

Apparent flow coefficient of carbon dioxide through wheat bulks

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¹Department of Biosystems Engineering, 438 Engineering Building, University of Manitoba, Winnipeg, MB, Canada R3T 5V6; and ²Agriculture and Agri-Food Canada, Winnipeg Research Centre, 195 Dafoe Road, Winnipeg, MB, Canada R3T 2M9. Received 28 March 1994; accepted 19 January 1996.

Alagusundaram, K., Jayas, D.S., Muir, W.E., White, N.D.G. and Sinha, R.N. 1996. **Apparent flow coefficient of carbon dioxide through wheat bulks.** *Can. Agric. Eng.* 38:069-073. Laboratory experiments were conducted to determine the apparent flow coefficient, an empirical quantity that quantifies the rate of movement of carbon dioxide (CO₂) gas through wheat bulks. Dry ice was used as a source of CO₂ gas. The effects of temperature (-10 to 30°C), wheat moisture content (11 to 18.5%), and the mass of introduced dry ice (30 to 120 g) on the apparent flow coefficient of CO₂ gas through wheat bulks were determined. The apparent flow coefficient increased with an increase in temperature and the amount of introduced dry ice. No significant variation in apparent flow coefficient was observed with a change in moisture content. At all temperatures, moisture contents, and masses of introduced dry ice, the natural logarithm of apparent flow coefficient and time had a linear relationship. Keywords: controlled atmosphere, wheat, storage, carbon dioxide, flow coefficient

Le coefficient d'écoulement apparent, un paramètre empirique qui sert à quantifier les mouvements du dioxyde de carbone (CO₂) à travers une masse de blé, a été déterminé lors d'expériences en laboratoire. De la glace sèche a été utilisée comme source de CO₂. On a déterminé les effets de la température (-10 à 30°C), du taux d'humidité du blé (11 à 18,5%) et de la masse de glace sèche introduite (30 à 120 g) sur le coefficient d'écoulement apparent du dioxyde de carbone dans une masse de blé. Le coefficient d'écoulement apparent a augmenté avec la température et la quantité de glace sèche introduite. Aucune variation du coefficient d'écoulement apparent due au changement de taux d'humidité n'a été enregistrée. La relation du logarithme naturel du coefficient d'écoulement apparent en fonction du temps est linéaire, quelles que soient la température, le taux d'humidité et la quantité de glace sèche introduite.

INTRODUCTION

In a stored-grain ecosystem the composition of intergranular gas is an important abiotic factor that influences the growth and survival of pests. Respiration of insects, mites, fungi, and the grain itself causes a reduction in oxygen (O₂) concentration and an increase in CO₂ concentration in the intergranular air (White et al. 1982a, 1982b). Consequently, CO₂ can be used as a detector of incipient spoilage of grain (Singh et al. 1983). In airtight storage structures the depleted O₂ and elevated CO₂ levels have been effectively used to control stored-product pests (Banks and Annis 1977). Controlled atmosphere (CA) storage is a pesticide-free method of controlling pests in stored grain. In CA storage the gaseous composition of the intergranular air is altered by injecting either CO₂ to create high-CO₂ atmospheres or nitrogen (N₂) to create low-O₂ atmospheres lethal to pests (Banks and

Annis 1977).

The rate of movement of gases introduced into a CA storage or the gases produced in a hermetic storage is an important material property that can be used to determine the distribution and maintenance of these gases in the grain bulks. In the absence of convection currents, diffusion due to concentration gradients will be the predominant mechanism of transport of gases through the interstitial space (Singh et al. 1983, Jayas et al. 1988). Quantifying the rate of diffusion of different gases through agricultural grains has been a subject of study for more than 50 years (Henderson and Oxley 1944; Bailey 1959; Haugh and Isaacs 1967; Adamczyk et al. 1978; Singh et al. 1984, 1985). The diffusion coefficient of gases through agricultural grains is about one-third of the diffusion coefficient of gases in air (Henderson and Oxley 1944; Bailey 1959; Haugh and Isaacs 1967).

In addition to the diffusion due to a concentration gradient, other factors such as natural convection currents caused by temperature differentials in a grain bulk or the bulk movement caused by the pressure with which the gas is applied also play roles in the distribution of gases within the grain bulks. In a CA treatment with CO₂ gas, for example, liquid CO₂ is vaporized and pumped into the grain bulk (Jay 1980) or dry ice pellets are introduced into the plenum or on the grain surface and allowed to sublimate (Banks and Sharp 1979; Jay and D'Orazio 1984; Alagusundaram 1993). In both modes of application, a bulk movement of CO₂ occurs through the grain bulk because of the pressure with which the gas is pumped into the grain bulk or the pressure created by the sublimation of dry ice. The knowledge of the rate of bulk movement of introduced CO₂ gas (apparent flow coefficient) through grain bulks can assist in a cost efficient design with minimal use of gases and effective CA treatment.

