

Composition change model for sealed atmosphere in coal mines

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ABSTRACT: A sealed atmosphere in a mined-out area of an underground coal mine is simply a volume with homogeneous composition governed by boundary conditions. This paper presents a mathematical model based upon the conservation of mass principle that describes the flow of air (nitrogen and oxygen), methane and carbon dioxide into and out of a sealed atmosphere and the time-dependent changes in gas concentration within the sealed atmosphere. As boundary conditions, the model includes the inflow of methane and carbon dioxide from the surrounding strata, the inflow of nitrogen as an inert gas, the production of carbon dioxide from coal oxidation and the related depletion of oxygen. The model also considers the barometric pressure which can either cause air to flow into the sealed atmosphere or gas to flow out of that volume, depending on the pressure differential with the sealed atmosphere. The mathematical model is implemented into a MATLAB[®] program for calculation and data display. Using a range of realistic input parameters, the model shows that the atmosphere within sealed atmospheres tends to become fuel-rich inert and the pressure tends to increase due to the inflow of methane gas from the surrounding strata. Sealed atmospheres may therefore have a natural tendency to outgas, i.e. to release gas into the mine atmosphere as leakage around and through the seals. The pressure within the sealed atmosphere will depend on the leakage gas flow resistance of the mine seal and the surrounding rock between the sealed atmosphere and the active mine. If this resistance is high enough, it appears possible to maintain the sealed atmosphere in a fuel-rich inert condition and outgassing at all times despite changes in the barometric pressure. Designing the seal and the sealed area to control leakage such that the sealed atmosphere remains inert could result in safer sealed areas with minimal explosion hazard.

1 Introduction

1.1 Need for a Composition Change Model

The Sago Mine disaster of 2006 and the ensuing changes to mine sealing regulations caused the U.S. coal industry to become more aware of the atmospheric composition within sealed atmospheres and how that composition can change over time. The composition of the atmosphere behind seals determines the design explosion pressure that they must resist. Under certain conditions, the sealed atmosphere may become self-inert, and the time required for self-inertization to occur may receive consideration prior to conducting a sealing operation. During the construction and cure time for seals, the sealed atmosphere must remain inert (non-explosive), until the seal achieves its design strength. Sealed atmospheres may “breathe” and exchange gases with the mine atmosphere, causing the sealed atmosphere composition to change.

The sealed atmosphere behaviour and the factors controlling it have not received extensive scientific study. Actual measurements of the sealed atmosphere composition are not available because sealed areas may not be readily accessible for direct measurements. However, evidence suggests that many sealed atmospheres tend to become and remain inert by themselves.

1.2 Objectives

This paper presents a mathematical model describing the condition and composition changes of sealed atmospheres in coal mines. The model considers the following factors affecting the sealed atmosphere composition:

- Methane (CH₄) inflow from remnant coal or CH₄ reservoirs in the roof and floor strata.
- Addition of the inert gases nitrogen (N₂) or carbon dioxide (CO₂).
- CO₂ production from coal oxidation.
- Oxygen (O₂) depletion from coal oxidation.
- Seal leakage resistance.
- Barometric pressure changes.

Presenting this mathematical composition change model may facilitate the understanding and interpretation of actual measurements of the sealed atmosphere composition should they become available. With this theoretical model, it is demonstrated that sealed atmospheres will become inert and will remain inert if the air leakage into the sealed atmosphere is controlled. Maintaining the sealed atmosphere inert by minimizing leakage may result in safer sealed area with minimal explosion hazard.

1.3 Related Prior Work

Mining engineers have considered the atmosphere behind seals and how barometric pressure changes will affect that atmosphere. Dawson (1956) noted the practical difficulty in building air-tight seals that prevent gas from entering or exiting sealed atmospheres. Stevenson (1968) found a correlation between decreasing barometric pressure and increased CH_4 concentration in a bleeder system. Fauconnier & Beukes (1978) correlated measured barometric and sealed atmosphere pressure changes, and noted the time lag between the two. Neethling (1989) described how CH_4 could migrate closer to the active face during periods of falling barometric pressure and migrate away during rising pressure. Fauconnier (1992) conducted statistical analyses of explosions in South African coal mines and found that barometric pressure drops longer than 1 day were a contributing factor to gas explosions. Timko *et al.* (1987) measured gas velocity through longwall gob and sealed atmospheres that ranged from 0.0051 to 0.0150 m/s. At this rate, gas might take about 8 hrs to cross a 300-m wide longwall panel. The measured gas leakage through each 140 kPa seal ranged from 0.12 to 0.24 m^3/s . However, the magnitude of the pressure differential causing that gas flow is not known. While the changes to the sealed atmosphere are known qualitatively and some measurements of those changes are available, researchers have not explored the composition of the sealed atmosphere with any quantitative models to better understand the processes and the interrelationships between important parameters affecting the processes.

