

Numerical modelling of the movement of carbon dioxide through stored-wheat bulks

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Abstract

A step-by-step approach was taken in an attempt to model the three-dimensional movement of introduced CO₂ gas through stored-wheat bulks. Experimental data on the distribution of CO₂ in wheat bulks contained in three 1.42 m diameter bins were collected to validate the model. These bins were equipped with three different partially perforated floors (0.3 m diameter floor opening near the centre, 1.14 × 0.36 m rectangular floor opening, and 0.3 m diameter floor opening near the wall). In the experiments the grain surfaces were left open or covered with polyvinylidene chloride sheets. Dry ice was used to create high CO₂ concentrations in the wheat bulk. A model that assumes pure diffusion as the transport mechanism did not predict the CO₂ distribution well.

Later the model was modified to predict CO₂ distribution using experimentally determined flow coefficients (apparent flow coefficient) during the dry ice sublimation period and then a diffusion coefficient afterwards. Although model predictions improved in this approach, there were still high errors during the initial time period. The model predictions were further improved when the sorption of CO₂ by the wheat was included. The sorption rates for the predicted CO₂ concentrations were calculated by extrapolating from the available sorption data which are for a 100% initial CO₂ concentration. The importance of including the sorption for accurate model predictions is demonstrated by assuming various rates of sorption from 0 to 100% of the measured sorption rate. The need for sorption data at lower initial concentrations, empirical data on the gas loss from grain storage structures, and the inclusion of convection terms in the model is highlighted.

Introduction

Computer simulation models of physical parameters are integral parts of research and development in many fields of science. These models, based on physical principles and validated against measured experimental data, become powerful design and management tools. They eliminate the need for time- and labour-intensive experimental studies. Furthermore, experimental data are specific to the system on which they were observed and cannot be generalised. For example, the temperatures measured in grain bulk-stored near Winnipeg (Canada) cannot be extrapolated to predict the temperatures of grain bulk-stored near Darwin (Australia) as the weather conditions in these two places are entirely different from each other. Winnipeg experiences temperate weather

conditions while Darwin experiences tropical conditions. On the other hand, mathematical models with fewer assumptions may be more general in nature. In a stored-grain ecosystem, for example, the damaging insects, mites, and microorganisms grow and multiply under optimum conditions of grain temperature, moisture content, and intergranular gas composition. A farmer, manager of a commercial storage facility, or a grain storage scientist who must determine the management practices required to safeguard the grain before any damage occurs should know the changes in these abiotic factors in relation to the local conditions. Numerous mathematical models have been developed to simulate the grain temperatures and moisture contents (Jayas 1994) but only limited research work has been done to model the changes in the intergranular gas composition (Singh et al. 1983; Jayas et al. 1988; Nguyen 1986). The intergranular gas composition, initially at atmospheric level, is altered due to the respiration of the insect pests, microflora and the grain, or by artificially introducing different compositions of atmospheric gases as in controlled atmosphere (CA) storage.

The success of CA storage relies on the uniformity of distribution of the introduced gases in the grain bulk and the maintenance of these gases for the minimum required exposure period. A knowledge of the distribution and maintenance of the introduced gases is important for the design and management of CA storage systems. The application and management of CA storage systems are often based on experience and rules of thumb. A comprehensive mathematical model that will predict with accuracy the distribution and maintenance of the introduced gases would be helpful in efficiently designing and operating CA storage systems. The present work was undertaken to develop a finite element model for predicting the three-dimensional distribution of carbon dioxide (CO₂) in stored-wheat bulks. In this paper we will explain the step by step procedure we followed in developing and validating the model and the assumptions we made at each step.

Experimental Data for Model Validation

Carbon dioxide concentrations were measured at various locations (Fig. 1) in wheat bulks contained in three experimental bins, 1.42 m in diameter and 1.47 m tall. The CO₂ data were collected from 5 levels in each bin (beginning at the floor, and then spaced 0.33 m apart in the vertical direction). At each level there were 11, 13, and 12 sampling points for Bins 1, 2, and 3, respectively (Fig. 1). Metal boxes of size 0.5 × 0.5 × 0.37 m for Bins 1 and 3 and 1.22 × 0.46 × 0.36 m for Bin 2 were mounted centrally under the floor openings. Known quantities of dry ice were placed in these boxes. The CO₂ concentrations were measured using a gas chromatograph at 1, 3, 6, 9, 12, and 21 hours after the introduction of dry ice. The grain surfaces were left open or covered with a polyvinylidene chloride sheet. Three replicates were conducted for each experimental combination.