The objective of the present study was to determine the apparent flow coefficient of CO₂ through wheat bulks as affected by the temperature and moisture content of the grain and the mass of introduced dry ice.

MATERIALS AND METHODS

Apparatus

The apparatus used for determining the apparent flow coefficient of CO₂ through a wheat bulk was similar to the one used by Singh et al. (1984). In addition to the gas sampling ports used by Singh et al. (1984), we also installed two ports near

the inlet end of the grain chamber (Fig. 1). Two tubes of semi-rigid nylon and outside diameter of 3.2 mm were inserted through rubber septa fitted to these ports to take gas samples from the grain and gas chambers near the perforated screen (ports 4 and 5, Fig. 1).

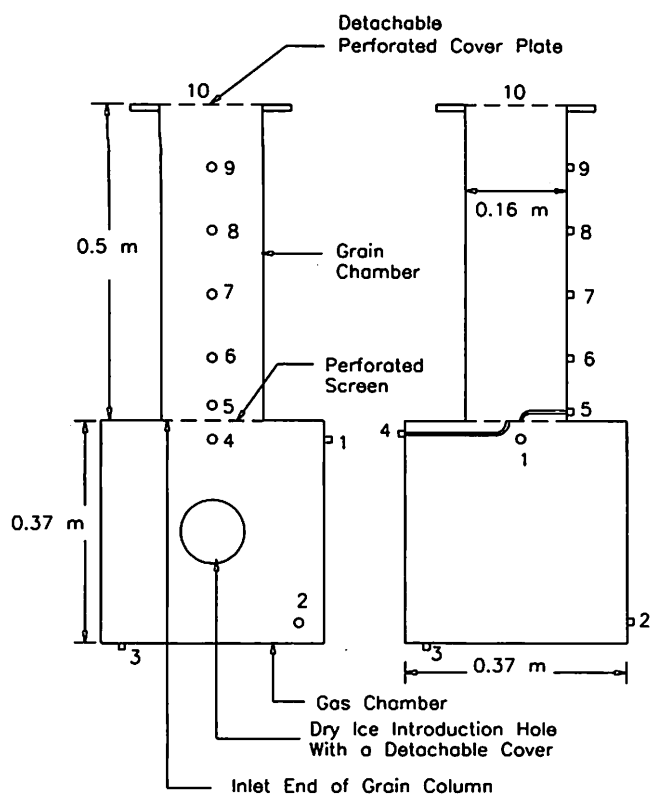


Fig. 1. Schema of the apparatus used for measuring apparent flow coefficient of CO₂ through stored wheat bulks.

Sample preparation

Canadian hard red spring wheat graded No.1 by the Canadian Grain Commission, Winnipeg, MB was used in the experiments. The wheat obtained from a local farmer had 0.5% dockage by mass and 12.8% moisture content (wet mass basis). Wheat samples of about 25 kg each were conditioned to five different moisture contents (11.0, 12.3, 14.0, 16.5, and 18.5% wet mass basis) by adding predetermined quantities of distilled water and mixing in a small concrete mixer or by spreading the wheat on the floor and allowing it to dry until the desired low moisture content was reached. The prepared samples were sealed in plastic bags and allowed to equilibrate at room temperature for about 24 h and then stored at -20°C until used in the experiments. Before the start of the experiment, the samples were conditioned for about 48 h at the experimental temperature. The moisture contents of the wheat samples were determined on a wet mass basis before each experiment using the procedure given in ASAE Standard S352.2 (ASAE 1992). An environmental chamber equipped with a relative humidity (RH) controller was used to create the required experimental temperatures. The RH of the envi-

ronmental chamber was set at 75% during all the experiments.

Experimental procedure

The grain chamber was filled with wheat by manually pouring from the end of the grain chamber with detachable perforated cover plate. The grain chamber was filled by pouring the grain from near the top end of the grain column to its brim in all the experiments and was left undisturbed. In most experiments the mass of the grain in the grain chamber was measured to calculate the in-situ bulk density of the wheat. The particle densities of wheat samples with various moisture contents were determined using a toluene displacement method (Mohsenin 1970). The porosity of the wheat bulk in the grain chamber was calculated from measurements of the in-situ bulk density and the particle density (Mohsenin 1970).

