Predictive Modelling of Concentration of Dispersed Natural Gas in a Single Room

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Abstract

This paper aimed at developing a mathematical model equation to predict the concentration of natural gas in a single room. The model equation was developed by using theoretical method of predictive modelling. The model equation developed is as given in equation 28.

The validity of the developed expression was tested through the simulation of experimental results using computer software called MathCAD Professional. Both experimental and simulated results were found to be in close agreement. The statistical analysis carried out through the correlation coefficients for the results of experiment 1, 2, 3 and 4 were found to be 0.9986, 1.0000, 0.9981 and 0.9999 respectively, which imply reasonable close fittings between the experimental and simulated concentrations of dispersed natural gas within the room. Thus, the model equation developed can be considered a good representation of the phenomena that occurred when there is a leakage or accidental release of such gas within the room.

Keywords

Natural gas, Dispersion, Modelling, Simulation and Correlation coefficient

Introduction

The possibility of a release of natural gas within a single room depends upon the flow rate. Such continuous release may result in its build up, thus resulting into a gas-air mixture 3]. The ignition of such an accumulated flammable mixture may cause a very serious physical damage to the properties, injury or death to anyone in the vicinity. [3]

Natural gas is a flammable gaseous mixture consisting mostly of hydrocarbons (chemical compounds that contain carbon and hydrogen). [2] Along with coal and petroleum, natural gas is a fossil fuel that contains about 85% methane (CH_4), 10% ethane (C_2H_6) while propane (C_3H_4), butane (C_4H_{10}), pentane (C_5H_{12}) and other alkane present in small proportions made up the remaining percentages. Natural gas, which is usually found together with petroleum deposits, when extracted and refined into fuels that provide approximately 25 percent of the world energy supply. This reason, therefore, gave natural gas more consideration as a domestic source of energy in the homes. [2]

Apart from when the natural gas is being used as a source of energy, for example, cooking in homes, which is ideological controlled. Its uncontrolled release may be attributed to some accidental reasons such as tube leakages (rupture). However, literature revealed that certain researches have been carried out in these areas most especially, as regards the modelling of natural gas release within the accidental areas. Hill & Pool (1998) developed a model for the build and dispersion of natural gas in a house. This work gave more emphasis to the build ups of natural gas.

[14] developed a model that provides tools to enable one to assess human exposure to chemicals emitted by domestic appliances. This model based its approach on the level of contact, exposure and uptake. The model gave a general framework that joins the particular exposure and uptake together.

Considering the past works carried out so far on the release of natural gas in a single room, little or nothing has been said on the concentrations of natural gas dispersion. Obviously, when natural gas is released, its concentration changes as it disperses. It is therefore desired, in this work, to obtain a mathematical equation that can represent the concentration of dispersed natural gas in a single room wit respect to time. This can be achieved through the realization of the following objectives:

- Collection of data on the concentrations of a natural gas released in a single room with respect to variable such as time.
- Development of a mathematical model equation to predict concentration of dispersed gas within a single room with time.
- Simulation of the model equation using MathCAD software.
- Compare the simulated and experimental results.

On completion of this project, the model equation can be used to predict the concentration of the natural gas released at any given time within a residential area. Therefore enable us to projects and come up with policies that can assist in eliminating and preventing any danger or accident that may arise from the release and dispersion of such gases within the residential areas.

Methodology

Experimental determination of dispersion of natural gas in a single room [3]

The majority of release experiments consisted of a build up phase, during which gas builds up was measured within each room in the house, and a decay phase when the gas in mixture was left to dispersed under the influence of natural ventilation provided by opening specific window/doors within the property.

The typical experiment began by initiating the computer program which logged the build-up phase and opening the electrical control valve to enable the gas to flow into the test room. The rate of flow into the single room was regulated to a pre-determined value using a rotameter. Once this flow had stabilised, the rotameter was checked periodically using a dedicated video camera to ensure no significant fluctuation in flow rate occurred during a test.

When sufficient data on the build up of a gas had been collected, the electric control valve was turned off and the time noted for which gas has been released. The computer program recording the build-up phase information was then turned off.

Within the test house, the build-up of the gas was monitored using up to 49 sample line positions using probes attached to stands. Each sample stand has 7 sample probes installed to provide measurements of gas concentration at positions on a vertical axis between the floor and the ceiling in each room. The probes were sampled sequentially via a stream selection unit controlled by a computer-based data logging/analysis system. The time taken to measure the gas concentration in each sample was 20s, and in order to accommodate such a large number of sample probes, two computer-based logging/analysis systems were employed thereby reducing the time taken to sequence through and log all the data.

