# Heat production in wet wheat under adiabatic conditions

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Zhang, Q., Muir, W.E., Sinha, R.N. and Cenkowski, S. 1992. **Heat production in wet wheat under adiabatic conditions**. Can. Agric. Eng. **34**:233-239. Heat production in wheat rewetted to moisture contents of 27.2% w.b. (wet basis) and 23.0% w.b. was measured using a computer controlled calorimeter. The heat production rate increased with time during the initial stage of heating, reached its peak (150 mW/kg for 27.2% moisture content) at about 45°C, then approached a lower constant rate (70 mW/kg). Directly measured heat production was higher than that calculated from $CO_2$ production using the respiration equation. The respiratory quotient increased to over 4.0 during the initial heating stage (4 to 6 days) and decreased to about 0.8 after 14 to 20 days when the temperature rose above 52°C. An exponential model was fitted to the heat production data.

Key Words: wheat storage, microflora, metabolic heat, respiratory quotient, calorimeter, adiabatic

La production de chaleur dans le blé réhumecté pour contenir 27,2% et 23% d'humidité a été mesurée à l'aide d'un calorimètre commandé par ordinateur. Au cours de la première étape de chauffage, la production de chaleur augmentait en fonction du temps pour atteindre un taux de pointe de 150 mW/kg à une température d'environ 45°C dans le blé contenant 27,2% d'humidité, puis revenait ensuite à un taux constant plus bas de 70 mW/kg. La production de chaleur directement mesurée était plus élevée que celle de $CO_2$, calculée à l'aide de l'équation de la respiration. Le quotient respiratoire augmentait à plus de 4 au cours de la première étape (de 4 à 6 jours) et déclinait à environ 0,8 après 14 à 20 jours, alors que la température s'élevait à plus de 52°C. Un modèle exponentiel a été adapté aux données sur la production de chaleur.

Mots clés : entreposage du blé, microflore, chaleur métabolique, quotient respiratoire, calorimètre, adiabatique.

## INTRODUCTION

Wheat produced on the Canadian Prairies is normally stored over winter and into the following summer in farm granaries without drying or ventilating systems. Most of these granaries, particularly after a few years of use, allow the entrance of blown snow and rain. This entering moisture along with moisture migration within the grain bulk can create pockets of wet grain. Measured moisture contents (m.c.) in such pockets have been as high as 27.3% w.b. (wet basis) in a farmer-owned granary (Wallace and Sinha 1962), 24.3% in an experimental bin (Muir et al. 1978) and 43.6% in an open pile (Muir et al. 1980). Sinha and Wallace (1965) showed that a 27.2-kg pocket of wet wheat (23% m.c.) in a 13.5-t bulk could develop into a hotspot where the temperature increased from 10°C to 65°C in 11 days. The heat produced within a pocket of wet moldy grain is not dissipated rapidly because of the low thermal conductivity of the grain and the slow free convection currents in the granular bulk. The elevated grain temperature and moisture content of the pocket provide a favourable environment for further growth of microorganisms, thereby making the heating process self-accelerating. Heating induced by seed-borne microflora is a complicated process involving many physical, chemical and biological factors including temperature, water activity, intergranular gas composition, and microfloral species associated with the grain. No adequate theories have been advanced to explain and predict heat production in stored grain ecosystems, although the respiration equation has been often used to estimate heat production during heating (Lassik 1986, Multon 1988):

$$C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O + HEAT \qquad (1)$$

For each gram of dry matter ($C_6H_{12}O_6$) broken down, 15.7 kJ of heat is produced. The respiration equation incorporates many successive steps involved in oxidation of carbohydrates (glucose) under aerobic conditions. It provides a simple way of calculating heat production from $CO_2$ production, which can be more readily measured than heat production in grain storage ecosystems. According to Eq. 1 the respiratory quotient should be equal to 1.0, however, measured quotients frequently deviate from 1.0 (Milner and Geddes 1946). Thus an exploration of possible errors in applying Eq. 1 to the calculation of heat production in grain storage ecosystems was considered desirable.

Objectives of this study were: (1) to develop a method for direct measurements of heat production under adiabatic conditions similar to those in a naturally occurring pocket of wet wheat, and (2) to determine whether heat production in a pocket of wet grain can be predicted from measured $CO_2$ production using the standard aerobic respiration equation, Eq. 1.