A known quantity of dry ice was placed in the gas chamber and the opening was sealed using the detachable lid. The inlet end of the grain chamber was always open to the gas chamber. Gas samples were taken at 10 min and at 1 h intervals for 8 h after the introduction of dry ice. When drawing gas samples, about 5 mL of gas were flushed out and about 8 mL of gas were taken in 10-mL syringes. These gas samples were analysed for CO₂ concentrations using a gas chromatograph (Model HP 5890, Hewlett Packard, Avondale, PA) equipped with a thermal conductivity detector and a 1 mL fixed-volume injection-loop. The column temperature was set at 70°C and the detector temperature was set at 150°C.

A total of 16 experiments was conducted (five moisture contents at 20°C with 40 g dry ice, five temperatures at 12.3% moisture content with 40 g dry ice, and six amounts of dry ice at 20°C and at 12.3% moisture content). Each experiment was repeated three times.

CALCULATION OF APPARENT FLOW COEFFICIENT OF CO₂ THROUGH WHEAT BULKS

The apparent flow coefficient of CO₂ through wheat bulks was calculated assuming that at all times the conditions approximated a steady state condition, i.e. the concentration gradient in the grain column and the diffusion flux at any time were those that would be found if the concentration at the inlet end was maintained at the instantaneous measured value. This assumption was similar to that made by Cowie and Watts (1971) for calculating the diffusion of methane and chloromethane in air and that made by Singh et al. (1984) for calculating the diffusion coefficient of CO₂ through wheat bulks. The apparent flow coefficient was calculated using:

$$D_{app} = \frac{Q_m \cdot \Delta x}{A \cdot \Delta c} \quad (1)$$

where:

- D_{app} = apparent flow coefficient of CO₂ through wheat bulk (m²/s),
- Q_m = mass flow rate of CO₂ through wheat (g/s),
- A = cross sectional area of the grain column (m²),
- Δc = concentration difference between the inlet end of the grain column and a sampling point along the grain column (g/m³), and

Δx = distance between the inlet end of the grain column and the sampling point at which c was calculated (m).

The mass flow rate Q_m was calculated for two time periods in the experiment as Q_{m1} and Q_{m2} , where Q_{m1} is the mass flow rate during the time period up to when the dry ice sublimated and Q_{m2} is the mass flow rate during the time period beginning from when the dry ice was completely sublimated and up to the end of the experiment (8 h). Q_{m1} and Q_{m2} can be expressed as:

$$Q_{m1} = \frac{M_{dryice} - (CO_2)_{subl}}{t_{subl}} \quad (2)$$

$$Q_{m2} = \frac{(CO_2)_{subl} - (CO_2)_{8h}}{8 \times 3600 - t_{subl}} \quad (3)$$

where:

- m_{dryice} = mass of introduced dry ice (g),
- $(CO_2)_{subl}$ = CO₂ remaining in gas chamber and grain column at the time all dry ice has sublimated (g),
- $(CO_2)_{8h}$ = CO₂ remaining in gas chamber and grain column after 8 h (g), and
- t_{subl} = time at which all dry ice has sublimated (s).

Our observations showed that 180 to 740 g of dry ice pellets exposed to room temperature sublimated in 45 min to 1 h. Therefore we determined Q_{m1} at 1 h and Q_{m2} between 1 h and 8 h.

At any given sampling time, the concentration gradient, $\Delta c/\Delta x$, was estimated between the inlet end of the grain column to each of the five sampling points along the grain column (Fig. 1) and D_{app} estimated for each of these values. The average of these five D_{app} values was taken as the D_{app} for that sampling time. Similarly, the D_{app} values were calculated for all the sampling times.

The D_{app} decreased with time from 0 to 8 h. The natural logarithm of D_{app} and time were related as:

$$\ln(D_{app}) = A + B \ln(t) \quad (4)$$

where:

- t = time (h), and
- A and B = empirical constants.

The GLM procedure of SAS (SAS 1982) was used to estimate the constants A and B for various experiments (Table I).

RESULTS AND DISCUSSION

Effect of temperature

The D_{app} increased with an increase in temperature from -10 to 30°C. Bailey (1959) observed an increase in the diffusion rate of O₂ through wheat with an increase in temperature in the range of 1.7 to 42°C. Singh et al. (1984) also observed an increase in the diffusion rate of CO₂ through grain bulks with an increase in temperature from -10 to 30°C. Both Bailey (1959) and Singh et al. (1984) observed a quadratic relationship between the diffusion rate of gases through grain bulks and the temperature. In this study, we observed a linear

Table I: Empirical constants A and B (in Eq. 4) at various temperatures, wheat moisture contents, and with different amounts of dry ice used to determine the apparent flow coefficient of CO₂ through wheat bulks