The grain was aerated using a 1.5 kW centrifugal fan for about 1 hour immediately after each replicate and for about 15

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minutes just before the next replicate to bring the intergranular CO₂ concentrations to atmospheric level. The grain was left undisturbed for about 24 hours between replicates. Grain samples were collected after each experiment for determining the moisture content. The moisture contents of the wheat samples were determined by drying triplicate samples of about 15 g each in an air convection oven at 130°C for 19 hours (ASAE 1992). The moisture content of the wheat did not vary appreciably during the course of the experiments. The average moisture content of the wheat used in the experiments was 12.6 ± 0.4% (wet basis). In addition to the CO₂ samples, the grain temperatures were also monitored at all sampling times. The grain temperatures were measured at five locations in Bin 1 and at 15 locations in each of Bins 2 and 3 (Fig. 1). The grain temperatures were fairly constant in any given experiment. The maximum observed deviation from the mean grain temperature in any experiment was ±2.7°C.

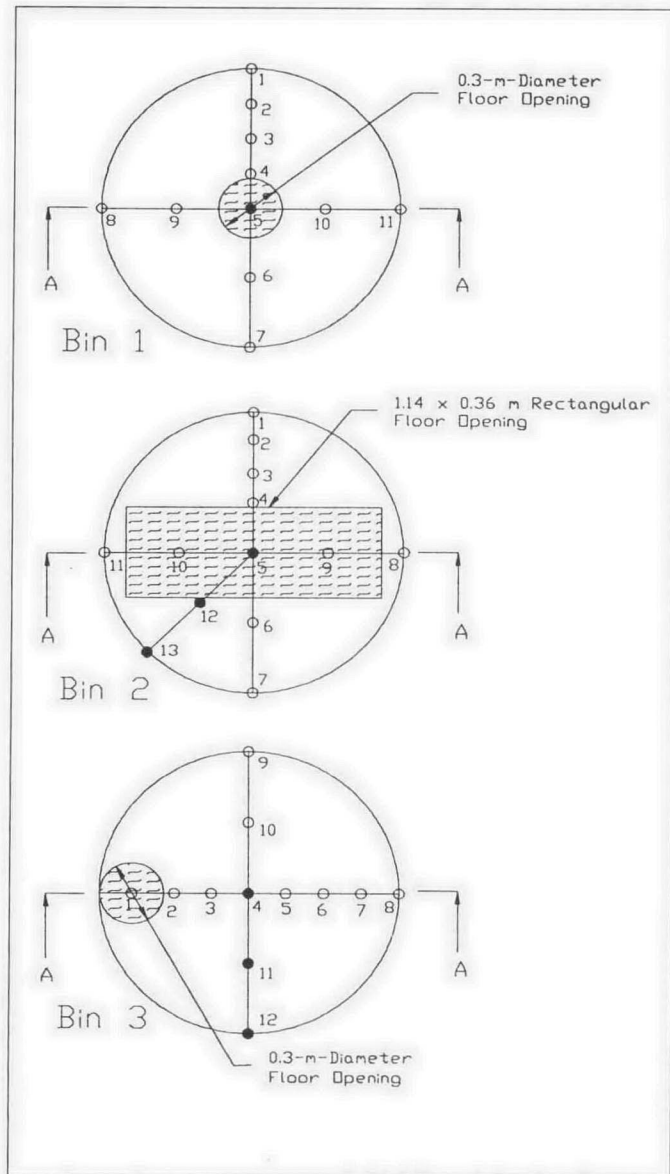


Fig. 1. Schematic diagram of the temperature and gas sampling locations in 1.42 m diameter × 1.47 m tall bins. (● = temperature and gas samples; ○ = only gas samples)