The "Gob Assistant Program" (Foster-Miller, 1988) may have been the first effort to understand the sealed atmosphere quantitatively and to calculate leakage quantity in and out. The intent of the Gob Assistant Program was to aid mine ventilation planning in order to: 1) reduce the CH_4 in return airways from outgassing seals, 2) reduce spontaneous combustion potential and 3) reduce explosion potential within sealed atmospheres behind ingassing seals.

The Gob Assistant Program solved the differential form of a conservation of mass equation for a sealed atmosphere as it "breathes" in and out due to atmospheric pressure fluctuations. As input, the program required the volume of the sealed atmosphere, the mine ventilation pressure (barometric pressure), the seal leakage constant and the CH_4 inflow rate into the sealed atmosphere. As output, the program calculated the pressure within the sealed atmosphere, and then determined the leakage rate either in or out. The program appeared to compute the CH_4 concentration within the sealed atmosphere, but it did not consider other important gases such as O_2 , N_2 or CO_2 . Unfortunately, the Gob Assistant Program is no longer available.

The work described in this paper attempts to extend the concepts behind the Gob Assistant Program and provide a practical tool to understand the composition of the sealed atmosphere and the factors affecting it.

2 Derivation of the Composition Change Model

2.1 Volume of Sealed Atmosphere

Figure 1 shows the assumed volume for the Composition Change Model (CCM). This volume, V , contains 4 gas species, namely, CH_4 , O_2 , N_2 and CO_2 , denoted by subscripts m, n, o and c. Total mass, M , is the sum of the masses of each gas species. The total pressure P_t inside the volume is the sum of the partial pressures of each species, P_m , P_n , P_o and P_c . The mass, concentration and partial pressure for each species varies in time. This model treats the partial pressures for each species as the four unknown quantities.

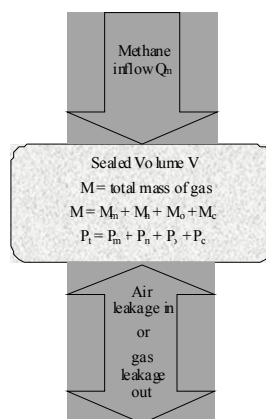


Figure 1 Volume, V , of sealed atmosphere containing total mass of gas, M , with constant CH_4 inflow rate and leakage in or out depending on barometric pressure.

2.2 Boundary Conditions

Figure 1 also indicates the two primary boundary conditions on the volume, namely, CH_4 inflow rate and leakage either in or out. The CH_4 inflow rate, Q_m , is the CH_4 volume liberated within the sealed atmosphere per unit time, and it has units of m^3/s . In addition to the CH_4 inflow rate, the model includes a N_2 inflow rate, Q_n , and a CO_2 inflow rate, Q_c , to simulate inert gas addition to the sealed atmosphere.

The model also considers coal oxidation and the related CO_2 production and O_2 depletion. These quantities depend upon the O_2 partial pressure and the rate constants r_o and r_c , which have units mass (O_2 or CO_2) per unit time per unit of O_2 partial pressure. This simple approximation of coal combustion is not intended to simulate spontaneous combustion. Full discussion of these additional model capabilities for inert gas addition and coal oxidation will appear in related papers.

The other boundary condition on the sealed atmosphere is leakage. Outside the sealed atmosphere, the barometric pressure denoted by $P_v(t)$ changes as a function of time. The gas quantity, Q_L , leaking through seals is defined as:

$$Q_L = L_c \sqrt{|P_i(t) - P_v(t)|} \quad (1)$$

where: L_c = leakage coefficient

$P_i(t)$ = total pressure of the sealed atmosphere,
and

$P_v(t)$ = barometric pressure outside sealed atmosphere.

When $P_i(t) < P_v(t)$ the seal is ingassing, i.e. air is flowing into the sealed atmosphere. Conversely, when $P_i(t) > P_v(t)$ the seal is outgassing, i.e. gases are flowing out of the sealed atmosphere. During an ingassing condition, the leakage quantity is air with composition of 79% N_2 and 21% O_2 . CH_4 and CO_2 , which are present in the mine atmosphere in small quantities, are neglected. During an outgassing condition, the leakage quantity has the composition of the sealed atmosphere.

