L\bullet s^{-1}\bullet m^{-3}$ assuming that the air velocity varied inversely proportional to the grain height above the floor between the minimum and maximum air velocities in a bin of 5.5 m diameter with 15% and 40% minimum perforated area (Manitoba Agriculture 1987), respectively. Therefore, the air velocities leaving the perforated area were 0.0379 and 0.0711 m/s at 1 and 5 $L\bullet s^{-1}\bullet m^{-3}$, respectively, while the air velocities at the top were 0.0057 and 0.0284 m/s, respectively.

RESULTS AND DISCUSSION

Execution time

The average execution time for the equilibrium model using an IBM 370, model 3090 mainframe computer was about 0.15 s per 100 h of simulation for each grain layer using a 1 h time interval. The non-equilibrium mathematical model was about 30% faster than the equilibrium model.

Changes of moisture content, temperature, and ASTE

The moisture content, temperature, and ASTE simulated using the non-equilibrium model at standard conditions with linear airflow were similar to those obtained for non-linear airflow (Fig. 1). The deterioration was lower for the non-linear airflow because the higher air velocity increased the speed of the cooling front although the average grain moisture content was slightly higher for non-linear airflow. Increased air velocity may increase the speed of the drying or wetting front depending on the air conditions during the ventilation period but the speed of the cooling front was the main factor affecting the rate of grain spoilage for Winnipeg weather conditions.

The deterioration (ASTE) after 3 months of storage predicted by the equilibrium model was slightly lower than that predicted by the non-equilibrium model for most grain layers (Figs. 2 and 3). The differences in ASTE predicted by the models decreased as the air velocity decreased. Because of the dry climate in Winnipeg, the higher prediction of drying was not cancelled by a higher prediction of wetting and therefore resulted in a lower prediction of spoilage. Several researchers have found that equilibrium models overpredict the drying and wetting rates especially in the bottom layers (Morey et al. 1979; Van Ee and Kline 1979a; Mittal and Otten 1982).

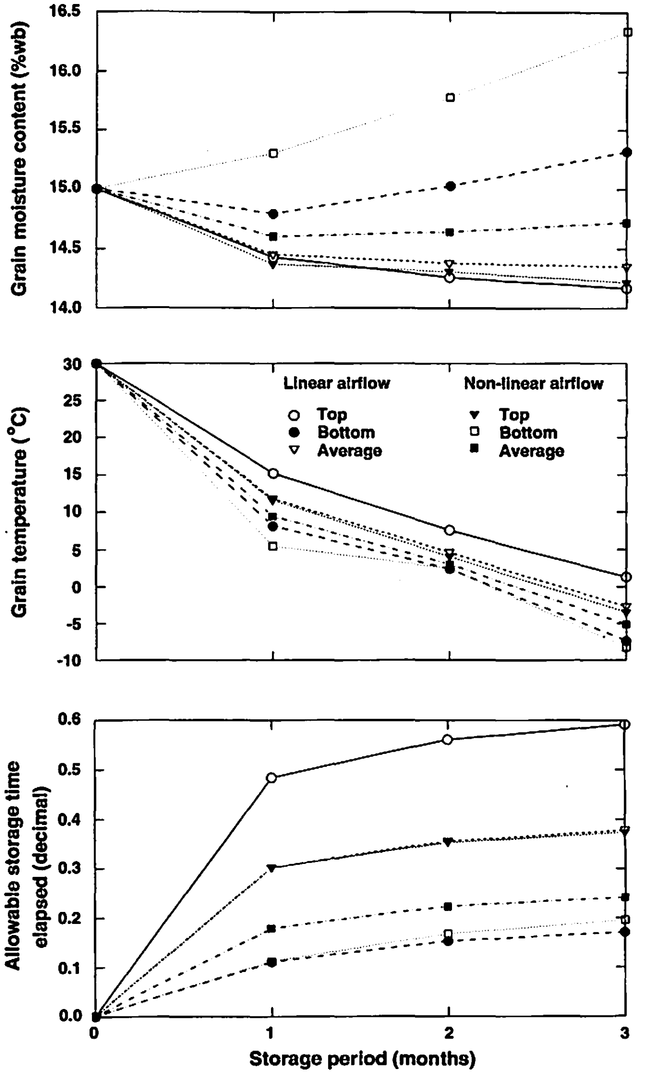

Fig. 1. Moisture content, temperature, and allowable storage time elapsed (*ASTE*) predicted by the non-equilibrium mathematical model for wheat stored at Winnipeg, Canada and aerated for September to November, 1979 at standard conditions with linear and non-linear airflow distributions.