Model Development and Validation

Step 1: The diffusion model

In a model of the gas transport through a porous medium, the first and the simplest assumption is that the mechanism of transport is by pure diffusion. In addition to this basic assumption we also assumed that the sorption of CO₂ by the wheat was negligible and that there was no gas loss from the grain bin. The partial differential equation governing the diffusion of a gas through porous material under these assumptions is given as:

$$\nabla(D\nabla C) = \frac{\partial C}{\partial \tau} \quad (1)$$

subject to the boundary conditions:

$$C = C_{s1} \quad \text{on } S1 \quad (2)$$

$$\frac{\partial C}{\partial \eta} = 0 \quad \text{on } S2 \quad (3)$$

and the initial condition:

$$C(x, y, z, \tau = 0) = C_i \quad \text{on } \Omega \quad (4)$$

For the movement of CO₂ through a stored-grain bulk, the various notations used in the above equations are:

C = concentration of CO₂ at time $\tau > 0$ (g/m³),

C_i = initial CO₂ concentration in the grain bulk (g/m³),

C_{s1} = specified CO₂ concentration on the boundary $S1$ (g/m³),

D = Diffusion coefficient of CO₂ through wheat bulk (m²/s),

Ω = problem domain (the grain bulk),

η = outward pointing normal,

τ = time (seconds), and

$S1$ and $S2$ = boundary segments.

Boundary segment $S1$ may be made of more than one segment. For example, $S1$ may represent the surface of the grain where concentration may be specified as constant at the atmospheric level in a ventilated head space. Another portion of $S1$ may represent the portion of a grain boundary where CO₂ is injected. Similarly $S2$ may comprise the bin wall, bin floor other than the floor opening, and a grain surface covered with a sheet impermeable to CO₂. $S1$ and $S2$ together make the total boundary of the domain Ω .

The system of equations 1–4 was solved using the finite element method (Segerlind 1984; Rao 1982), resulting in a set of algebraic equations:

$$\left[\frac{[K1]}{\Delta \tau} + \theta [K2] \right] \{C\}_{n+1} = \left[\frac{[K1]}{\Delta \tau} - (1 - \theta) [K2] \right] \{C\}_n \quad (5)$$

where:

$[K1]$ = matrix of constants,

$[K2]$ = matrix containing diffusion coefficients,

$\{C\}_n$ = vector of nodal CO₂ concentrations at time τ ,

$\{C\}_{n+1}$ = vector of nodal CO₂ concentrations at time $\tau + \Delta \tau$,

θ = a constant.

By choosing the value of θ between 0 and 1, the following schemes can be obtained (Wood and Lewis 1975) (0—forward difference scheme; 0.5—Crank-Nicholson scheme; 0.667—Galerkin's scheme; and 1.0—backward difference scheme). Equation 5 can be solved to obtain the CO₂ concentrations at time $\tau + \Delta \tau$ by using the CO₂ concentrations at time τ .

Simulation of CO₂ distribution

A FORTRAN program was written to solve the system of equations (equation 5). For simulating the distribution of CO₂

in the grain bulk, half of the grain bulk (cut along section A-A of Fig. 1) was discretised into linear elements with 445 nodes for Bin 1, 430 nodes for Bin 2, and 390 nodes for Bin 3. The measured CO₂ concentrations near the floor opening (sampling point 5 of Bin 1, the average of sampling locations 5, 9, and 10 of Bin 2, and sampling location 1 of Bin 3) were specified for the nodes lying inside or on the boundary of the floor opening. To include this boundary condition in the program, the measured CO₂ concentrations at these locations were fitted using procedure NLIN of SAS (SAS 1982) to an equation of the form:

$$\%CO_2 = a e^{-b.t} \quad (6)$$

where:

%CO₂ = measured CO₂ concentration at the inlet boundary,
a and *b* = empirical constants, and
t = time (hours).