This leakage quantity relationship is identical in form to the typical air flow relationship:

$$H = RQ^2 \quad (2)$$

where: H = head loss

R = resistance and

Q = flow quantity

Therefore, this leakage quantity relationship implies turbulent airflow. Stokes (1985) measured the air flow velocity and flow resistance through a longwall gob and concluded that turbulent flow relations applied. Depending on the magnitude of the leakage quantity, laminar flow may exist, and a linear leakage quantity relationship may apply; however, leakage quantity data measured by Weiss *et al.* (1993; 1996) tends to support the non-linear relationship used.

2.3 Assumptions

The Composition Change Model (CCM) shown in Figure 1 makes numerous critical assumptions:

1. Composition throughout the sealed atmosphere is homogeneous.
2. Mixing of any added gases, such as CH_4 , inert gas or air from leakage, occurs instantaneously and completely so that homogeneity of the sealed atmosphere is maintained at all times.
3. Temperature (T) is constant throughout the sealed atmosphere.
4. The volume (V) is constant.
5. Total pressure ($P(t)$) varies with time but is independent of location within the sealed atmosphere.
6. Leakage in and out of the sealed atmosphere is the sum of leakage through all seals, around all seals and through the rock surrounding the seals.
7. The composition of leakage inflow is that of air. The CH_4 concentration in the active mine atmosphere is neglected and assumed zero.
8. The composition of leakage outflow is identical to that of the sealed atmosphere.

The model does not consider any spatial dimensions or the geometry of the sealed atmosphere. Composition gradients into the sealed atmosphere due to leakage or point sources of gas are neglected. The sealed atmosphere is simply a volume with homogeneous composition governed by boundary conditions. This simple model, however, appears to be the first model of its kind for examining the composition of the sealed atmosphere and considering the main factors controlling that atmosphere. It may provide useful guidance for later, more complex models that properly consider spatial variations in composition.

2.4 Equations for the Composition Change Model

Based on the conservation of mass principle, and the ideal gas law, $P = \rho RT$ the following system of ordinary differential equations was developed to describe the composition of a sealed atmosphere.

For the ingassing condition where $P_i(t) < P_v(t)$

$$\frac{dP_m(t)}{dt} = \frac{\rho_m R_m T}{V} Q_m \quad (3)$$

$$\frac{dP_n(t)}{dt} = \frac{N_p \rho_n R_n T}{V} Q_{IG} + \frac{A_p \rho_n R_n T}{V} L_c \sqrt{|P(t) - P_v(t)|} \quad (4)$$

$$\begin{aligned} \frac{dP_o(t)}{dt} = & \frac{(1 - N_p) \rho_o R_o T}{V} Q_{IG} - \frac{r_o R_o T}{V} P_o(t) \\ & + \frac{(1 - A_p) \rho_o R_o T}{V} L_c \sqrt{|P(t) - P_v(t)|} \end{aligned} \quad (5)$$

$$\frac{dP_c(t)}{dt} = \frac{\rho_c R_c T}{V} Q_c + \frac{r_c R_c T}{V} P_o(t) \quad (6)$$

For the outgassing condition where $P_i(t) > P_v(t)$

$$\frac{dP_m(t)}{dt} = \frac{\rho_m R_m T}{V} Q_m - P_m(t) \frac{L_c}{V} \sqrt{|P(t) - P_v(t)|} \quad (7)$$

$$\frac{dP_n(t)}{dt} = \frac{N_p \rho_n R_n T}{V} Q_{IG} - P_n(t) \frac{L_c}{V} \sqrt{|P(t) - P_v(t)|} \quad (8)$$

$$\begin{aligned} \frac{dP_o(t)}{dt} = & \frac{(1 - N_p) \rho_o R_o T}{V} Q_{IG} - \frac{r_o R_o T}{V} P_o(t) \\ & - P_o(t) \left(\frac{L_c}{V} \right) \sqrt{|P(t) - P_v(t)|} \end{aligned} \quad (9)$$

$$\frac{dP_c(t)}{dt} = \frac{\rho_c R_c T}{V} Q_c + \frac{r_c R_c T}{V} P_o(t) - \frac{P_c(t)}{V} L_c \sqrt{|P(t) - P_v(t)|} \quad (10)$$

The variables and constants in these equations are defined as follows:

P_m , P_n , P_o and P_c are the partial pressures for CH_4 , N_2 , O_2 and CO_2 , respectively, as a function of time.

P = the total pressure or the sum of the partial pressures for each gas species and is a function of time.

P_v = the barometric pressure and is a function of time.

Q_m = the CH_4 inflow rate.

Q_{IG} = the N_2 inert gas inflow rate at purity N_p .