Comparison of predictions of *ASTE* by the equilibrium and non-equilibrium models

The results produced by the equilibrium and non-equilibrium mathematical models were not different when using a ventilation time of 0000 to 0600 h, initial moisture content of 15% wb, and grain layer thickness 284 mm (Tables III and IV) because the maximum absolute deviations in *ASTE* were equal to or less than 30% for almost all tests. The results produced by the models, however, were different for Tests 22

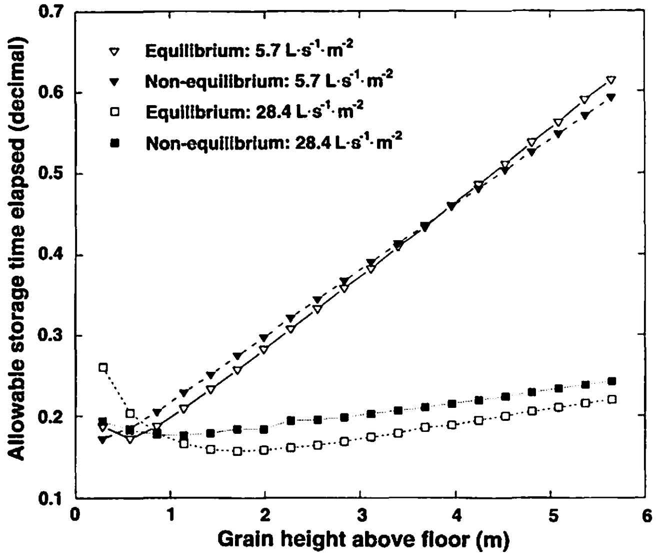

Fig. 2. Allowable storage time elapsed predicted by the equilibrium and non-equilibrium mathematical models for wheat stored at Winnipeg, Canada and aerated for September to November, 1979 with linear airflow distribution and 1°C fan temperature rise.

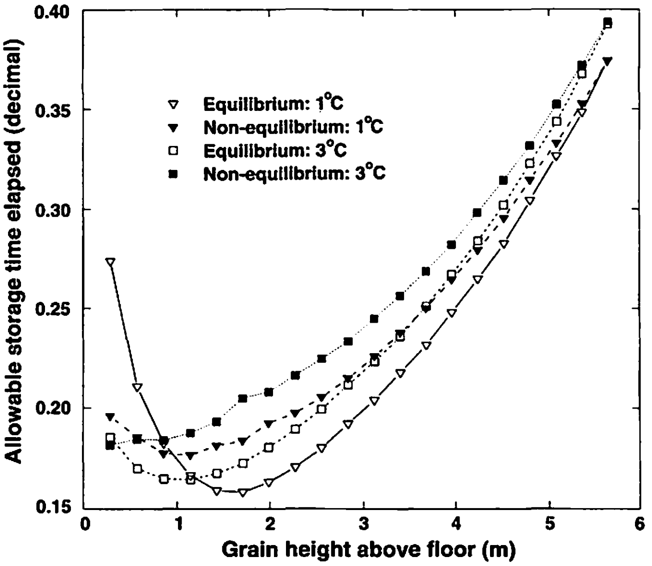

Fig. 3. Allowable storage time elapsed predicted by the equilibrium and non-equilibrium mathematical models for wheat stored at Winnipeg, Canada and aerated during 3 months with air velocities varying from 5.9 L•s^{-1}•m^{-2} at the top to 35.1 L•s^{-1}•m^{-2} at the bottom.

and 35 because the maximum absolute deviations in ASTE for these tests were 37 and -34%, respectively (Table IV). The equilibrium model predicted higher drying and wetting rates depending on the air conditions during the ventilation period, particularly in the bottom layers.