A total of seven sample stands were employed for the majority of experiments. Data from four stands were logged using one data logging/analysis system whilst a second system recorded data from the other three. As this arrangement caused a complete cycle of the sample probes to take a different time on each system, the concentration-height profiles used to determine the distribution of gas-air mixture were generated by re-calculating the linearly interpolated concentrations determined using the system logging three sample stands in order to provide a set of profiles plotted at times similar to those obtained using the other system.

Modelling and Simulation Methodology

The proposed model equation was developed using the work developed by Shepherd (2002) as the basis. Simulation of the developed model was carried out with the aid of computer software called MathCAD 2000 Professional, while Spreadsheet Program was used to analyze the results to determine their conformities with the experimental results. (Giwa, 2004)

Conceptualization of Modelling

Modelling of Concentrations of Natural Gas in a Room and Assumptions

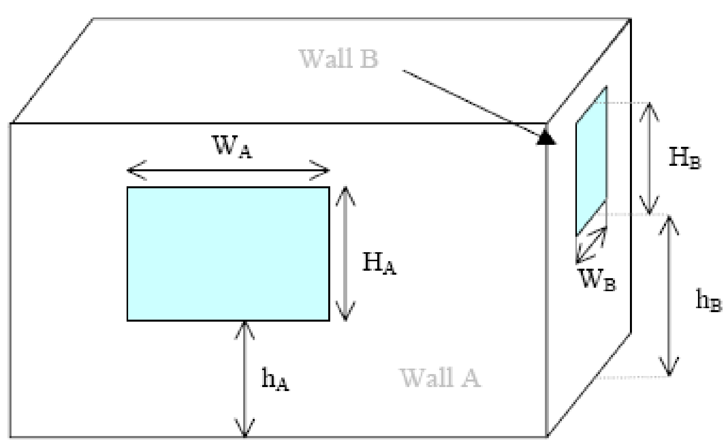

Figure 1. *Schematic diagram of the test room*

In order to develop a good mathematical model that can be used to determine the concentration of a natural gas in a single room, a series of assumptions were made and these include:

- The room dimensions are that of a cuboid. If a room of complex geometry is to be modelled then a set of regular pseudo-dimensions should be calculated to maintain the correct room surface area and volume.
- Calculations are performed assuming a homogeneous mixture. The natural gas phase is then re-distributed to be below the datum height, thus increasing the concentration in this layer, due to the smaller volume. These modified concentrations are used for the ventilation calculations.
- Pressurised liquid natural gas enters the room at ambient (storage) temperature.
- The room may be defined to have many combination of openings to the environment up to a maximum of four (one in each wall, labelled A, B, C)
- The ideal gas law applies to the gas/air mixture in the room.
- Initially the room is full of air under ambient conditions, and is therefore in thermal equilibrium with the environment.
- If the external pressure at an opening is greater than the room pressure, then fresh air will enter the room at ambient temperature.
- If the external pressure at an opening is less than the room pressure then, depending upon the position of the dense gas layer relative to that opening, natural gas/air mixture or air at the room temperature will be vented.
- All physical properties of air and the methane are assumed to remain constant.

Development of the Model Equation

During the transient, it is possible that conditions within the room may change from being unsaturated to being saturated. Thus, an equation describing the rate of change of concentration of natural gas is required to determine the concentration of the natural gas in a single room [15].

The basis for the formulation of the model equations is that there are three constituent mediums contributing to the room volume; these are the components in gaseous and liquid phases (M_g and M_l) and ambient air (M_a). These are such that the total mass within the room (M_t) is given by (Shepherd, 2002):

$$M_g + M_l + M_a = M_t \tag{1}$$

Or dividing through by M_t, equation 1 becomes

$$\frac{M_g}{M_t} + \frac{M_l}{M_t} + \frac{M_a}{M_t} = \frac{M_t}{M_t} \tag{2}$$

That is,

$$\frac{M_g}{M_t} + \frac{M_l}{M_t} + \frac{M_a}{M_t} = 1 \tag{3}$$

Denoting mass fraction by 'c', equation 3 can be written as:

$$c_g + c_l + c_a = 1 \tag{4}$$

The pressure in the room is assumed to be related by the ideal gas law to the average molecular mass, the density of the gaseous mixture and the temperature in the room (from assumption v). Hence:

