INTRODUCTION

Over 90 Mt of grain and oilseeds — worth about 7 billion dollars — are stored annually in elevators and on farms in Canada (Anonymous 1982). Generally, little or no equipment is used to detect any loss in quality or quantity of this stored food caused by the activity of various biotic agents. The most commonly employed monitoring system for grain bulks is the point measurement of temperature. In principle, the detection of metabolic heat produced by harmful organisms is a sound procedure because the existence of a hot spot in a grain bulk indicates that the grain in the affected area is in an advanced stage of decay. However, because of the low thermal diffusivity of bulk grain a single temperature measurement must be within about 0.5 m of an active spoilage spot to detect the spoilage (Yaciuk and Wallace 1965). Measured temperatures cannot be readily interpreted without the temperature history of the stored grain. As an example, temperature of 35°C in a large bin in mid-winter may mean that there is an active hot spot or that the grain has not yet cooled at the center of the bin (Yaciuk et al. 1975).

Olfactory sensing of a mouldy odor is a method frequently used by elevator managers to detect spoiled rapeseed; but the managers report that considerable spoilage occurs before it can be detected by this method (Mills 1976). Consequently, there is a need for a better monitoring system that can be used to warn the storage manager or farmer when his stored product begins to undergo unacceptable deterioration.

Previous work (Muir et al. 1980a) has shown that in grain bulks intergranular carbon dioxide (CO$_2$) concentrations above ambient atmospheric level (0.03%) can be indicators of the activity and respiration of grain storage pests, viz. microorganisms, insects and mites. The measured CO$_2$ concentrations can be readily compared with the CO$_2$ level in ambient air which can be used as a standard, thus eliminating the need for knowledge of the storage history to interpret the readings. Using this principle a project to develop a scientifically valid and commercially feasible monitoring system to detect deterioration of cereal grain and oilseeds during storage in large bulks was undertaken.

Rates of production of CO$_2$ in wheat and rapeseed at different temperatures and moisture contents (White et al. 1982a, b) and diffusion properties of CO$_2$ through wheat and rapeseed (Singh et al. 1983) have been studied to provide the basic data required for implementation of this concept. Currently, rates of diffusion of CO$_2$ through and out of large bulks of cereals and oilseeds stored in various types and sizes of bins are being measured in farm granaries to provide in-the-field confirmation. The objectives of this report are (1) to describe the use of a finite element model for predicting the required instrument resolution and the most suitable bin location for a spoilage-sensing device; and (2) to compare the concentration levels which can be monitored by available instruments with the requirements determined above.

ASSUMPTIONS AND LIMITS OF MATHEMATICAL MODEL

Carbon dioxide produced by a pocket of deteriorating grain can move from that pocket by mass movement of the intergranular air and by diffusion. Preliminary analysis of incomplete results being measured in 47 farm bins of 35- to 3000-m$^3$ capacity suggests that wind may cause significant movement of the intergranular air. But in bins containing deteriorating grain, levels of CO$_2$ concentration higher than that in ambient air can be detected (Muir et al. 1980a). The location of the CO$_2$ sampling point must be chosen assuming no wind because the wind effect changes with the unpredictable wind direction. Free convection currents established in the grain bulk because of temperature gradients appear to be negligible (Muir et al. 1980b).

The diffusion of CO$_2$ from a pocket of deteriorating grain was assumed to be modelled by Fick's second law of diffusion (Jost 1960). Biological activity of the grain surrounding the pocket was assumed to be negligible and thus not generating CO$_2$. The surrounding grain mass was considered homogeneous with a constant CO$_2$ diffusivity independent of direction and force of gravity (Singh et al. 1983).

The grain absorbs CO$_2$ from the air until it comes into equilibrium with the CO$_2$ concentration in the intergranular air. The CO$_2$ concentrations in the intergranular air are predicted for the steady state conditions developed after the absorbed CO$_2$ comes into equilibrium with the CO$_2$ in the intergranular air. Based on a straight-line interpolation of the data of Yamamoto and Mitsuda (1980) equilibrium could be reached in about 3–6 days after initiation of deterioration.

The diffusion of CO$_2$, in a circular steel bin with a concrete floor, 6 m in diameter and filled to a height of 4.6 m with wheat was modelled mathematically.
ture content of the wheat was assumed to be 13% wet mass basis and the CO₂ diffusion coefficient was set at 0.0373 cm²/sec (Singh et al. 1983; Singh 1982).

The concrete floor of the bin was assumed to be impermeable to the diffusing carbon dioxide gas thus resulting in the homogeneous boundary condition $\partial c/\partial n = 0$ (as in Neuman and Narasimhan (1977), Narasimhan et al. (1977)). As a consequence of assuming no variation in the CO₂ concentration with the angle $\theta$, i.e. around the bin, there is no CO₂ flow across the center axis and the boundary condition is $\partial c/\partial n = 0$.