The comparison of mathematical models using non-linear airflow (Table IV) showed almost the same trend as shown for the linear airflow case. The deviations in *ASTE*, however, were different for the non-linear airflow because the air velocity range was higher than that used for linear airflow. The increased air velocity increased the drying or wetting rates according to the air conditions thus resulting in higher or lower prediction in *ASTE* especially in the bottom layers. The deviations in *ASTE* between the equilibrium and non-equilibrium models increased or decreased over the storage period depending on the conditions used for the simulations such as airflow, fan temperature rise, year of simulation, and initial grain conditions but the average absolute deviations in ASTE generally decreased over the storage period.

The differences in grain temperature predicted by both models decreased slightly for most cases when the airflow was increased. The differences in *ASTE* predicted by the models, probably, are caused by higher drying or wetting rates depending on the air conditions during the aeration period. Decreasing the fan temperature rise from 1 to 0°C resulted in a higher prediction of the maximum *ASTE* by the equilibrium model in comparison with the non-equilibrium model, particularly when the airflow was increased (Tests 1 and 3, 2 and 5, 15 and 17, or 16 and 19, Table III and Tests 21 and 23 or 31 and 33, Table IV). Conversely, increasing the fan temperature rise from 1 to 3°C, resulted in a lower prediction of the maximum *ASTE* by the equilibrium model (Tests 1 and 4, 2 and 6, 15 and 18, or 16 and 20, Table III and Tests 21 and 24, 22 and 25, 31 and 34, or 32 and 35, Table IV). The higher prediction in ASTE was caused by a higher prediction of the wetting rate by the equilibrium model and the lower prediction in ASTE was caused by a higher prediction of the drying rate. The average absolute deviations in ASTE for the same airflow, however, did not change when the fan temperature rise was changed (e.g. Tests 1, 3, and 4 or 2, 5, and 6, Table III).

The maximum deviations in *ASTE* between the two models were high for ventilation time from 1200 to 1800 h (Test 7, Table III) indicating the trend of the equilibrium model in predicting higher drying rate. The prediction of higher drying rate was increased for non-linear airflow (Table IV) because the increased air velocity (Test 26, Table IV). Because of this, equilibrium mathematical models should not be used for grain drying simulation when the airflow rates are usually higher than 5 L•s^{-1}•m^{-3} (Manitoba Agriculture 1987). These results agree with the results of Metzger and Muir (1983a) for simulating ventilation of stored wheat. They observed that equilibrium was not a good assumption for airflow rates as high as 9.0 L•s^{-1}•m^{-3} while the assumption of equilibrium gave relatively accurate moisture content predictions for airflow rates of 1.9 L•s^{-1}•m^{-3}.

The deviations in *ASTE* increased when the initial moisture content was decreased from 15 to 12% wb (Tests 1 and 12, Table III) or from 15 to 13% wb (Tests 21 and 29, Table IV). The deviations in *ASTE* were high because there was a higher prediction of the wetting rate.

A 5% offset in the equilibrium relative humidity in moisture adsorption did not change the deviations in *ASTE* for

Table III: Comparison of equilibrium and non-equilibrium mathematical models, determined by the maximum and average absolute deviations in *ASTE*, to simulate aeration of stored wheat in Winnipeg, Canada after 3 months of storage, using linear airflow distribution

Test #	Parameter	Deviation in *ASTE* (%)	
		Maximum	Average
1	standard conditions[1]	-9	4
2	airflow: 28.4 L•s^{-1}•m^{-2}	26	14
3	fan temperature rise: 0°C	12	4
4	fan temperature rise: 3°C	-11	4
5	fan temperature rise: 0°C; airflow: 28.4 L•s^{-1}•m^{-2}	28	15
6	fan temperature rise: 3°C; airflow: 28.4 L•s^{-1}•m^{-2}	-19	13
7	ventilation time: 1200 - 1800 h	-34	5
8	grain layer thickness: 947 mm	33	13
9	grain layer thickness: 142 mm	17	5
10	grain depth: 4 m; grain layer thickness: 200 mm; airflow: 4.0 L•s^{-1}•m^{-2}	-9	4
11	grain depth: 6 m; grain layer thickness: 200 mm; airflow: 6.0 L•s^{-1}•m^{-2}	-13	5
12	initial moisture content: 12% wb	42	8
13	initial grain temperature: 15°C	11	3
14	offset in the equilibrium relative humidity in the equilibrium model: 5%	-10	4
15	worst year: 1963	-6	3
16	worst year: 1963; airflow: 28.4 L•s^{-1}•m^{-2}	-12	7
17	worst year: 1963; fan temperature rise: 0°C	7	3
18	worst year: 1963; fan temperature rise: 3°C	-5	3
19	same as Test 16 and fan temperature rise: 0°C	15	8
20	same as Test 16 and fan temperature rise: 3°C	-22	9