From:

$$PV = nRT \tag{5}$$

Assuming a unit (1) mole of the gas:

$$PV = RT \tag{6}$$

and, since:

$$\rho = \frac{M}{V} \tag{7}$$

$$V = \frac{M}{\rho} \tag{8}$$

Substituting for V in the gas law gives:

$$P = \frac{M}{\rho} = RT \tag{9}$$

Making P, pressure, the subject of the formula

$$P = \frac{\rho RT}{M} \tag{10}$$

Now, for the gaseous mixture,

$$P = \frac{\rho_{ga} RT}{M_{ga}} \tag{11}$$

The average molecular mass of the gaseous mixture in the room is given by:

$$m_{ga} = x.m_g + (1 - x).m_a = x.(m_g - m_a) + m_a \tag{12}$$

where the volumetric concentration of gas in the gas/ air mixture, χ, is given in terms of the mass fractions c_g and c_l as [15]:

$$x = \frac{m_a . c_g}{m_g(1 - c_l) - c_g.(m_g - m_a)} \tag{13}$$

Therefore the average molecular mass of the gaseous mixture in the room is given by [15]:

$$m_{ga} = \frac{m_a . m_g(1 - c_l)}{m_g(1 - c_l) - c_g.(m_g - m_a)} \tag{14}$$

The average density of the mixture can be obtained by considering the mass of the gaseous natural gas / air mixture. This may be derived by two similar approaches, i.e. (Shepherd, 2002)

$$M_{ga} = c_{ga}.M_t = (c_g - c_a).M_t = (1 - c_l).\rho_t V_r \tag{15}$$

$$M_{ga} = \left[V_r - \frac{M_l}{\rho_l}\right].\rho_{ga} = V_r\left[1 - c_l.\frac{\rho_t}{\rho_l}\right].\rho_{ga} \tag{16}$$

Equating (15) and (16) yields an expression describing the average density of the gaseous natural gas/air mixture, i.e.

$$\rho_{ga} = \frac{(1 - c_l).\rho_t.\rho_l}{\rho_l - c_l.\rho_t} \tag{17}$$

Application of the law of conservation of mass generates an equation for the rate of change of mass of the liquid phase gas.

$$\frac{d}{dt} M_l = (1 - F_f).M.M_e \tag{18}$$

'F_f ' describes the flash fraction - the proportion of natural gas that 'flashes off' due to sudden expansion when the material experiences a violent change in pressure as it enters the room. Hence the initial term on the right hand side of Equation (18) describes the contribution of liquid phase natural gas to the room. The 'M_e' term represents the rate of evaporation to the vapour phase from any pool formed on the floor of the room or contained within the bounds of a bund wall.

The mass of liquid component may be written in terms of the liquid mass fraction and the total density of the room contents, i.e.:

$$M_l = V_r.\rho_t.c_l \tag{19}$$

Differentiating (19) with respect to time and inserting into (18) yields:

$$V_r.\left[\rho_t.\frac{d}{dt}c_l + c_l\frac{d}{dt}\rho_t\right] = (1-F_f).M - M_e \tag{20}$$

The rate of change of natural gas mass in the gas phase is governed by the flash fraction, the amount of material that vaporises or evaporates from the pool, and the fraction discharged through the openings (if any) and/or the scrubber unit.

$$\frac{d}{dt}M_g = F_f.M + M_e - c_g.(M_{outg} + M_{scg}) \tag{21}$$

Where, M_{outg} and M_{scg} are defined as the total discharge rates of the air/natural gas mixture through all openings, and the scrubber unit respectively.

As in Equation (19), the mass of gaseous natural gas may be written in terms of the vapour mass fraction and total room density:

$$M_g = V_r.\rho_t.c_g \tag{22}$$

Differentiating (13) with respect to time and inserting into (12) gives:

$$V_r.\left[\rho_t.\frac{d}{dt}.c_g + c_g.\frac{d}{dt}\rho_t\right] = F_f.M + M_e - c_g.(M_{outg} + M_{scg}) \tag{23}$$

The rate of change of air is determined by establishing whether fresh air is entering the room or air (as a constituent part of the gas/air mixture) is leaving the room through at least one opening or the scrubber unit, i.e.

$$\frac{d}{dt}M_a = M_{in} - c_a.(M_{outg} + M_{scg}) \tag{24}$$

Where, 'M_{in}' is defined as the rate of fresh air intake through individual openings A, B, C and D, from the environment.