For tests with uncovered top grain surfaces, the measured CO₂ concentrations near the surface of the grain were specified at the nodes lying on this boundary, and when the grain surface was covered with a plastic sheet, this boundary was assumed impermeable to flow of CO₂ ($\partial C/\partial \eta = 0$). The bin wall and the bin floor, excluding the floor opening, were assumed impermeable to CO₂. A diffusion coefficient of 4.15 mm²/second for red spring wheat at 12% moisture content (Singh et al. 1985) was used in the simulations. It was assumed that the diffusion coefficient was independent of the direction of diffusion (Singh et al. 1984), and of concentration (Cunningham and Williams 1980). The predicted CO₂ concentrations were much lower than the measured concentrations at every sampling point and at all times. The mean relative percent error of prediction (*e*) was calculated as:

$$e = \frac{1}{N} \sum \frac{|M_i - P_i|}{M_i} \times 100 \quad (7)$$

where:

M_i = measured CO₂ concentration at sampling point *i*,
P_i = predicted CO₂ concentration at sampling point *i*, and
N = number of data points.

The relative error for replicate 1 of Bin 1 with an uncovered top grain surface ranged from 71% at 3 hours to 31% at 21 hours. Similar high relative errors were observed for other test combinations.

The governing partial differential equation and the associated boundary conditions (equations 1–3), on which the model was based, assume that the mechanism of transport is by diffusion only. In the experiments, 180 to 740 g of dry ice were placed in the metal boxes under the floor openings. When the dry ice sublimated into CO₂ gas, a pressure must have developed inside the box which would have caused a bulk movement of CO₂ through the grain bulk. This may have caused the large errors in prediction. To account for the bulk movement of CO₂ a model of forced mass transport must be included in the model.

Step 2: Model of bulk movement of CO₂

It was hypothesised that replacing the diffusion coefficient with an experimentally determined flow coefficient of CO₂ through wheat bulks (apparent flow coefficient, *D_{app}*) during the sublimation period of the dry ice would improve the accuracy of the model. To achieve this, laboratory experiments were conducted to determine the *D_{app}* values (Alagusunda-

ram 1993). The natural logarithm of *D_{app}* values and time were linearly related as:

$$\ln(D_{app}) = A + B \ln(t) \quad (8)$$

The constants *A* and *B* were separate linear functions of grain temperature in the range of –10 to 30°C and expected pressure drops across the grain column due to the sublimation of dry ice were in the range of 77 to 310 kPa. No definite pattern of variation of the constants *A* and *B* with an increase in the grain moisture content (in the range 11–18.5% w.b.) was observed. The *D_{app}* values in the horizontal direction were greater than in the vertical direction and were related as follows:

$$\frac{D_{app}H}{D_{app}V} = 4.011 - 0.212 \ln(t) \quad (9)$$

Using these empirical equations, *D_{app}* was determined for the experimental conditions. Estimated *D_{app}* was used in place of *D* for the first 3 hours of simulation. It was assumed that at the end of this arbitrarily chosen time period the pressure created by the expansion of the CO₂ was dissipated and that the movement of CO₂ through the wheat bulk was purely due to the concentration gradient.

The relative error (Table 1) was calculated using equation 7. At sampling times 6 hours and afterwards, the predicted CO₂ concentrations were close to the measured values in all three bins with 180 or 370 g of dry ice. In most of the experiments, and particularly in Bin 1 with 540 g of dry ice and an open grain surface, the errors were lower in the first four levels (0, 0.33, 0.66, and 0.99 m above the floor) than in all five levels (shown as 4 L and 5 L, respectively, in Table 1). This might be because, in the model predictions, the grain surface was assumed perfectly levelled. But at sampling level 5, which was only 0.05 m below the grain surface, small undulations in the grain surface would cause a relatively large difference in the measured CO₂ concentrations. For example, a difference of 0.02 percentage points in a CO₂ concentration of 0.05% causes an error of 40% while at a CO₂ concentration of 10% the error is only 0.2%.

During the initial periods after the introduction of the dry ice (sampling times 1 hour and 3 hours), the relative errors were very high (Table 1). At these sampling times the predicted CO₂ concentrations at heights of 0.33 m and more above the floor were higher than the measured concentrations. For example, in replicate 1 of Bin 1 with 180 g of dry ice and an open grain surface the error at a height of 0.33 m above the floor was 53% and that near the floor was only 17%. Similar high errors at heights of 0.33 m and above were observed in the other two bins. The reason for this cannot be explained.