[1] Standard conditions were used as follows unless a parameter is specified otherwise — initial moisture content: 15% wb; initial grain temperature: 30°C; ventilation time: 0000 - 0600 h; storage period: 1 September - 30 November 1979; airflow: 5.7 L•s^{-1}•m^{-2}; fan temperature rise: 1°C; total grain depth: 5.7 m; grain layer thickness: 284 mm; and offset in the equilibrium relative humidity was not simulated in the equilibrium model.

linear airflow (Test 1 and 14, Table III) but the maximum absolute deviation in ASTE was reduced for non-linear airflow (Test 28, Table IV). Higher prediction of wetting changed to higher prediction of drying when the offset in relative humidity was included. Sanderson et al. (1989) found that a 5% offset in the equilibrium relative humidity improved the predictions of grain moisture content and temperature. Therefore, it is reasonable that the non-equilibrium model has more accuracy when predicting aeration of stored wheat than the equilibrium model. Schultz et al. (1984) obtained the best correlations to predict wheat aeration using the equilibrium model of Thompson (1972) in drying and the non-equilibrium model of Thompson et al. (1968) in wetting.

The deviations in *ASTE* between the equilibrium model with and without a 5% offset in the equilibrium relative humidity were not important for airflows of 5.7 and 28.4 L•s^{-1}•m^{-2} and fan temperature rises of 1 and 3°C. The maximum deviations in *ASTE* after 3 months of storage were between 15 and 16% at 28.4 L•s^{-1}•m^{-2} and 1°C fan temperature rise. This shows that a simple inclusion of an offset in the equilibrium relative humidity is not sufficient to generate differences between the equilibrium model with and without the offset. The higher prediction in *ASTE* was decreased for the Test 28 when the offset in the equilibrium relative humidity was assumed, indicating that the offset improved the equilibrium model compared with the non-equilibrium model, especially at high airflow rates. Schultz et al. (1984) stated that adsorption should be considered separately and hysteresis must be included if the model is to accurately predict wetting. Schultz et al. (1984) found that the equilibrium model over predicted wetting while the non-equilibrium model over predicted drying.

The deviations in *ASTE* were changed when simulating for the worst year (Tests 15 to 20, Table III and Tests 31 to 35, Table IV). The equilibrium model predicted higher drying rate in the worst year, 1963, and predicted higher wetting rate in the median year, 1979, because 1963 was drier and warmer than 1979.

Sensitivity analysis

The parameter *N* in the thin-layer drying equation was the parameter which presented the highest maximum deviations in *ASTE* among all parameters (Tables V to VII) when adding a fixed uncertainty. The maximum deviations in *ASTE* for all parameters and tests were much lower than the uncertainty in predicting *ASTE*. Therefore, the mathematical model used to simulate aeration of stored grain can be simplified based on

Table IV: Comparison of equilibrium and non-equilibrium mathematical models, determined by the maximum and average absolute deviations in *ASTE*, to simulate aeration of stored wheat in Winnipeg, Canada after 3 months of storage, using non-linear airflow distribution

Test #	Parameter	Deviation in *ASTE* (%)	
		Maximum	Average
21	standard conditions[1]	28	10
22	airflow: 29.0 - 69.0 L•s^{-1}•m^{-2}	37	15
23	fan temperature rise: 0°C	28	11
24	fan temperature rise: 3°C	-19	9
25	fan temperature rise: 3°C; airflow: 29.0 - 69.0 L•s^{-1}•m^{-2}	-18	14
26	ventilation time: 1200 - 1800 h	-76	17
27	grain layer thickness: 568 mm	18	7
28	offset in the equilibrium relative humidity in the equilibrium model: 5%	-19	9
29	initial moisture content: 13% wb	60	16
30	initial grain temperature: 15°C	27	4
31	worst year: 1963	-8	5
32	worst year: 1963; airflow: 29.0 - 69.0 L•s^{-1}•m^{-2}	-15	8
33	worst year: 1963; fan temperature rise: 0°C	15	6
34	worst year: 1963; fan temperature rise: 3°C	-23	7
35	same as Test 32 and fan temperature rise: 3°C	-34	13

[1] Standard conditions as given in Table III and airflow: 5.9 - 35.1 L•s^{-1}•m^{-2}.