## METHODOLOGY

### Calorimeter

A computer controlled calorimeter was developed for measuring heat production in wet grain (Fig. 1). The grain sample was contained in two identical one-liter Dewar flasks which were housed in a 1.0 m x 0.8 m x 0.8 m insulated chamber (Fig. 1). One of the flasks, from which grain was sampled regularly for determination of moisture content and microfloral infection, was used as the reference flask. The use of this flask avoided disturbance of the test flask during grain sam-

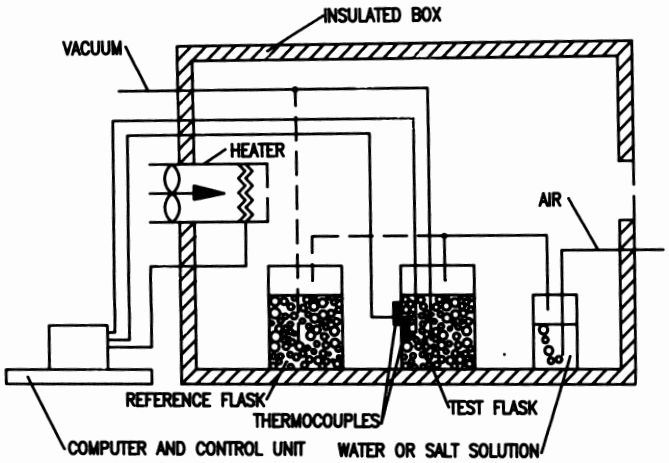


**Fig. 1. Schematic of computer controlled calorimeter.**

pling. Temperatures inside and outside the test flask were continuously monitored by a computer controlled data acquisition and control system (HP 3497 data acquisition system and HP 85 computer, Hewlett-Packard Co., Palo Alto, PA) through six thermocouples, three inside and three outside. When grain in the test flask started to heat, presumably due to metabolic activity of the seed and microorganisms associated with it, the inside temperature rose, thus causing a difference between the inside and outside temperatures. If the difference exceeded the preset value (0.5°C to 0.7°C), the computer turned on an electric heater to heat the air in the chamber, and thus to equalize the temperature outside the flask to the elevated temperature inside the flask. The temperature gradient across the flask wall was minimized throughout the course of heating; consequently, no heat was transferred from or to the grain contained in the flask. Under adiabatic condition, metabolic heat produced inside the flask by the seed and microflora was measured directly. To test the stability of the calorimeter, the flask was filled with hot water at 52°C. The change in water temperature was less than 1°C over 7 days of continuous operation.

The calorimeter also included a vacuum flushing system, which was used to flush the flasks regularly to maintain an adequate oxygen level inside both test and reference flasks during the tests (Fig. 1). During flushing, the respired gas was drawn out from the bottom of the flask by vacuum while conditioned air entered the head space of the flask. Before the air entered the flask, it was brought to a temperature and relative humidity in equilibrium with the grain by passing it through a salt solution or water bottle in the insulated box. This ensured that flushing did not alter the temperature and moisture content of the grain. Because high moisture grain (23.0% and 27.2% w.b.) was used in the experiments, the intergranular air was assumed to be saturated in the flask. Therefore, water was used in the air conditioning bottle.

## Material

Canada Western Red Spring wheat (cv. Katepwa), harvested in August 1988, was used in the experiments after being cleaned by a seed cleaner and by hand to remove foreign materials and damaged kernels. The initial germination rate of the wheat was 98% and the moisture content was 12.9% w.b. For each test, wheat was rewetted by adding distilled water to obtain the desired higher moisture contents. Because the experiments focused on naturally occurring heating by biological agents, there was no sterilization treatment. Major fungi occurring in unconditioned wheat, which were determined by the filter paper method of Wallace and Sinha (1962), included *Alternaria alternata, Aspergillus versicolor* (Vuill) Tiraboshi, *Penicillium spp. and Rhizopus* (Table I).