Q_c = the CO_2 inert gas inflow rate that is assumed to be 100% pure.

- N_p = the purity of the N_2 inert gas, which is usually in the range of 90 to 95%. The balance of the N_2 inert gas is assumed to be O_2 .
- A_p = the N_2 fraction in air leaking into a sealed volume and is assumed to be 79%. The balance is 21% O_2 . All other gases in the mine air such as CO_2 , water vapour, argon and other gases are neglected as insignificant.
- R_m , R_n , R_o and R_c are the specific gas constants for CH_4 , N_2 , O_2 and CO_2 , respectively.
- ρ_m , ρ_n , ρ_o and ρ_c are the gas densities at standard pressure and temperature for CH_4 , N_2 , O_2 and CO_2 , respectively.
- L_C = the leakage coefficient for the sealed volume.
- T = the temperature and is assumed constant.
- V = the sealed volume and is assumed constant.
- r_o and r_c are the rate of O_2 depletion and the rate of CO_2 production as a function of O_2 partial pressure.

3 MATLAB® Implementation of CCM

3.1 Computational Scheme

The system of ordinary differential equations for ingassing conditions (Equations 3 through 6) or outgassing conditions (Equations 7 through 10) have the following form:

$$\frac{dP_i(t)}{dt} = f_i(t, P_m(t), P_n(t), P_o(t), P_c(t), P_v(t)) \quad (11)$$

To integrate the ingassing and outgassing systems of differential equations, the fourth- and fifth-order-accurate Runge-Kutta method in MATLAB® was used. By this method, the next values in time for P_m , P_n , P_o and P_c are computed as:

$$P_m(t_{i+1}) = P_m(t_i) + \Delta t f_1(t_i, P_m(t_i), P_n(t_i), P_o(t_i), P_c(t_i), P_v(t_i)) \quad (12)$$

$$P_n(t_{i+1}) = P_n(t_i) + \Delta t f_2(t_i, P_m(t_i), P_n(t_i), P_o(t_i), P_c(t_i), P_v(t_i)) \quad (13)$$

$$P_o(t_{i+1}) = P_o(t_i) + \Delta t f_3(t_i, P_m(t_i), P_n(t_i), P_o(t_i), P_c(t_i), P_v(t_i)) \quad (14)$$

$$P_c(t_{i+1}) = P_c(t_i) + \Delta t f_4(t_i, P_m(t_i), P_n(t_i), P_o(t_i), P_c(t_i), P_v(t_i)) \quad (15)$$

where Δt = the time step,
 t_i = the current time step and
 t_{i+1} = the next time step.

A typical time step ranges from 50 to 500 seconds, depending on the problem.

Given the physical constants, input parameters, barometric pressure and initial conditions for partial pressures of CH_4 , N_2 , O_2 and CO_2 , the model calculates new values for the partial pressure of each gas species at future times, using both the ingassing and the outgassing sets of ordinary differential equations. The total pressure in the sealed atmosphere is then calculated as:

$$P_t(t_{i+1}) = P_m(t_{i+1}) + P_n(t_{i+1}) + P_o(t_{i+1}) + P_c(t_{i+1}) \quad (16)$$

Depending on whether the ingassing condition $P_i(t) < P_v(t)$ or the outgassing condition $P_i(t) > P_v(t)$ applies, the updated values for partial and total pressure are selected from the appropriate computation. Finally, the leakage volume in or out is computed with Equation 1.

3.2 Data Input for CCM

Figure 2 shows the data input interface in the CCM program. All units used by CCM are SI, i.e., kilogram, meter, second, Pascal for pressure and Kelvin for temperature. Major input parameters are the time step, the volume of the sealed atmosphere, leakage coefficient, CH_4 inflow rate and the initial volumetric concentration of the gas species. Other parameters include the gas constants, gas densities and the initial temperature, which are not normally changed by the user.

Figure 2 Input screen for Composition Change Model (CCM).

CCM uses a sine function to describe barometric pressure changes. Key parameters for this model include the average pressure, the maximum pressure change (amplitude), period and time offset for the sine wave. With this sine function, it is possible to consider longer-term barometric pressure changes from or low and high pressure weather systems as well as cyclic changes due to diurnal variations. A constant pressure case can be defined by setting the amplitude equal to zero. Constantly increasing or decreasing barometric pressure can be specified by setting the period very long and adjusting the time offset. It is also possible to input measured barometric pressure change data directly, and this option will be explored by further research.