Table V: Sensitivity of the non-equilibrium mathematical model to airflow, grain specific heat, and EMC equations determined by the maximum deviations in *ASTE* (%), to simulate aeration of stored wheat in Winnipeg, Canada after 3 months of storage, using linear airflow distribution[1]

Airflow (L•s^{-1}•m^{-2})	Fan temperature rise (°C)	Parameter change (%)	Maximum deviations in *ASTE* (%) caused by changes in parameters			
			Airflow	Grain specific heat	EMC equations	
					Adsorption	Desorption
5.7	1	+6	4	-4	-2	-8
	1	-6	-5	4	2	8
	3	+6	4	-4	-1	-9
	3	-6	-5	4	-1	10
28.4	1	+6	-2	-4	-3	-8
	1	-6	-4	2	3	8
	3	+6	2	-2	-2	-8
	3	-6	-2	3	1	11

[1] Aeration conditions — ventilation time: 0000 - 0600 h; total grain depth: 5.7 m; grain layer thickness: 284 mm; initial moisture content: 15% wb; initial grain temperature: 30°C; storage period: 1 September - 30 November 1979.

the results of sensitivity analyses. The uncertainty generated by equations which describe the resistance to airflow is not important for simulating aeration of stored wheat because the maximum deviations in *ASTE* resulting from changes in airflow are much lower than the uncertainty in predicting *ASTE* (Table V).

Changes in wheat bulk density caused no deviations in *ASTE* (maximum deviations in *ASTE*=0%). The results for wheat bulk density were obtained assuming no change in the air velocity due to a variation in the bulk density. The maximum deviations in *ASTE* for wheat bulk density, when the air velocity was changed in proportion to the changes in grain volume, were practically the same as those obtained for the airflow (Table V). Therefore, these deviations were caused by a change in the airflow and not by a change in the bulk density. Consequently, a constant bulk density can be used in

Table VI: Sensitivity of the non-equilibrium mathematical model to fan temperature rise and thin-layer equations determined by the maximum deviations in *ASTE*, to simulate aeration of stored wheat in Winnipeg, Canada after 3 months of storage, using linear airflow distribution[1]

Airflow (L•s^{-1}•m^{-2})	Fan temperature rise (°C)	Maximum deviations in *ASTE* (%) caused by changes in parameters									
		Fan temperature rise		Thin-layer drying equation				Thin-layer wetting equation			
				Parameter *K*		Parameter *N*		Parameter *K′*		Parameter *N′*	
		Change (°C)	Deviation (%)	Change (%)	Deviation (%)	Change (%)	Deviation (%)	Change (%)	Deviation (%)	Change (%)	Deviation (%)
5.7	1	+0.5	-2	+20	4	+30	10	+90	-4	+10	-1
	1	-0.5	2	-20	-5	-30	-18	-90	4	-10	1
	3	+0.5	-3	+20	4	+30	11	+90	-2	+10	-1
	3	-0.5	3	-20	-5	-30	-18	-90	2	-10	0
28.4	1	+0.5	7	+20	4	+30	10	+90	-8	+10	-3
	1	-0.5	-9	-20	-5	-30	-16	-90	8	-10	3
	3	+0.5	-3	+20	5	+30	10	+90	-3	+10	-1
	3	-0.5	4	-20	-5	-30	-16	-90	4	-10	-1

[1] See Table V for aeration conditions

simulations, i.e. it can be assumed that the grain does not shrink or expand significantly during storage. Grain bulk density has a greater importance in grain drying than aeration processes, because during drying bulk density varies over a greater range. Also, variation of bulk density affects the airflow due to a variation in the resistance to airflow.