## Procedures

The two moisture contents studied were 27.2% w.b. and 23.0% w.b., which are typical in naturally occurring pockets of wet grain. The initial grain temperature in all tests was 30°C. Each moisture content was repeated twice on two separate calorimeters, i.e., four replicates of each condition. A test involved six steps: (1) wheat was cleaned to eliminate foreign materials and damaged kernels, (2) wheat was moistened with distilled water and stored in plastic bags at 2°C for 48 h, (3) the conditioned wheat stored in plastic bags was placed in an environment chamber at 30°C for 12 h to allow it to reach the desired initial temperature, (4) the test and reference flasks were filled with 650 g of conditioned wheat and the calorimeters were started (grain was totally exposed to air before it was filled into the calorimeters), (5) intergranular gas samples were taken from the test flasks and wheat samples (20 to 30 g) were taken from the reference flasks at every 4°C temperature rise, and (6) both flasks were flushed after the gas and grain samples were taken. A test was terminated when a slowing-down of the temperature increase became apparent. Flushing maintained $O_2$ concentration in flasks between 10% and 21% in all tests. According to Pitt et al. (1985), the estimated decrease in the aerobic respiration rate was about 15% when the $O_2$ concentration decreased to 10%.

During each test, the temperature inside the test flask was recorded by the computer automatically at every 2°C rise. Cumulative heat production was then determined from the temperature increase as:

$$h = \Delta T\,(m_g c_p + C_f) \qquad (2)$$

where:

**Table I. Major fungi identified in unconditioned wheat at 12.9% w.b. moisture content, % seeds infected**

| Medium | *Alternaria alternata* | *Aspergillus versicolor* | *Penicillium spp.* | *Rhizopus* |
|---|---|---|---|---|
| $H_2O$ | 65 | 0 | 39 | 96 |
| NaCl | 27 | 19 | 36 | 0 |

$h$ = cumulative heat production (kJ),
$\Delta T$ = cumulative temperature increase (°C),
$m_g$ = mass of grain in flask (kg),
$c_p$ = specific heat of grain (kJ•kg$^{-1}$•°C$^{-1}$), and
$C_f$ = heat capacity of calorimeter (kJ/°C).

The heat capacity of the calorimeter (flask and thermocouples) was determined in the temperature range of 20 to 65°C by using an electrical heater (0.65 W) to heat distilled water in the test flask. A linear regression analysis of the relationship between the measured temperature rise of the water and the measured electrical energy input to the heater was used to calculate the heat capacity of the calorimeter less the heat capacity of the water. Measured heat capacities of the two calorimeters used in the experiments were 699 J/°C with a standard deviation of 19 J/°C, and 604 J/°C with a standard deviation of 9 J/°C.

Because the specific heat of grain varies with moisture content, an empirical equation proposed by Muir and Viravanichai (1972) was employed to estimate the specific heat of wheat used in the experiments:

$$c_p = 1.098 + 0.0405MC_d \quad (3)$$

where $MC_d$ = moisture content in dry basis (%).

To validate the adequacy of Eq. 3, the specific heat of wheat at 27.2% w.b. moisture content was measured using the calorimeters. The mean of the measured specific heat was 2.51 kJ•kg$^{-1}$•°C$^{-1}$ with a 95% confidence interval of 2.12 to 2.90 kJ•kg$^{-1}$•°C$^{-1}$, while the specific heat predicted by Eq. 3 was 2.61 kJ•kg$^{-1}$•°C$^{-1}$. There was no significant difference between the measured and predicted specific heat at the significance level of 0.05.

Intergranular gas samples were taken from the test flask using a syringe before and after each flushing. Gas samples were then injected into a gas chromatograph (HP 5890A with a thermal conductivity detector, Hewlett-Packard Co., Palo Alto, PA) to determine $CO_2$, $O_2$ and $N_2$ concentrations in the gas samples. $CO_2$ production and $O_2$ consumption were calculated from the measured concentrations as:

$$v = (C_b - C_a)\left(V_f - \frac{m_g}{\rho}\right) \quad (4a)$$

$$m = \frac{pvM}{RT} \quad (4b)$$

where:
$v$ = volume of gas (m$^3$),
$C_a$ = concentration measured after previous flushing (fraction),
$C_b$ = concentration measured before current flushing (fraction),
$V_f$ = volume of flask (m$^3$),
$m_g$ = mass of grain in flask (kg),
$\rho$ = particle density of grain (kg/m$^3$),
$m$ = mass of gas (kg),
$p$ = pressure inside flask (Pa),
$M$ = molar mass of gas (kg/mol),
$R$ = universal gas constant (J•K$^{-1}$•mol$^{-1}$), and
$T$ = absolute temperature (K).

The pressure, $p$, inside the flasks increased as more $CO_2$ was produced than $O_2$ consumed. By assuming a constant mass of $N_2$ in the flask during heating, the pressure was calculated as:

$$p = \frac{C_{NO}}{C_N} p_a \quad (5)$$

where:
$C_{N0}$ = $N_2$ concentration measured after previous flushing (≈78%),
$C_N$ = $N_2$ concentration measured before current flushing (%), and
$p_a$ = pressure after previous flushing (= atmospheric pressure) (Pa).