The errors were high at all sampling times in Bin 2 with 740 g of dry ice and a covered grain surface (Table 1). At all sampling times the predicted CO₂ concentrations were much higher than the observed values. That observed values were low was probably the result of sorption of CO₂ by the wheat. A mass balance, assuming no loss from the bin, indicated that in Bin 2 with 740 g of dry ice and covered grain surface, about 330 g of CO₂ had been absorbed by the wheat. So, based on the hypothesis that inclusion of CO₂ sorption by the wheat might improve the predictions of the model, we decided to include it.

Table 1. Mean relative percent errors between the measured and predicted CO₂ concentrations in wheat bulk. Predictions were based on mass flow during the first 3 hours and molecular diffusion during the remaining time period.

Bin	Top grain surface	Mass of dry ice (g)	Replicate	Mean relative percent error											
				1 hour	3 hours	6 hours		9 hours		12 hours		21 hours		24 hours	
						5L ^a	4L ^{ba}	5L	4L	5L	4L	5L	4L	5L	4L
Bin 1	Open	180	1	35	20		6	9	8	7	6	10	4		
			2	35	16		9	9	10	9	9	8	4		
			3	35	13		7	9	7	10	8	17	7		
			4 ^d	34	13		7	10	7	10	8	18	8		
	Covered	180	1	54	25		14			16	11	11	10		
			2	29	33		14			13	9	11	9		
			3	35	31		12			15	10	9	8		
			4 ^d	39	30		12			14	10	10	9		
		540	1	103	64	34	17	44	18	53	17	53	23		
			2	104	60	44	17	40	10	41	8	58	16		
			3	110	48	26	14	21	9	22	13	21	13		
			4 ^d	106	56	33	15	31	10	31	10	37	17		
Bin 2	Open	370	1	21	29		10			7	11	21	23		
			2	24	22		9			8	9	22	27		
			3	20	10		19			10	15	11	10		
			4 ^d	19	13		11			5	9	18	17		
	Covered	370	1	28	15		22			13	18	6	8		
			2	31	16		22			15	20	7	9		
			3	23	15		10			7	9	10	9		
			4	22	12		11			8	11	7	7		
		740	1	97	113	122	70			96	69	102	80	101	80
			2	118	165	157	93			116	88	124	101	129	104
			3	113	101	102	56			85	60	93	74	96	75
			4 ^d	105	121	124	71			96	70	103	82	105	83
Bin 3	Open	180	1	127	48		27	22	21	18	18	11	11		
			2	103	50		23	16	18	14	15	9	10		
			3	159	55		30	26	22	22	18	18	13		
			4 ^d	151	61		32	19	21	16	17	14	14		
	Covered	180	1	93	56		35	26	27	17	18	12	11		
			2	189	49	26	17		17	14	13	8	7		
			3	144	65	36	22		22	14	14	10	10		
			4 ^d	127	55	30	20		21	14	15	9	9		

$$\text{Mean relative percent error (\%)} = \frac{1}{N} \sum \frac{|\text{Measured} - \text{Predicted}|}{\text{Measured}} \times 10$$

^a the mean relative percent errors were calculated for all 5 levels; ^b the mean relative percent errors were calculated for bottom 4 levels; ^c Bins are illustrated in Fig. 1; ^d The measured data for the three replicates were averaged and compared with the simulation results. N number of data points (25 in Bin 1, 50 in Bin 2, and 45 in Bin 3)

Step 3: Including sorption of CO₂ by wheat in the model

The governing partial differential equation that includes the sorption or desorption (sink or source term) of CO₂ by the wheat can be written as:

$$\nabla(D\nabla C) + q = \frac{\partial C}{\partial \tau} \quad (10)$$

where q is the sorption or desorption of CO₂ by the wheat (g/m³/s). The solution of this equation using the Galerkin weighted residual method will result in the following set of algebraic equations (Segerlind 1984; Rao 1982):

$$\left[\frac{[K1]}{\Delta \tau} + \theta[K2] \right] \{C\}_{n+1} - \left[\frac{[K1]}{\Delta \tau} - (1-\theta)[K2] \right] \{C\}_n = \left[\theta\{F\}_{n+1} + (1-\theta)\{F\}_n \right] \quad (11)$$

where F is a vector that contains the sorption term.