Once again, the mass of air may be written in terms of the natural gas concentrations, via Equation (4).

$$M_a = V_r.\rho_t.c_a = V_r.\rho_t.(1-c_g-c_l) \tag{25}$$

Hence, differentiation of (25) with respect to time and insertion into (24) provides:

$$V_r.\left[(1-c_g-c_l).\frac{d}{dt}\rho_t\right] - \rho_t.\frac{d}{dt}c_g - \rho_t.\frac{d}{dt}c_l = M_{in} - (1-c_g-c_l).(M_{outg} + M_{scg}) \tag{26}$$

Addition of (20), (23) and (26) enables an equation to be formulated for the rate of change of total density:

$$\frac{d}{dt}\rho_t = \frac{1}{V_r}.\left[M + M_{in} - c_g.(M_{outg} + M_{scg}) - (1-c_g-c_l).(M_{outg} + M_{scg})\right] \tag{27}$$

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This may then be substituted back into Equation (23) to formulate the rate of change of natural gas as:

$$\frac{d}{dt}c_g = \frac{1}{V_r.\rho_t}.(F_f - c_g).M + M_e - c_g.\left[M_{in} + (1 - c_g).(M_{outg} + M_{scg}) + (c_l + c_g - 1).(M_{outg} + M_{scg})\right] \quad (28)$$

In summary, equation (28) represents the model equation developed for the determination of the concentrations of natural gas in a room.

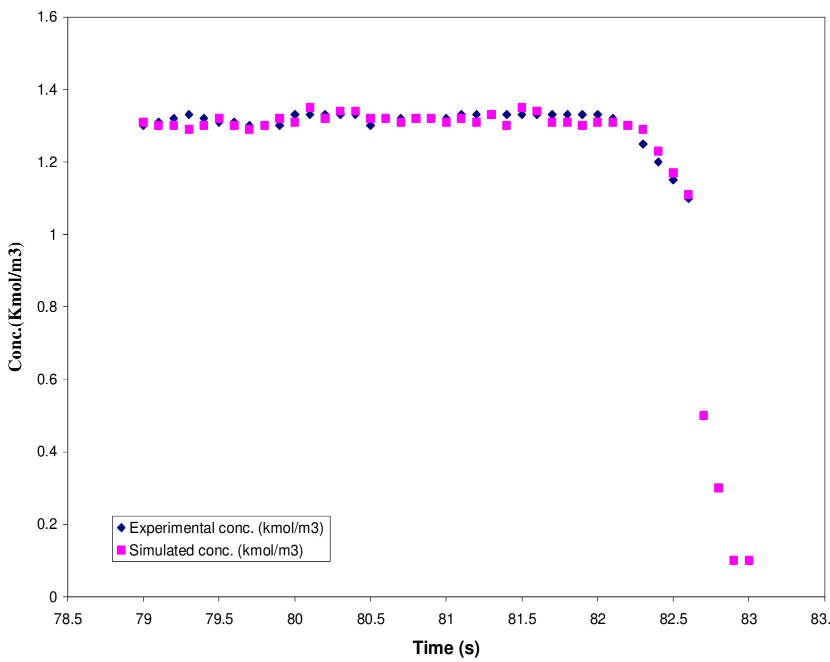

Figure 2. *Variation of Concentration with Time for Test 1*

Experimental result for test 1 (Figure 2), indicates that as time increases, the concentration of dispersed natural gas in the single room does not have a defined response pattern (fluctuates). For example, when the time was 79 seconds, the concentration of dispersed natural gas in the room was 1.30kmol/m^3 and when the time increased to 81 seconds, the concentration also increased to 1.32kmol/m^3 but the concentration decreased to 1.31kmol/m^3 when the time was increased to 83 seconds. So, it can be observed that the concentration first increased as the time increased while it (the concentration of natural gas in the single room) later decreased when the time of dispersion increased further. The same trends of fluctuation between the time of dispersion and the concentration of natural gas in the single room were observed in the remaining three tests. The fluctuation in the concentration of natural gas in the single room can be attributed to the fact that at the beginning of the experiment there was a fixed quantity of natural gas, while the effect of the velocities of the wind in the room at the different times of the experiment also can not be ignored.