## RESULTS AND DISCUSSION

### Heat production

Directly measured heat production (kJ of heat per kg of dry matter, kJ/kg) was determined using Eq. 2 and the measured cumulative temperature increase, whereas $CO_2$ based heat production was calculated using Eq. 1, which assumed that 10.7 kJ of heat was produced per gram of $CO_2$ produced. Accuracy of the heat production calculated by Eq. 2 was influenced by many factors associated with procedures and instrumentation in measuring quantities $T$, $m_g$, $C_f$, and $c_p$. The possible maximum error due to instrumentation was estimated as (Dally et al. 1984):

$$\varepsilon = \frac{dh}{h} = \sqrt{2\left(\frac{d\Delta T}{\Delta T}\right)^2 + \left(\frac{dm_g}{m_g}\right)^2 + \left(\frac{dC_f}{C_f}\right)^2 + \left(\frac{dc_p}{c_p}\right)^2} \quad (6)$$

where: $\varepsilon$ = overall error in heat production measurement.

Based on the specifications of the instruments, the overall error estimated by Eq. 6 was between 4.0% and 4.5% for direct measurement of heat production. Although this error was relatively small, experimental data appeared scattered (Fig. 2). This was because of the complexity of interrelations among measured and unmeasured factors in grain storage ecosystems and slight differences in initial conditions from

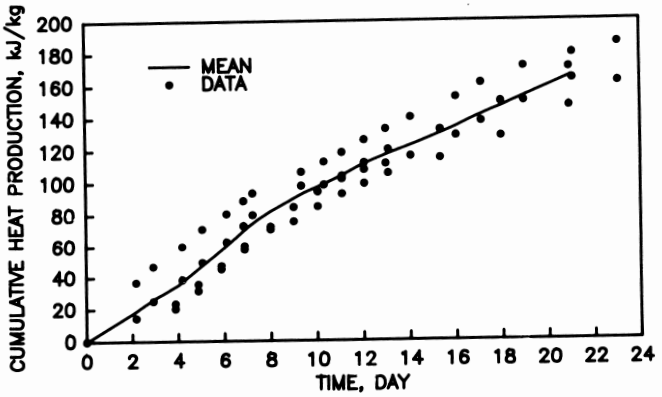


**Fig. 2. Measured cumulative heat production under adiabatic conditions for wheat at 27.2% w.b. moisture content.**

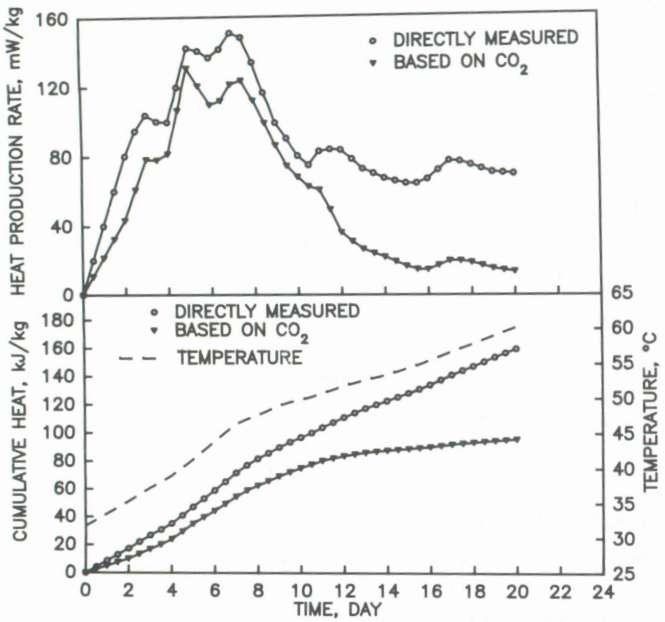


**Fig. 3. Means of measured cumulative heat production, heat production rate and temperature of wheat at 27.2% w.b. moisture content under adiabatic conditions.**

test to test. To facilitate discussions of general relationship patterns, mean values were calculated.