Variable	A	B	R ²
Temperature (°C)			
-10	7.526	-0.614	0.891
0	9.067	-0.761	0.923
10	9.838	-0.835	0.935
20	10.566	-0.935	0.892
30	11.426	-0.941	0.863
Grain moisture content (%)			
11.0	9.273	-0.780	0.927
12.3	10.566	-0.935	0.892
14.0	7.855	-0.640	0.851
16.5	10.203	-0.872	0.917
18.5	9.214	-0.761	0.907
Amount of dry ice (g)			
30	11.268	-1.015	0.879
40	10.566	-0.935	0.892
50	12.437	-1.137	0.923
60	13.172	-1.202	0.887
80	16.509	-1.553	0.825
120	21.533	-1.995	0.829

increase in A and a linear decrease in B with an increase in temperature in the range of -10 to 30°C. According to Jost (1960), true diffusion generally shows a relatively strong dependence on temperature while the effect of temperature on bulk flow of gases through capillaries is rather small. The results of Bailey (1959) and Singh et al. (1984) were for pure diffusion while in our study, due to the pressure created by dry ice sublimation, a bulk movement of CO₂ gas occurred. The relationship between the constants A and B of Eq. 4 and temperature were:

$$A = -16.6455 + 0.093T \quad R^2 = 0.974 \quad (5)$$

$$B = 1.5273 - 0.00828T \quad R^2 = 0.927 \quad (6)$$

where T = temperature (K).

Effect of moisture content

No definite pattern of increase or decrease in D_{app} was observed with an increase in the moisture content of wheat from 11 to 18% (Table I). The in situ porosity increased from 42% at 11% moisture content to 47.3% at 18% moisture content. This increased pore space, however, did not cause an increase in D_{app} . The mass displacement of CO₂ created by the dry ice sublimation process may have reduced the effect of increased porosity at higher moisture contents.

Effect of the amount of dry ice

As expected, the D_{app} increased with an increase in the mass

of dry ice introduced. The increased volume of CO₂ caused an increase in pressure in the gas chamber thus increasing the mass displacement of CO₂ through the wheat bulk. Even though the constants *A* and *B* of Eq. 4 increased linearly with an increase in the mass of dry ice, such a relationship may not be useful in a mathematical model to predict the CO₂ distribution in grain bulks. This is because the mass of dry ice used in the experiments for determining the *D_{app}* will be different from the amount of dry ice that would be used in a farm bin. The pressure drop across the grain column created by the various amounts of dry ice, if all of it were sublimated at once, is a more realistic quantity for use in the mathematical models. The pressure drop across the grain column was estimated using:

$$\frac{P}{L} = \frac{m}{V} \frac{RT}{L} \quad (7)$$

where:

- P* = pressure created by the dry ice if all the dry ice introduced in the gas chamber sublimated at once (kPa),
- L* = length of the grain column (m),
- m* = mass of dry ice introduced (kg),
- R* = CO₂ gas constant (0.1889 kJ•kg⁻¹•K⁻¹),
- T* = temperature (K), and
- V* = volume of the gas chamber (m³).

The relationships between the constants *A* and *B* of Eq. 2 with the pressure drop across the grain column created by various amounts of dry ice introduced in the gas chamber were of the form:

$$A = 6.3683 + 0.0482(P/L) \quad R^2 = 0.970 \quad (8)$$

$$B = -0.5448 - 0.00465(P/L) \quad R^2 = 0.967 \quad (9)$$

PRACTICAL USE OF *D_{app}*

Diffusion is the mechanism of CO₂ transport in a grain bulk with uniform grain temperature and at normal atmospheric pressure. During application period, however, the pressure with which the gas is applied causes a bulk movement. The bulk movement of gas through the grain bulk can be modelled by replacing the diffusion coefficient in the governing partial differential equation with the *D_{app}*. After the application period is over, the diffusion coefficient should be used to further model the distribution of CO₂. Using the pressure with which the gas is applied and Eqs. 4, 7, 8, and 9, the *D_{app}* at 20°C can be estimated. The calculated *D_{app}* can be corrected for temperature using Eqs. 4, 5, and 6. Using *D_{app}* and diffusion coefficient for modelling the movement of CO₂ through grain bulks is an easier and quicker method compared to attempting to model the bulk movement based on physical principles.

CONCLUSIONS

The apparent flow coefficient of CO₂ gas through stored wheat bulks is an important bulk property required to determine the movement and distribution of introduced CO₂ gas. The *D_{app}* increased with an increase in the temperature from -10 to 30°C and an increase in the mass of introduced dry ice from 30 to 120 g. The moisture content of wheat did not have

any influence on the *D_{app}* in the range of 11 to 18%. At all temperatures, the masses of dry ice introduced, and moisture contents used in this study, the logarithmic values of *D_{app}* decreased with an increase in time. The relationship between the variables and time on logarithmic scales was linear.

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