3.3 Data Display from CCM

CCM creates three different plots of calculated data:

1. Gas species volumetric concentration versus time as shown in Figure 3.

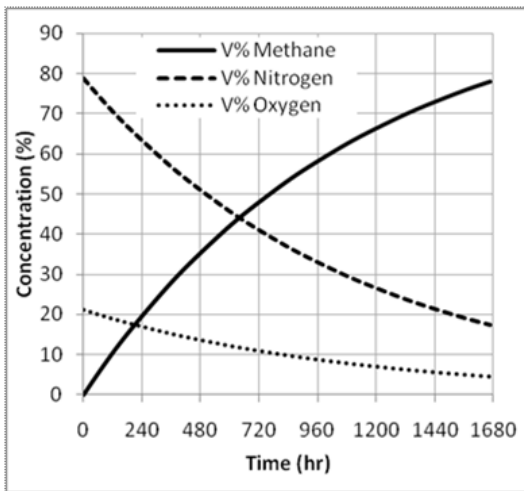


Figure 3 CH_4 , N_2 and O_2 concentration versus time for sealed atmosphere with $0.25 \text{ m}^3/\text{s}$ CH_4 inflow rate, $1,000,000 \text{ m}^3$ volume and $0.00625 \text{ m}^3/\text{s}/\text{Pa}^{1/2}$ leakage coefficient. CO_2 concentration remains zero. This example considers a non-reactive coal which does not consume O_2 or produce CO_2 .

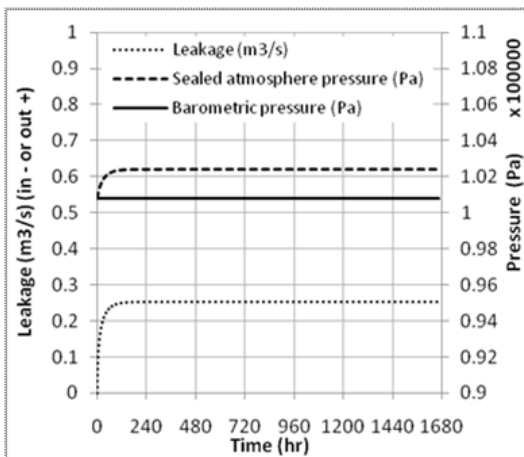


Figure 4 Leakage from and pressure within sealed atmosphere versus time with constant barometric pressure.

2. Leakage rate (Q_L), the barometric pressure and the sealed atmosphere pressure versus time as shown in Figures 4 and 5.
3. Leakage rate and pressure difference between the sealed atmosphere pressure and the barometric pressure versus time (not shown).

The user can manipulate the scales as the data dictates.

3.4 A Note on Rounding Errors and Time Step

CCM employs an explicit method for numerical integration of the system of ordinary differential equations. Depending on the time step set by the user, rounding errors can occur, leading to apparent numerical instabilities. These errors may arise when the system transitions from an ingassing to an outgassing condition or vice versa. To eliminate such errors, the MATLAB[®] code sets the leakage flow to zero when the absolute difference between the total seal pressure and the barometric pressure is less than 5 Pa.

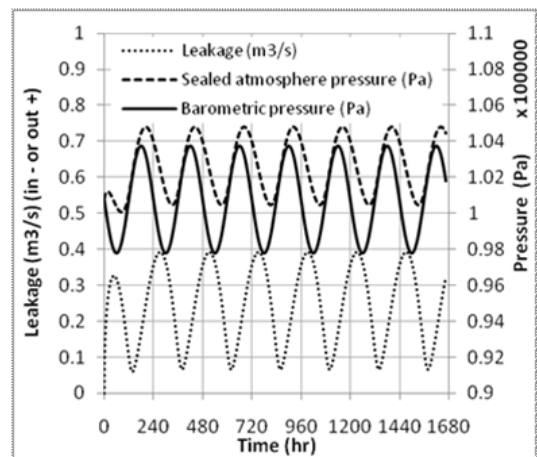


Figure 5 Leakage from and pressure within sealed atmosphere versus time with cyclic barometric pressure.

4 Estimating Input Parameters for CCM

Tables 1, 2 and 3 provide bounds for the major input parameters for CCM, namely, the volume V of the sealed atmosphere, the CH_4 inflow rate Q_m , and the leakage coefficient L_C .

Estimating the volume is a critical first step, and knowing the volume mined-out provides an upper bound for this parameter. Subsidence and flooding of mined-out areas can only decrease the volume from this upper bound estimate. The user should calculate the volume from a mine map, taking into account the mining history and mine subsidence. The volumes presented in Table 1 are based on typical coal mine dimensions and show that the volume may range from about 10^4 to 10^7 m^3 .