Rate of heat production (mW per kilogram of dry matter, mW/kg) increased rapidly with time in the initial heating stage (Fig. 3). Peaks occurred when temperature reached about 46.5°C for 27.2% m.c. wheat and 43.0°C for 23.0% m.c. wheat. The peak heat production rates were 150 mW/kg and 98 mW/kg for the two moisture contents, respectively. When the temperature reached 52°C (11th day), the heat production rates levelled out at lower levels presumably due to decreased microfloral activities. The rate however did not decrease to zero. Even after the temperature went above 65°C, heat production remained at about 70 mW/kg for 27.2% m.c. wheat and 31 mW/kg for 23.0% m.c. wheat. The variation of heat production rate reflected effects of temperature on microfloral and chemical activities. In the initial stage of heating, increasing temperatures accelerated microorganism growth, thus resulting in an increasing rate of heat production. When the temperature exceeded the most favourable condition for the microorganisms, heat production rate started to decrease. Further temperature rises (above 52°C) may have killed or reduced the respiration rate of some species of microorganisms. Continuation of heat production may have been caused by chemical oxidation or thermophilic microflora or both (Milner and Geddes 1946).

During the initial 11 days, the heat production rate calculated from measured $CO_2$ followed the directly measured rate of heat production (Fig. 3). On average, the directly measured rates were 27% and 14% higher than those calculated from $CO_2$ production for 23.0% and 27.2% moisture contents, respectively. These discrepancies might be attributed to: chemical reactions at the elevated temperatures, $CO_2$ absorption by the grain, and bacterial activities. Chemical reactions may produce heat in addition to heat of respiration and $CO_2$ absorption by the grain can reduce the amount of $CO_2$ released to the intergranular air, i.e., the measured $CO_2$ was less than actual $CO_2$ production. The high moisture contents and temperatures are conducive to bacterial growth, but no attempt was made to identify the species of bacteria. Because of continuous changes in $O_2$ and $CO_2$ concentrations in the calorimeters (in extreme cases $CO_2$ increased from near 0% to above 30% between flushings), both aerobic and facultative bacteria may have been present along with aerobic fungi. Co-existence of aerobic and anaerobic microorganisms was also suggested by the high respiratory quotients measured during the initial 11 days (Fig. 4). This implied that oxidation of carbohydrates through both aerobic and anaerobic metabolisms contributed to the heat and $CO_2$ production. Further research is needed to investigate grain heating by bacteria under partial anaerobic conditions.

After the 11th day the directly measured rates of heat production became much higher than those calculated from $CO_2$ (Fig. 3). The average differences were 72% and 39% for 27.2% and 23.0% moisture contents, respectively. The large difference may be attributed to chemical oxidation, such as browning, after thermal killing of the microorganisms (Multon 1988). For 27.2% m.c. wheat, the rate calculated from $CO_2$ dropped 89.7% when temperature rose from 46.5°C to 60.2°C, while the corresponding drop in the directly measured rate was 53.7%.

Large differences in heat production rate resulted in large discrepancies in accumulated heat production (Fig. 3). In 20 days, the directly measured cumulative heat production was 159.1 kJ/kg for 27.2% m.c. wheat and 103.7 kJ/kg for 23.0% m.c. wheat, whereas the corresponding heat production calculated from measured $CO_2$ was 93.7 kJ/kg and 87.5 kJ/kg, respectively. The directly measured heat productions were 1.7 times and 1.2 times higher than those calculated from $CO_2$ for the two moisture contents, respectively.

### Respiratory quotient

Variations of respiratory quotients for the two moisture contents followed a similar pattern. The following discussion is focused on the test with 27.2% m.c. wheat. Both $CO_2$ production and $O_2$ consumption rates increased with time during the initial heating stage (Fig. 4), reaching peaks at the same time and temperature as did the heat production rate. As temperature approached the thermal killing point, both $CO_2$ and $O_2$ rates began to decrease. The production of $CO_2$ dropped more rapidly than did $O_2$ consumption probably because of greater consumption of $CO_2$ and release of $O_2$ by the anaerobic bacteria.

The respiratory quotient was not constant during adiabatic heating (Fig. 4). It increased rapidly from 1.0 to 4.2 in 4 days, then decreased gradually to about 0.8 after about 12 days (corresponding to a temperature of 52°C) and stayed constant thereafter. The peak respiratory quotient occurred on the 4th day at a temperature of 39°C, whereas other peaks (heat production, $CO_2$ and $O_2$) occurred on the 7th day at 46.5°C.