Van Ee and Kline (1979b) found that a change of +0.5% wb in the EMC of shelled corn had an effect on the calculated final grain moisture content and the rate of movement of the drying front. Because of this, Sharp (1982) recommended caution on the selection of an accurate EMC equation when simulating drying of corn at near ambient temperatures. The uncertainty used in the EMC (6% which correspond to 0.9% wb in the EMC at 15% wb) during 3 months of aeration of stored wheat did not generate significant deviations in *ASTE*.

Neglect of the net heat of sorption caused a maximum deviation in ASTE of -4% for airflows of 5.7 and 28.4 L•s^{-1}•m^{-2} and fan temperature rises of 1 and 3°C with linear airflow distribution. The net heat of sorption is the amount by which the latent heat of vaporization or condensation of the water in the grain differs from that of free water. Therefore, the latent heat of vaporization equations for adsorption and desorption by wheat, which were used to calculate the net heat of sorption, are not necessary in the computer model.

A maximum deviation in *ASTE* of 3% was obtained when the air velocity was reduced to one-half by doubling the bin area for a constant airflow per grain volume (1 and 5 L•s^{-1}•m^{-3}) for fan temperature rises of 1 and 3°C with linear airflow distribution. Consequently, the ratio of bin diameter to bin height is not important to simulate aeration of stored wheat when only forced convection is simulated.

The parameter *N* in the thin-layer drying equation showed great variation in moisture content and *ASTE* when adding or subtracting a fixed increment (Fig. 4). Subtracting an increment was more important than adding it because decreasing the drying front speed increased the drying time and grain deterioration. The maximum deviations in ASTE were approximately constant over the storage period and the maximum absolute difference in *ASTE* over the 3 months storage period for each parameter was less than 5%. The relative importance of most parameters changed when the airflow or the fan temperature rise was changed. The relative importance of the parameter *N* in the thin-layer drying equation, however, was not changed.

The maximum deviations in *ASTE* varied when non-linear airflow was used. There was no apparent trend in these variations. For most tests increasing the air velocity increased the over prediction of drying or wetting depending on the airflow and fan temperature rise. The maximum deviations in *ASTE*, when using non-linear airflow and 1°C fan temperature rise (Table VII), are only shown for the parameters which caused the maximum deviations in *ASTE*.

Grain depths of 4 and 6 m and grain layer thickness less than 300 mm did not affect the model's sensitivity. The maximum deviations in ASTE were 24% for the EMC desorption equation and 11% for the parameter N in the thin-layer drying equation when using 567 mm grain layer thickness. Therefore, excessively increasing the grain layer thickness increases the possibility of errors due to uncertainty in parameters such as the EMC equation.

The relative importance of fan temperature rise, EMC desorption equation, and parameter *K′* in the thin-layer wetting equation changed when simulating for the worst year and median year. The relative importance of the parameter N in the thin-layer drying equation was not changed but the fan temperature rise was equally important for 1963 with non-linear airflow distribution.