Immediately prior to sealing a volume, the CH_4 inflow rate is determined by measuring the CH_4 concentration difference between the concentration in the return and that in the intake air and the volume flow rate of the ventilating air. The CH_4 inflow rate used by CCM depends on the size of the sealed area and the CH_4 influx rate. Three CH_4 influx rates are defined, low, medium and high. At low, medium or high CH_4 influx rate a sealed atmosphere will reach a fuel-rich inert condition defined as 20% CH_4 by volume in 50, 10 or 2 days, respectively. Kingery & Dornenberg

(1957) provided measurements of the CH₄ influx rate into mined-out areas. Depending on the coal seam and the age of the mined-out volume, the CH₄ influx ranged from 0.018 to 3.76 m³/s/10⁶ m².

Table 1 Order of magnitude estimates for typical volumes in a coal mine.

Mined-out component	Volume range – m ³
Single entry – 1 to 5 km	10,000 to 50,000
3 entry gate road – 1 to 5 km	50,000 to 200,000
7 entry mains – 1 to 5 km	100,000 to 500,000
Room-and-pillar panel	50,000 to 1,000,000
Longwall panel	500,000 to 1,500,000
Approximate range	10,000 to 10,000,000

Table 2 Approximate ranges for CH₄ inflow rate Q_m.

Volume, m ³	Low influx rate, m ³ /s (50 days to > 20% CH ₄)	Medium influx rate, m ³ /s (10 days to > 20% CH ₄)	High influx rate, m ³ /s (2 days to > 20% CH ₄)
10,000	0.0005	0.0025	0.01
100,000	0.005	0.025	0.1
1,000,000	0.05	0.25	1
10,000,000	0.5	2.5	10

Table 3 Values for leakage coefficient into sealed atmosphere (Weiss *et al.*, 1993, 1996).

	Leakage quantity (m ³ /s)	Pressure differential (Pa)	Leakage coefficient (m ³ /s/Pa ^{1/2})
Lowest values measured at NIOSH	0.019	1000	0.0006
Old MSHA guideline for 140 kPa seals	0.047	250	0.0030

From an estimate of the CH₄ inflow rate obtained prior to sealing, measuring the time required to achieve a certain CH₄ concentration provides an approximate check on the volume estimate for the sealed atmosphere. The volume is estimated as:

$$V = \frac{t_c Q_m}{C_m} \tag{17}$$

where: Q_m = CH₄ inflow rate
C_m = CH₄ concentration at time t_c
t_c = time to achieve CH₄ concentration C_m.

This relation assumes that leakage in or out of the sealed atmosphere is negligible during the initial self-inertization phase immediately after seal construction and that the CH₄ concentration is uniform throughout the volume.

The leakage coefficient is used in Equation 1 to determine the gas quantity flowing in or out of a sealed area given the pressure differential across the seals. Weiss *et al.* (1993; 1996) used a method to estimate L_C from direct measurements of the leakage quantity through a test seal. In conducting the quantity measurements, researchers erected an airtight brattice curtain in front of the test seal

that had a 0.30 x 0.30-m hole cut into it to concentrate the flow. Using a vane anemometer to detect flow, researchers could measure flow quantities as low as 0.019 m³/s at differential pressure of up to 1,000 Pa. With this experimental setup, the smallest detectable value for the leakage coefficient is about 0.0006 m³/s/Pa^{1/2}.

Another method to measure the leakage coefficient for a sealed area uses indirect measurements of the leakage quantity developed from measurements of CH₄ concentration in the ventilating air upstream and downstream of a seals. For an outgassing set of seals, the leakage quantity flowing from the sealed atmosphere is

$$Q_L = \frac{(C_{mD} - C_{mU})}{(C_{mSV} - C_{mD})} Q_V \tag{18}$$

where: Q_V = ventilation airflow past a set of seals
C_{mU} = CH₄ concentration upstream of the set of seals
C_{mD} = CH₄ concentration downstream of the set of seals
C_{mSV} = CH₄ concentration within the sealed atmosphere.

Application of this method requires precision measurements of the CH₄ concentration using a gas chromatograph on air samples. Simple measurements with handheld methanometers may not have sufficient precision for reliable determination of Q_L.

Whether a direct or indirect measurement of leakage quantity from a sealed atmosphere is made, the leakage coefficient is calculated as:

$$L_c = \frac{Q_L}{\sqrt{\Delta P}} \tag{19}$$

where ΔP is the measured pressure differential between the sealed atmosphere and the mine atmosphere.