### Effect of moisture content

Comparing 27.2% m.c. wheat and 23.0% m.c. wheat, the

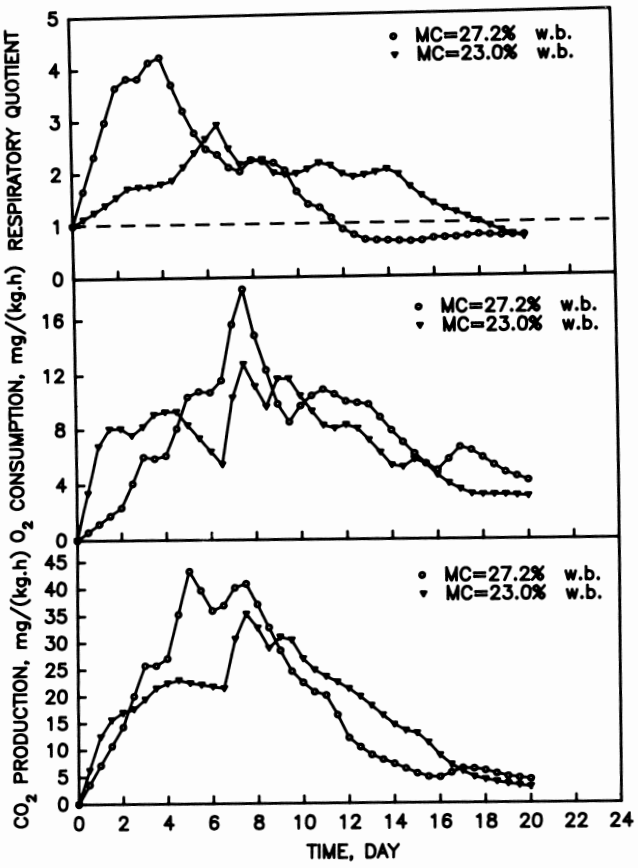


**Fig. 4. Comparison of $CO_2$ production and $O_2$ consumption between wheat at 27.2% and wheat at 23.0% w.b. moisture content under adiabatic conditions.**

higher moisture content provided a more favourable environment for a higher heat production rate (Fig. 5). Directly measured heat production was affected more by moisture content than was that calculated from $CO_2$. On the 20th day, the directly measured cumulative heat production for 27.2% m.c. wheat was 1.5 times higher than that for 23.0% m.c. wheat, while heat calculated from $CO_2$ for 27.2% m.c. was 1.1 times higher than that for 23.0% m.c. One reason for this difference might be the greater activity of anaerobic microflora in wheat with higher moisture content.

For the two moisture contents, rates of $CO_2$ production and $O_2$ consumption followed the same pattern (Fig. 4), with the higher moisture content (27.2%) showing slightly higher rates. The peak respiratory quotient for 27.2% m.c. wheat was higher and occurred earlier than that for 23.0% m.c. wheat. At both moisture contents, the respiratory quotient stayed at about 0.8 after temperature reached 52°C.

## Empirical model

Adiabatic heating developed in two distinct stages (Fig. 3): (1) the initial stage during which the heat production rate, $H$, increased with time, $t$, until it reached a peak, $H_p$, at time $t_p$ and (2) the post-peak stage during which the heat production rate decreased with time and eventually became constant, $H_r$.

Two exponential functions were used to describe the heat production rate during the two stages:

$$H = H_p e^{-a(t-t_p)^2} \qquad t<t_p \tag{7a}$$

$$H = (H_p - H_r)e^{-b(t-t_p)^2} + H_r \qquad t \geq t_p \tag{7b}$$

where:

$H$ = heat production rate (mW/kg),
$H_p$ = peak heat production rate (mW/kg),
$H_r$ = constant heat production rate after thermal killing (mW/kg),
$t$ = time (d),
$t_p$ = time of peak heat production rate (d), and
$a$, $b$ = empirical constants ($d^{-2}$).

The peak heat production rate, $H_p$, constant rate, $H_r$, and peak time, $t_p$, were determined from the measured heat production rate data (Table II). Equations 7a and 7b were rewritten to determine constants $a$ and $b$:

$$\ln\left(\frac{H}{H_p}\right) = -a\,(t-t_p)^2 \qquad t<t_p \tag{8a}$$

$$\ln\left(\frac{H-H_r}{H_p-H_r}\right) = -b\,(t-t_p)^2 \qquad t \geq t_p \tag{8b}$$

The slopes of the two straight lines obtained by plotting Eqs. 8a and 8b were constants $a$ and $b$ (Table II). The heat production rate calculated by the exponential model compared reasonably well with the experimental data (Fig. 6).