The effect of initial moisture content and temperature of

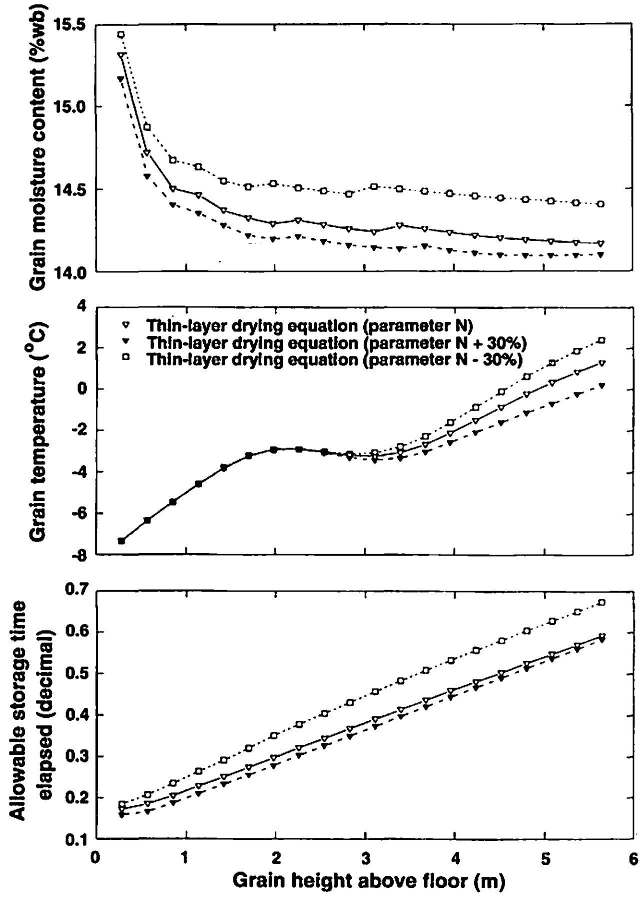

Fig. 4. Moisture content, temperature, and allowable storage time elapsed obtained when adding or subtracting 30% from the parameter *N* in the thin-layer drying equation to simulate aeration of stored wheat in Winnipeg, Canada after 3 months of storage at standard conditions with linear airflow distribution.

the grain on the maximum deviations in *ASTE* was simulated for the median year at the standard conditions with linear airflow for all parameters. The deviations in *ASTE* were increased 47 to 117% when the initial moisture content was decreased from 15 to 13% wb for the parameter N¢ in the thin-layer wetting equation, EMC adsorption equation, and fan temperature rise. The deviations in *ASTE* were decreased 49 to 65% when the initial temperature was decreased from 30 to 15oC for the parameter *N* in the thin-layer drying equation, airflow, and specific heat 49 to 65%. The deviations in *ASTE* for the EMC desorption equation were not affected by the initial moisture content or temperature of the grain.

Parameter interaction when using fixed increments in the parameters Different conditions interacting may cause an important change in the maximum deviations in ASTE. For instance, the maximum deviation in *ASTE* for the interaction of the thin-layer drying equation (parameter *N* - 30%) and EMC desorption equation (EMC - 6%) was -11% at the standard conditions with linear airflow. Therefore, an error introduced by one parameter may cancel the error introduced by another parameter. The maximum deviation in *ASTE* was -14% when the airflow (airflow - 6%) was added to that interaction. The results of sensitivity analysis, with fixed increments in the parameters, give a good estimate of the maximum errors that could be introduced in the mathematical model by each parameter and also about the relative importance of all parameters.

Parameter interaction when using random variation in the increments The maximum deviations in *ASTE* for all parameters interacting with random variation in the increments varied from 4 to 5% for three repetitions of the simulations at standard conditions with linear airflow distribution. Maximum deviations in *ASTE* between -3 and 7% were generated when using 13% wb initial moisture content or 15°C temperature, at 1 and 3°C fan temperature rise or at 1 and 5 L•s^{-1}•m^{-3}, respectively. The results of sensitivity analysis, with random variation in the increments, indicated that in computer simulation the errors introduced in the mathematical model by the thermal and physical properties of the grain and weather data will be much lower than normally expected because the error introduced by one parameter may cancel the error of another parameter.

Comparison with published data

The research of Sinicio and Muir (1996) for Curitiba, Brazil, which has a humid and warm climate, showed that the results produced by the equilibrium and non-equilibrium models were significantly (α=0.05) different for all conditions analyzed when ventilating from 0600 to 1200 h for one year except when using a 5°C fan temperature rise with non-linear airflow. The differences between the models were not affected by initial moisture content and temperature of the grain and year of simulation but they were affected by the different climatic conditions in different geographic locations.

The higher wetting rate predicted in the bottom layers by the equilibrium model is increased in warm, humid climates compared with a cold, dry climate like that of Winnipeg when simulating aeration of stored wheat. For instance, Sinicio and Muir (1996) determined that the ASTE at the standard conditions after 3 months of storage, at Curitiba, Brazil, for the top and bottom layers, and the average of all layers were 0.7, 1.2, and 0.7, respectively, for the equilibrium model compared with 0.6, 0.7, and 0.6, respectively, for the non-equilibrium model. The standard conditions used by Sinicio and Muir (1996) for the simulations were practically the same as used here (Fig. 1) except that the initial moisture content was 13% wb, grain depth was 1 m, storage period was from December 1, 1965 to February 28, 1966, and ventilation time from 0600 to 1200 h.