Prior to 2006, MSHA had guidelines for the allowable leakage through 140 kPa seals as constructed and evaluated within the NIOSH Lake Lynn Experimental Mine (Weiss *et al.*, 1993; 1996). With a 250 Pa pressure differential, the leakage through a single seal could not exceed 0.047 m³/s. These obsolete guidelines implied a leakage coefficient less than 0.0030 m³/s/Pa^{1/2}. For multiple seals, the leakage coefficients of each seal are added to determine the total leakage coefficient.

5 General Behaviour of Sealed Atmospheres as Computed with CCM

Based on the input parameters shown in Figure 2, CCM calculated the concentration and partial pressure for each gas species as a function of time. The volume is 1,000,000 m³ which is typical of several open room-and-pillar panels. The CH₄ inflow rate is 0.25 m³/s which is considered a medium influx rate for this sealed atmosphere. At this inflow rate, the sealed atmosphere should reach a CH₄ concentration of 20% in about 9.3 days, as long as the leakage in or out of the sealed

atmosphere is small. The assumed *total* leakage coefficient is 0.00625 m³/s/Pa^{1/2}, which implies a tight set of seals.

Figure 3 shows the calculated concentration for each gas species versus time. As expected, the CH₄ concentration reaches 20% in about 240 hours (10 days). After 70 days, the concentration has reached 80% and the rise rate has decreased. N₂ and O₂ concentrations fall steadily and maintain a constant ratio of about 4-to-1, the same as the initial conditions. CCM calculations with a low or high CH₄ influx rate produce calculated concentration behavior similar to that shown in Figure 3, except the time to reach 20% CH₄ is longer or shorter, respectively. Note that CO₂ concentration remains zero, because the rate constants *r_o* and *r_c* are zero. This example does not consider a reactive coal.

Figure 4 shows the calculated leakage from the sealed atmosphere and the calculated pressure within. Also shown is the specified barometric pressure, which is assumed constant at 100,765 Pa. With the constant CH₄ inflow rate of 0.25 m³/s, the pressure within the sealed atmosphere must rise by some amount to drive an equivalent leakage volume. As expected, the leakage out from the sealed atmosphere reaches a constant value of slightly more than 0.25 m³/s in about 120 hours (5 days), and the sealed atmosphere pressure stabilizes at 102,365 Pa. The small difference between CH₄ inflow rate and leakage out of the sealed atmosphere arises due to density difference between CH₄ and the general sealed atmosphere.

6 Barometric Pressure Change Effects with CCM

In the previous calculations with CCM, barometric pressure remained constant at one standard atmosphere. Changes in the barometric pressure can cause a sealed atmosphere to outgas when the barometric pressure falls or to ingas when it rises. This section briefly examines how barometric pressure changes affect the sealed atmosphere.

Table 4 Range for variations in barometric pressure.

Cause of barometric pressure change	Period	Pressure change			
		mbars	In. Hg	In. H ₂ O	Pa
Diurnal variation	1 day	3–4	0.09–0.12	1.2–1.6	300–400
Weather systems	2–5 days	17–34	0.5 – 1.0	7–13	1,700–3,400
Severe storms	2–10 hours	34–68	1.0–2.0	13–27	3,400–6,800
Severe hurricane	2–5 days	166	5	68	16,600

Table 4 summarizes the range of barometric pressure variations for a variety of causes and the approximate time period or duration for each change. Low and high pressure weather systems can change the barometric pressure up to about 3,400 Pa (1 inch Hg) over a few days, while severe storms or passing weather fronts can induce pressure changes up to about 6,800 Pa (2 inch Hg) in a few hours. The worst case is that of a hurricane, which could depress

the barometric pressure by up to 16,600 Pa (5 inch Hg). To examine these pressure change effects, researchers input the cyclic barometric pressure function defined in Figure 2. Over a period of 10 days, pressure rises by 6,000 Pa and then falls by the same amount, simulating a series of severe storm systems.

Figure 5 shows the calculated leakage, calculated sealed atmosphere pressure and the prescribed barometric pressure versus time. The calculated CH₄ concentration versus time within the sealed atmosphere with the cyclic barometric pressure change did not differ substantially from that shown in Figure 3 where the barometric pressure remained constant. As shown in Figure 5, the peak sealed atmosphere pressure lags the peak barometric pressure by about 24 hours. The sealed atmosphere pressure remains greater than the barometric pressure at all times in this case, so the sealed atmosphere outgases continuously. The outgassing leakage rate ranges from about 0.06 to 0.39 m³/s, and as expected, averages about 0.25 m³/s.

This calculation demonstrates that if the leakage coefficient for a sealed atmosphere is less than a certain threshold, the sealed atmosphere can tolerate a substantial barometric pressure change and still outgas continuously.