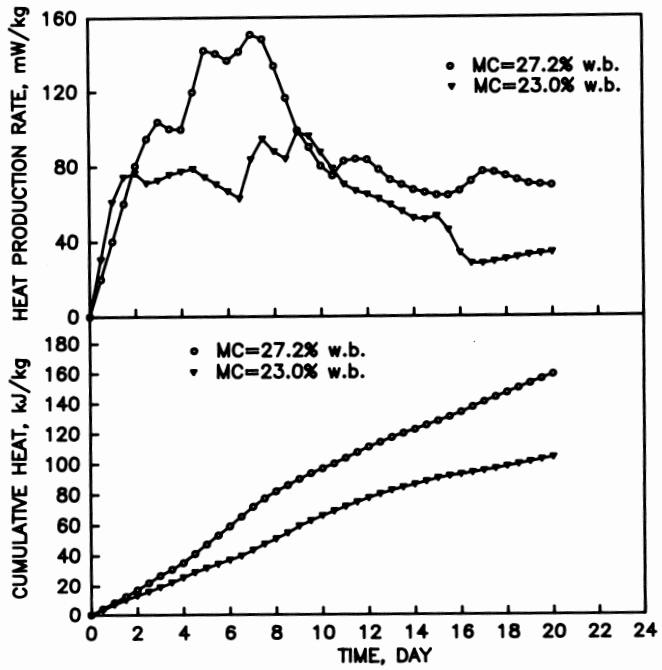


**Fig. 5. Comparison of directly measured heat production by wheat at 27% and wheat at 23.0% w.b. moisture content under adiabatic conditions.**

**Table II. Parameter values of exponential model of heat production for wheat at 27.2 % and 23.0% w.b. moisture contents**

| Moisture Content,% w.b. | $H_p$ (mW/kg) | $H_r$ (mW/kg) | $t_p$ (d) | $a$(d$^{-2}$) | $b$ (d$^{-2}$) |
|---|---|---|---|---|---|
| 27.2 | 150 | 70 | 7 | 0.036 | 0.12 |
| 23.0 | 98 | 31 | 9 | 0.0099 | 0.049 |

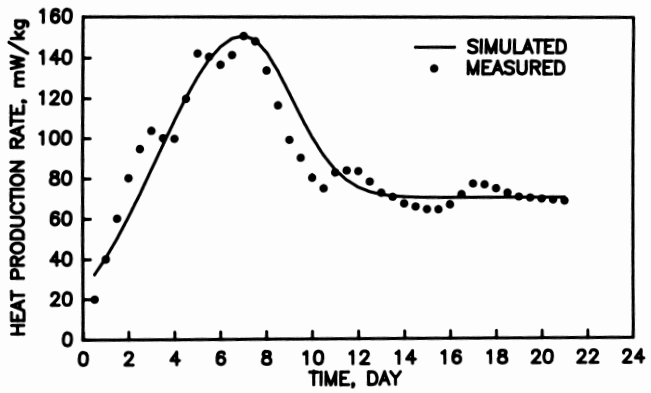


**Fig. 6. Comparison of simulated heat production rate with experimental data for wheat at 27.2% w.b. moisture content.**

## SUMMARY AND CONCLUSIONS

A computer controlled calorimeter was developed to study heating of stored grain caused by microfloral infection. Tests were conducted on wheat rewetted to moisture contents of 27.2% w.b. (wet basis) and 23.0% w.b. Heat and $CO_2$ production, and $O_2$ consumption were measured during the course of heating. Based on the study, the following conclusions were drawn for microflora-induced heating under adiabatic conditions:

1. Directly measured heat production was higher than that calculated from measured $CO_2$ production using the standard aerobic respiration equation.

2. The heat production rate increased with time in the initial heating stage and reached its peak when temperature was about 45°C. After peaking, the heat production rate decreased with time and approached a constant value. During the post-peak stage, the heat production rate calculated from $CO_2$ decreased more rapidly than that directly measured.

3. During heating, the respiratory quotient varied with time. It was higher than 1.0 during the initial heating stage, decreased to about 0.8 when temperature rose above 52°C, and stayed constant thereafter.

4.The heat production rate in wet wheat was modelled by a two-step exponential function.


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