In practice, the top surface of grain is open to atmospheric air under a ventilated roof. On the assumption that CO₂ leaving the top surface diffuses away instantaneously the CO₂ concentration at the top of the grain mass was defined to be constant and equal to the CO₂ concentration in the atmosphere (0.9 g·m⁻³).

The bin wall was assumed to be (1) infinitely permeable to CO₂ thus CO₂ concentration equals atmospheric air CO₂ concentration and (2) impermeable to CO₂ i.e. no flow across the bin wall ($\partial c/\partial n = 0$). These are two extreme cases which could occur in the field depending on the amount of leakage through the bin wall. Probably most steel bins would be between the two extremes tending towards the impermeable bin wall condition. Because the rates of diffusion of CO₂ through bin walls are not known, the two extreme possibilities have been considered.

The pocket of spoiling grain was assumed to be a disc 0.3 m deep and 1 m in diameter. The spoilage pocket was assumed to be at 30°C, 20% moisture content wet basis and producing CO₂ at a rate of 0.006 g·h⁻¹·kg⁻¹ of wheat, based on equations of White et al. (1982a).

Three locations for the spoilage disc (Fig. 1) were modelled. To simulate a hot spot (a localized area of intense biological activity manifested by the production of metabolic heat) near the top center of a bin that can occur due to moisture migration and snow blowing into a bin the disc was assumed to be 0.3 m below the top grain surface (Muir et al. 1978, 1980a). Moisture migration in the summer or the movement of snowmelt water from the top to the bottom of the bin may result in hot spots developing at the bottom of the bin (Muir et al. 1978).

A third location for the spoilage disc was taken at the center of the bin, 2.0 m from the top grain surface.

Carbon dioxide concentrations throughout the grain bulk were calculated using a finite element package (MANFEP) available on the University of Manitoba computer (Stevens and Wexler 1978a, b). Six sets of boundary conditions, i.e. two bin wall conditions, permeable and impermeable to CO₂, for three spoilage locations, top, mid-height and bottom of the bin (Fig. 1), were simulated.

**RESULTS AND DISCUSSION**

Initially, it was assumed that a constant concentration of CO₂, (18.5 g·m⁻³ or 1.0%) existed in the spoilage pocket. To maintain this constant concentration it was assumed that the rate of CO₂ production by the spoiling grain was equal to the calculated rate of diffusion from the bin. This rate was different for each of the six finite element models. With a permeable bin wall the rate of diffusion of CO₂ from the top surface of the grain decreased from 0.8 g·h⁻¹ with the spoilage pocket near the top of the bin to 0.07 g·h⁻¹ with the pocket at the bottom of the bin. The rate of diffusion through the bin wall is maximum (1.7 g·h⁻¹) when the pocket is near the center compared with 0.66 g·h⁻¹ with the pocket at the top and 1.28 g·h⁻¹ with the pocket at the bottom. This could be explained on the basis of geometrical considerations. For this bin, the distance from the pocket to the wall varies from 3 m to 5 m when the spoilage pocket is near the top or the bottom, whereas for the center location of the pocket the distance is 3.0–3.9 m. This results in nearly constant concentration gradients for the latter case in comparison with varied gradients for the former, and thus higher amounts of

![Figure 1](image-url)

Figure 1. Spoilage locations and boundary conditions assumed for the finite elements models ($c = $ carbon dioxide concentration (g·m⁻³); $c_a = $ carbon dioxide concentration in air (0.9 g·m⁻³); $c_e = $ CO₂ concentration in spoiling pocket (g·m⁻³); $\partial c/\partial n = $ concentration gradient in normal direction (g·m⁻³).
CO₂ diffused for the center location of the pocket than for the top or bottom locations. The rate of diffusion from the top of the bin for the bin wall impermeable to air reduces from 1.2 g·h⁻¹ to 0.6 g·h⁻¹ as the pocket is moved downward from the top to the bottom.

Grain can be stored under high levels of CO₂ to protect it from storage pests (Shejbal 1980). The development of gas leaks in the storage structure is a major problem of this grain preservation method. The CO₂ diffusion rates presented above could be used to predict the purging rate of CO₂ required to maintain an atmosphere lethal to storage pests.

In a second analysis of the finite element models, it was assumed that the rate of production of CO₂ in the spoilage disc was constant and equal for the six sets of boundary conditions (Fig. 1). This rate, 0.006 g·h⁻¹ per kilogram of dry wheat, was determined based on the results reported by White et al. (1982a) for the conditions assumed for the spoilage pocket. Concentrations of CO₂ in the spoilage pockets and throughout the bin that would result from a rate of diffusion from the bin equal to the set rate of CO₂ production in the spoilage disc were predicted (Fig. 2).