The most important parameters to simulate aeration of stored wheat in Curitiba, Brazil after one year storage period with linear airflow distribution determined by Sinicio et al. (1996), in decreasing order, were the fan temperature rise, parameter *K′* in the thin-layer wetting equation, and parameter *K* in the thin-layer drying equation, at airflows of 5.6 and 27.8 L•s^{-1} •m^{-2}. Fan temperature rise was the most important parameter for Curitiba because the maximum grain deterioration occurred in the first layer from the bottom, where the air enters the bin, and the grain deterioration in the bottom 1 m

Table VII: Sensitivity of the non-equilibrium mathematical model, determined by the maximum deviations in *ASTE*, to simulate aeration of stored wheat in Winnipeg, Canada after 3 months of storage, using non-linear airflow distribution[1]

Airflow (L•s^{-1}•m^{-2})	Maximum deviations in *ASTE* (%) caused by changes in parameters									
	Fan temperature rise		Thin-layer equations				EMC equations			
			Drying - Parameter *N*		Wetting - Parameter *K′*		Adsorption		Desorption	
	Change (°C)	Deviation (%)	Change (%)	Deviation (%)	Change (%)	Deviation (%)	Change (%)	Deviation (%)	Change (%)	Deviation (%)
5.9 - 35.1	+0.5	7	+30	11	+90	-8	+6	-4	+6	-8
5.9 - 35.1	-0.5	-11	-30	-18	-90	9	-6	3	-6	8
29.0 - 69.0	+0.5	6	+30	11	+90	-13	+6	-5	+6	-8
29.0 - 69.0	-0.5	-12	-30	-15	-90	13	-6	4	-6	9

[1] Aeration conditions — fan temperature rise: 1°C; ventilation time: 0000 - 0600 h; total grain depth: 5.7 m; grain layer thickness: 284 mm; initial moisture content: 15% wb; initial grain temperature: 30°C; storage period: 1 September - 30 November 1979.

was always greater than the average grain deterioration for a bin 5.6 m deep. An increased fan temperature rise reduces the wetting especially in the bottom layers reducing the risks of grain spoilage. Grain moisture content, therefore, is the major factor affecting the deterioration of stored wheat during aeration in warm and humid climates because the cooling by aeration is insufficient to compensate for the increase in grain moisture content due to wetting.

The results obtained for the grain bulk density, net heat of sorption, and ratio of bin diameter to bin height by Sinicio et al. (1996) in the sensitivity analysis agree with the results obtained here. The model's sensitivity for Curitiba, however, was not affected by the year of simulation and initial temperature of the grain but it was affected by location, and grain depth.

Validation of the non-equilibrium mathematical model of forced convection

The results of the sensitivity analysis suggest that validation of the mathematical model developed by Sinicio and Muir (1996) is not needed for Winnipeg conditions because the uncertainty in predicting grain deterioration is much higher than the maximum deviations in *ASTE* for all parameters within their expected range of uncertainty. Such a validation would be applicable only for a specific product and within the specific range of experimental conditions and the errors introduced in the mathematical model by several parameters will be much less than expected. Validation of computer models to simulate aeration of stored grain would require long duration tests and demand great economic resources. The tests would have to be repeated for different grain varieties and experimental conditions due to the random nature of the errors associated with the determination of thermal and physical properties of the grain, making such efforts economically unfeasible.

CONCLUSIONS

The equilibrium and non-equilibrium models were not significantly different for most test conditions analyzed when ventilating from 0000 to 0600 h. The most important parameters to simulate aeration of wheat stored for 3 months in Winnipeg, Canada are the parameter *N* in the thin-layer drying equation followed by the EMC desorption equation, fan temperature rise, and parameter *K′* in the thin-layer wetting equation, which are equally important. The deterioration model needs to be improved because the uncertainty in the calculation of wheat deterioration is much higher than the uncertainty generated by the equations used in the computer program for simulating aeration of wheat stored in Winnipeg, Canada. The wheat bulk density can be a constant, the net heat of sorption can be neglected and the ratio of bin diameter to bin height is not important in mathematical models to simulate aeration of stored wheat.

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