Estimation of sorption of CO₂ by the wheat

Cofie-Agblor et al. (1992) measured the sorption of CO₂ by wheat at various moisture contents (12, 14, 16, and 18%) and at various temperatures (0, 10, 20, and 30°C). They measured the sorption of CO₂ by wheat using an initial intergranular CO₂ concentration of 100%. Other than the work by Cofie-Agblor et al. (1992) we could find no other detailed study on the sorption of CO₂ by wheat. So we decided to extrapolate linearly their data to estimate the sorption at lower concentrations. Based on a study on the characteristics of CO₂ sorption by several grains, Yamamoto and Mitsuda (1980) concluded that the sorption of CO₂ by grains is completely reversible. The sorption and desorption curves were symmetric to the time axis, indicating that the sorption and desorption are two opposite phenomena. If the CO₂ concentration at any time is lowered from the original CO₂ concentration it is essential to account for the desorption of CO₂ by the grain. The value of q

for each element in the domain was estimated using the following equation:

$$q = (-1)^i \cdot \left(\frac{C_n + C_{n-1}}{2} \right) \frac{SCO_2 \rho_w}{\rho_{CO_2} \Phi 86400} \quad (12)$$

where:

- q = sorption or desorption of CO₂ by wheat (g/m³/s),
- SCO_2 = rate of sorption of CO₂ by wheat, linearly extrapolated from data of Cofie-Agblor et al. (1992) (g/kg/day),
- ρ_w = bulk density of wheat (kg/m³),
- ρ_{CO_2} = density of CO₂ gas (g/m³),
- C_n = average predicted CO₂ concentration of an element at the present time step (g/m³)
- C_{n-1} = average predicted CO₂ concentration of an element at the previous time step (g/m³)
- Φ = porosity of wheat,
- $i = 1$ when $C_{n-1} > C_n$, and
- $i = 2$ when $C_{n-1} < C_n$

Simulation results

In Bins 1 and 3 with 180 g of dry ice and with open or covered grain surfaces, the inclusion of sorption of CO₂ by the wheat slightly increased the accuracy of prediction in the first few hours after the introduction of dry ice (sampling times 1 and 3 hours), and reduced the accuracy of prediction later. At 21 hours after the introduction of dry ice, for example, in Bin 1 with covered grain surface the error increased from 9% when sorption = 0 to 11% when sorption > 0. It is possible that at low CO₂ concentrations (180 g dry ice will create a CO₂ concentration of approximately 10% in the intergranular space of Bins 1 and 3), the rate of sorption may be lower than the values obtained by linearly extrapolating the CO₂ sorption rate at 100% concentration.

In Bin 1 with 540 g of dry ice, and in Bin 2 with 370 or 740 g of dry ice, the accuracy of prediction was increased at all sampling times, indicating that including the sorption of CO₂ by wheat is essential for accurate model predictions. The errors with 370 g of dry ice in Bin 2 were around 10% at 21 hours after the introduction of dry ice. But with 540 g of dry ice in Bin 1 and 740 g dry ice in Bin 2, the errors were high even after the inclusion of sorption and desorption in the model. As mentioned earlier, linear extrapolation of sorption data at 100% initial CO₂ concentration might not be the

correct way to estimate sorption at lower concentrations. Further experimental data on the sorption of CO₂ by wheat at lower initial concentrations are needed.

To demonstrate the effect of including the sorption of CO₂ by wheat on the accuracy of model prediction, we simulated the CO₂ concentrations using various sorption rates (0 to 100% of sorption measured by Cofie-Agblor et al. (1992) in steps of 10%). The simulated CO₂ concentrations were compared with the measured concentrations averaged from three replicates of the 740 g dry ice experiment in Bin 2 with a covered grain surface. Table 2 shows the errors at various sampling times with various sorption values. The accuracy of prediction at 24 hours was the best (an error of 7%) with 60% of actual sorption. At 70 and 100% of actual sorption rate the predicted CO₂ concentrations were close to the measured values at 21 and 12 hours, respectively.