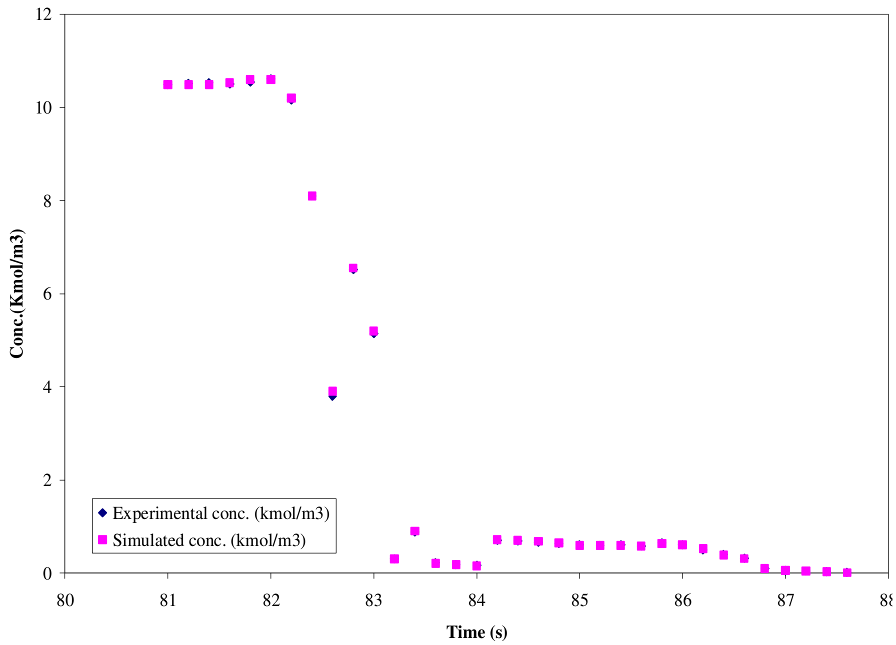

Figure 3. *Variation of Concentration with Time for Test 2*

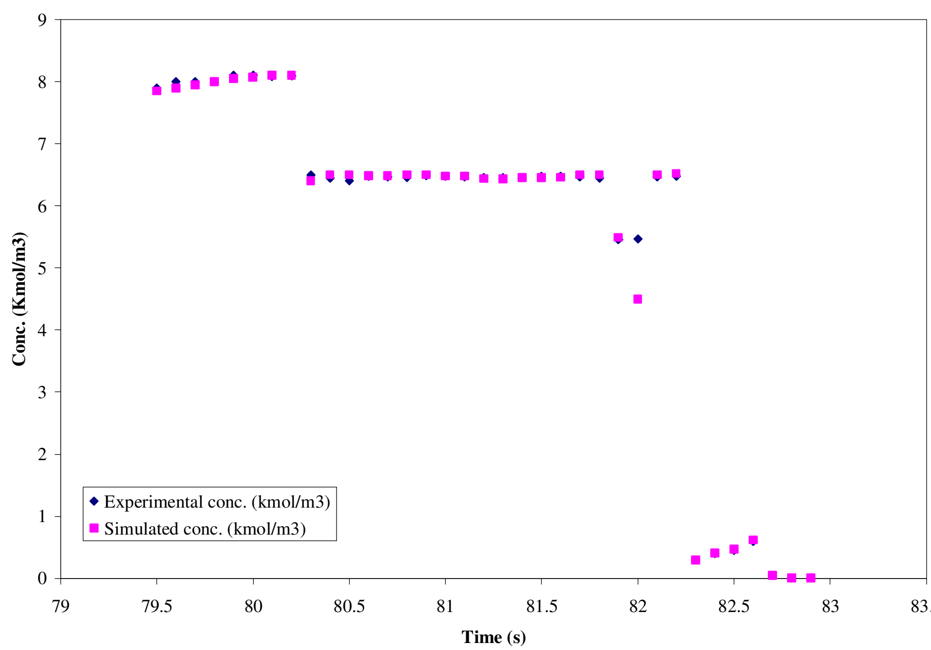

Figure 4*. Variation of Concentration with Time for Test 3*

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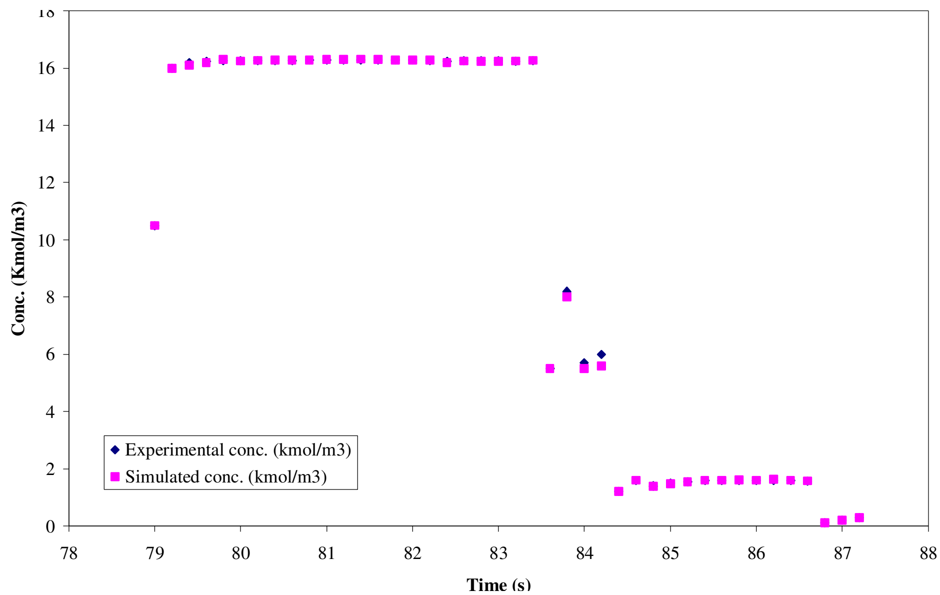

Figure 5. *Variation of Concentration with Time for Test 4*

Results and Discussion

A mathematical model equation for the prediction of concentration of dispersed natural gas in a single room (Equation 28) was developed. The equation shows the concentration of dispersed natural gas in a single room as a function of time of dispersion of the gas within the room.

Figure 2 to 5 shows the experimental and simulation results of dispersion of natural gas in a single room for four different tests carried out.

From the results, it will be noted that the time of dispersion starts at different times for the four different experiments. For instance, for experiment 1, the time of dispersion started at 79 seconds, while that of experiments 2, 3 and 4 started at 81, 79.5 and 79 seconds respectively. The difference in the time of dispersion of this natural gas as indicated in the four different experiments carried out can be attributed to the effect of wind on the dispersion of natural gas in the single room.

However, a mathematical model equation was developed for determining the concentration of dispersed natural gas in a single room with respect to time. The validity of the model was tested through the simulation of experimental results using computer software, MathCAD Professional.

Figure 2 to 5 show the simulated results obtained for the concentration of dispersed natural gas as a function of time in a singe room for four tests. The simulated concentration of dispersed natural gas in the single room was found to follow the same pattern as in the experimental results. For instance, when the time was 79 seconds, the concentration of natural gas was 1.31 kmol /m^3 for the first experiment while 1.32 kmol /m^3 was the concentration of natural gas in the room when the time was 81.10 seconds. The concentration decreased to 0.1 kmol /m^3 further, when the time increased to 83 seconds.