7 Tentative Design Principles

The Composition Change Model (CCM) shows how the sealed atmosphere changes in composition upon sealing from air to a self-inert state given sufficient time, a nominal CH₄ inflow rate and a reasonable leakage coefficient. On average, the CH₄ volume flowing into a sealed atmosphere must equal the leakage volume flowing out. CCM shows that because of the CH₄ inflow, the sealed atmosphere not only tends to become self-inert, but it also tends to re-pressurize slightly in order to drive the natural outgassing. Therefore, by designing seals and sealed atmospheres to minimize the leakage rate, it appears possible to create sealed atmospheres that become self-inert and remain inert by design. An atmosphere that is inert by design would minimize the explosion hazard from sealed areas.

The suggested steps necessary to design a sealed atmosphere to become inert and remain inert are as follows. A design example based on prior calculations in this paper is also provided.

1. Estimate the volume V and the CH₄ inflow rate Q_m prior to sealing. For this design example, V = 1,000,000 m³ and Q_m = 0.25 m³/s.
2. Estimate the time required to become fuel-rich inert with a CH₄ concentration greater than 20%. In this case that time is 10 days.
3. Determine a design barometric pressure change and time period based on typical conditions at the site. This decision dictates how much barometric pressure change that the sealed atmosphere must withstand and still continue to outgas. In this example, the design pressure change is 6,000 Pa decrease over 5 days, as was used in the prior calculations.

4. Estimate the design leakage coefficient as $L_c = Q_L / \sqrt{\Delta P}$ where $Q_L \approx Q_m$. In this example, maximum L_c is estimated as $0.0032 \text{ m}^3/\text{s}/\text{Pa}^{1/2}$, based on leakage coefficients presented in Table 3.
5. Calculate the actual design leakage coefficient. Using CCM to calculate the response of the sealed atmosphere to changes in barometric pressure, the maximum allowable leakage coefficient L_c is calculated as $0.01 \text{ m}^3/\text{s}/\text{Pa}^{1/2}$. With this maximum value for L_c , the sealed atmosphere always remains in an outgassing condition even under a barometric pressure decrease of 6,000 Pa over a 5 day period. Figure 5 shows leakage calculations for an L_c of $0.00625 \text{ m}^3/\text{s}/\text{Pa}^{1/2}$, and the sealed atmosphere always remains in an outgassing condition.
6. Design seals to meet the maximum allowable leakage coefficient $L_c = 0.01 \text{ m}^3/\text{s}/\text{Pa}^{1/2}$. This leakage coefficient represents the total leakage quantity emanating from a sealed atmosphere. If multiple seals are used to create a sealed atmosphere, the sum of the leakage coefficients for each seal must be less than the maximum allowable L_c . The earlier MSHA guidelines for evaluating 140 kPa seals at the NIOSH Lake Lynn Experimental Mine implied a leakage coefficient of $0.0030 \text{ m}^3/\text{s}/\text{Pa}^{1/2}$. In this design example, up to 3 such seals could be used to create the sealed atmosphere. New seals designed to withstand higher explosion pressure should have even lower leakage coefficients; however, no data is available at this time.
7. If by design, the sealed atmosphere is inert, the 345 kPa standard may apply. The sealed atmosphere will require monitoring of the composition until it becomes inert and the seal reaches its design strength. After the sealed atmosphere becomes self-inert, periodic monitoring is required to demonstrate that it remains inert and outgases continuously as designed. A differential pressure gauge installed through a seal can show that the sealed atmosphere is outgassing and therefore remains inert.

8 Conclusions

Using the conservation of mass principle, researchers present a theoretical mathematic model called CCM that describes how CH_4 , N_2 , O_2 and CO_2 concentrations change within a sealed atmosphere in response to gas inflow rates, leakage in or out and barometric pressure changes. Application of the model shows that because of the CH_4 inflow, sealed atmospheres tend to become fuel-rich and inert naturally if leakage in or out of the sealed atmosphere is controlled. A sealed atmosphere that is inert by design would minimize the explosion hazard in sealed areas.

CCM may help interpret and understand measurements of the atmospheric composition within sealed atmospheres. Engineering sealed atmospheres to become inert and remain inert through leakage-control-based design may lead to greater safety by preventing potentially explosive mixtures from ever developing within sealed atmospheres.

9 Disclaimers

The findings and conclusions in this report are those of the authors and do not necessarily represent the views of the National Institute for Occupational Safety and Health. Mention of any company or product does not imply endorsement by NIOSH.

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