The concentrations of CO₂ developed in the bin are low. A sensing instrument with high resolution is required to detect spoilage in the bin. To detect spoilage with a sensor located 2 m from an active hot spot in a bin with a wall permeable to CO₂ an instrument capable of detecting 2 g·m⁻³ (0.1%) CO₂ is required (CO₂ concentration in the ambient air is 0.9 g·m⁻³). To detect spoilage with a sensor 1 m from the pocket the equipment should detect a CO₂ concentration of about 4 g·m⁻³ (0.2%). When the bin wall is impermeable to CO₂, equipment capable of detecting CO₂ levels of about 6 g·m⁻³ (0.3%) would be required.

The concentrations of CO₂ in the spoilage pocket are about the same (12.0–14.8 g·m⁻³) for four of the models considered. A slightly lower concentration (8.7 g·m⁻³) occurs with the spoilage pocket at the center with a permeable wall, and almost double the concentration (26.2 g·m⁻³) occurs with the spoilage pocket at the bottom with an impermeable wall. Therefore, if the sensor can be located within the spoilage pocket it should be capable of accurately sensing CO₂ levels of at least 8 g·m⁻³ (0.4%). The best location to detect deterioration is in the vicinity of the active hot spot where the concentrations are highest, about 14–17 times that of atmospheric concentration.

To detect minimum CO₂ concentrations of 0.1% produced by spoiling grain in granaries five instruments were compared (Table I). Both analytical gas chromatographs are expensive and non-portable, therefore, it is not feasible to use them on farms. They could be used to analyze gas samples taken to a central location serving a large number of farmers. Equipment such as Drager tubes and Leakseekers are portable and not prohibitively expensive. A thermal conductivity sensor such as the Leakseeker is normally sufficiently accurate but it can give inaccurate readings with moist gas samples because water va-

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Figure 2. Lines of equi-concentration of CO₂ (g·m⁻³) in a 6-m-diameter bin predicted to occur for three locations of the spoilage pocket (0.3 m, 2.0 m and 4.3 m from top surface of grain). Left side, figures are for bin wall permeable to CO₂; and right side, figures are for a bin wall impermeable to CO₂.
### Table I. Minimum Resolution and Approximate Cost of Commercially Available Carbon Dioxide Sensing Devices

<table>
<thead>
<tr>
<th>Sensing devices</th>
<th>Source</th>
<th>Minimum resolution (% CO₂)</th>
<th>Approximate cost ($)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas chromatograph†</td>
<td>Perkin-Elmer (Canada) Ltd.,</td>
<td>0.0025</td>
<td>11 000</td>
</tr>
<tr>
<td>(P.E. Sigma 3B)</td>
<td>Richmond, B.C.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gas chromatograph†</td>
<td>Matheson Gas Products,</td>
<td>0.05</td>
<td>5 000</td>
</tr>
<tr>
<td>(Matheson 8430)</td>
<td>East Rutherford, N.J.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Drager tubes†</td>
<td>Safety Supply Canada,</td>
<td>0.01</td>
<td>75$</td>
</tr>
<tr>
<td></td>
<td>Toronto, Ont.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Leakseeker†</td>
<td>Ion Track Instruments, Inc.,</td>
<td>0.05</td>
<td>1 600</td>
</tr>
<tr>
<td></td>
<td>Burlington, Ma.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fyrite CO₂‡ (chemical analyzer)</td>
<td>Bacharach Instrument Co.,</td>
<td>1.0</td>
<td>350</td>
</tr>
<tr>
<td></td>
<td>Pittsburgh, Pa.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

†Non-portable.  
‡Portable.  
§Leakseeker may give inaccurate readings with moist gas samples as the thermal conductivity of water vapors obscures CO₂ effects.  
¶This technique requires an additional expenditure of up to $4.00 per sample tube.

por obscures the sensitivity to CO₂. The initial investment for Drager tube equipment is less than for a Leakseeker but the costs for replacement tubes can be high if a large number of gas samples are measured. The Fyrite analyzer is inexpensive and portable but it may not have sufficient resolution to detect CO₂ concentrations resulting from hot spots in stored grain.

### CONCLUSIONS

One possible method of detecting a pocket of deteriorating grain in a stored grain bulk is to measure the concentration of carbon dioxide in the intergranular air (Muir et al. 1980a). Based on mathematically simulated results for a cylindrical grain bulk of 6 m diameter and 4.6 m height the CO₂ concentration in a pocket of deteriorating grain along the central axis of the bin can be 8 g·m⁻³. To detect this deteriorating grain at a point up to 2 m away from the pocket would require an instrument that can be used to measure CO₂ concentrations of at least 2 g·m⁻³ (0.1%). If the location of a possible pocket of deteriorating grain is unknown but is expected to occur along the central bin axis the most suitable point to sample CO₂ concentrations is at the center of the bin.

The conclusions from this theoretical study are being tested in an experimental program with granaries in Manitoba and Minnesota. When the experiments are completed the results will be submitted for publication.

### ACKNOWLEDGMENTS

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### REFERENCES