The comparisons between the experimental and simulated results as shown in Figure 2 to 5 indicated that there was reasonable level of agreements between the experimental and simulated results. For instance, for test 1, when the time was 79 seconds, the concentration of dispersed natural gas in the room was found to be 1.30 and 1.31 kmol/m^3 for experimental and simulated results respectively. When the time was 81 seconds, the results were found to be 1.32 and 1.31 kmol/m^3 for the experimental and simulated results respectively.

The validity of the model equation developed was tested through the statistical analysis of the results by calculating the correlation coefficients. The values of correlation coefficients obtained using MathCAD Professional for tests 1, 2, 3 and 4 were found to be 0.9986, 1.0000, 0.9981 and 0.9999 respectively. The analysis showed that there is a reasonable level of agreement between the experimental and simulated results for the four tests because the values of the correlation coefficients were very to unity (1).

In conclusion, since the correlation coefficients for the results of experiment 1, 2, 3 and 4 were calculated to be 0.9986, 1.0000, 0.9981 and 0.9999 respectively, which imply reasonable close fittings between the experimental and simulated results as a function of time, then, the model equation developed can be considered a good prediction of the real system.

Conclusion

The experimental analysis shows that the concentration of dispersed natural gas in a single room initially increases, with increasing time, constant, later decreases with time. That is, no define regular response pattern. This may be attributed to the effect of wind velocity and the quantity of the gas available at the beginning of the analysis.

However, a mathematical model equation to predict the concentration of dispersed natural gas was developed. The model was simulated using MATHCAD Professional. The results obtained and the statistical analysis carried out through the correlation coefficient showed that the model developed is a good mathematical expression that can represent the real system.

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