Of the total amount of CO₂ sorbed by grains in 24 hours, 50 to 60% is sorbed in the first 4 to 6 hours (Yamamoto and Mitsuda 1980). Cofie-Agblor et al. (1992) observed that nearly 80% of the total amount of CO₂ sorbed by wheat occurred in the first 12 hours. From Table 2 it can be seen that the error was the minimum at 12 hours with 100% of the measured sorption rate. It is possible that at lower concentrations the sorption of CO₂ by wheat may be same as for 100% CO₂. Thus, using a high sorption rate in the initial few hours and a low sorption rate afterwards might give accurate model predictions. Further experimental evidence is required before such an approach is taken in the model.

Step 4 : The future model

Predicting CO₂ concentrations using an apparent flow coefficient in the beginning and a diffusion coefficient afterwards improved the accuracy of prediction but there were still high errors of prediction in the initial time periods. Theoretically, a differential equation of the form:

$$\nabla(D\nabla C - uC) + q = \frac{\partial C}{\partial \tau} \quad (13)$$

which includes both diffusion and convection terms can be solved to accurately predict the CO₂ distribution in the grain bulk. In this equation u stands for the average interstitial velocity of flow in x , y , and z coordinate directions. The values of u can be computed using the pressure at the inlet boundary

Table 2. Mean relative percent errors between the predicted CO₂ concentrations and the measured concentrations (average of 3 replicates) with 740 g of dry ice in Bin 2 with covered grain surface, and various sorption rates.

Sorption rate (% of actual q^a)	Mean relative percent error									
	1 hour	3 hours	6 hours		12 hours		21 hours		24 hours	
			5L ^b	4L ^c	5L	4L	5L	4L	5L	4L
10	105	119	117	67	87	64	89	70	88	70
20	105	116	111	64	78	57	74	59	72	0
30	104	113	104	60	69	51	60	47	55	43
40	103	110	97	56	59	44	45	35	39	30
50	103	108	90	52	50	37	30	24	23	17
60	102	105	84	49	41	31	16	12	7	4
70	102	102	77	45	31	24	4	3	11	11
80	101	99	71	41	23	18	12	14	27	23
90	101	97	64	38	13	11	28	23	43	36
100	100	94	57	34	7	6	43	34	59	49

^athe measured sorption data of Cofie-Agblor et al. (1992) were used to estimate the actual q

^bthe mean relative percent errors were calculated for all 5 levels

^cthe mean relative percent errors were calculated for bottom 4 levels

(the pressure created by the expansion of the CO₂) or using the inlet velocity (when liquid CO₂ is vaporised and pumped into the grain bulk). In both cases care must be taken to account for the anisotropy of the grain to the gas flow in horizontal and vertical directions. Resistance of grains and oilseeds to the bulk flow of gas is lower for horizontal flow than for vertical flow (Kumar and Muir 1986; Jayas et al. 1987; Alagusundaram et al. 1992). In a grain bulk with uniform temperatures equation 13 along with the calculated velocity components can be used during the CO₂ application period and equation 1 should be used afterwards. CO₂ distribution and maintenance in a farm bin is further influenced by natural convection currents caused by temperature differences in the grain bulk and gas loss from the store due to weather changes and leaks in the bin wall. These factors should be taken into account for accurate model predictions. In our current research we are attempting to solve equation 13 and to validate it against the CO₂ data measured in wheat bulks under isothermal conditions. Finally, the model will be further modified to include the CO₂ transport by natural convection currents and gas loss from the granary. The resulting model will be validated against CO₂ distribution data measured in farm bins.

Summary

A pure diffusion model was not sufficient to accurately model the distribution of CO₂ in a grain bulk, especially during the application period. Although, predicting the CO₂ concentrations using the experimentally determined apparent flow coefficients improved the accuracy of model predictions compared with the assumption of pure diffusion, another way to approach the problem is to solve the convection-diffusion equation. Including the sorption phenomenon in the model is important for accurate model predictions. We now have only limited data on the sorption of CO₂ by food grains which are for an initial CO₂ concentration of 100%. In a CA treatment we seldom observe 100% CO₂ concentration in the grain bulk. The sorption of CO₂ by food grains at various initial concentrations is essential for the model. Models of natural convection and gas losses from the grain storage structure are essential for predicting CO₂ distribution in farm granaries.

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