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Sizing of Explosion Pressure Relief for Gases with Low K_G Values using the Efflux Function

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Determination of deflagration venting requirements in chemical/process plants is usually carried out using well established standards employing an empirically based formula. However, this formula is shown to have severe shortcomings in the range of low K_G-values, where either negative or inconceivably large venting areas can be predicted. Due to these shortcomings a method has been developed using the efflux function for gases as a basis to predict the mass flow through a vent opening in a vessel during an internal explosion. The simulated rise in pressure due to the internal explosion is quantitatively determined from the K_G value, with the mass flow through the vent opening in the vessel resulting from the pressure difference between the vessel and its surroundings. This enables the maximum overpressure as a function of the pressure relief surface area to be predicted. The method takes account of the temperature of the efflux gases, and turbulence enhancement brought about by the venting process. The development, validation and limitations of this new method are presented along with suggestions for its further development.

1. Introduction

An area in the literature in which little work has been carried out is the vented deflagration of gases with low K_G values (i.e. ≤ 50 bar·m·s^{-1}). The safe handling of such gases are of extreme importance to many processes, a prominent example of which is the partial oxidation reaction. The product gas from such a reaction is normally a mixture of a combustible or mixture of combustibles in an oxygen depleted atmosphere. After leaving the reaction zone these gases are often further processed by heat exchangers, secondary reactors, condensers, separation equipment and their associated pipework, all of which requires protection from the overpressure associated with an unwanted explosion. Due to the shortcomings of the EN 14994 (2007) and NFPA 68 (2007) methodologies, the current method was developed in order to better describe the venting requirements of gases with low K_G vales. However, this method, after adaptation and appropriate validation, should be suitable for the determination of venting areas for the protection against any deflagration (i.e. also K_G > 50 bar·m·s^{-1}), assuming the explosion properties of the gas mixture are known. Both of the aforementioned standards use an equation, also known as the Bartknecht formula (Bartknecht, 1993), to determine the required venting area based on the reduced explosion pressure (p_{red} / barg), the static activation pressure of explosion venting (p_{stat} / barg), the volume of the vessel to be vented (V / m^3) and the K_G value of the mixture.

2. Shortcomings of the Bartknecht formula at low K_G values

There are a number of constraints attached to the application of the EN 14994 and NFPA 68 methodologies. The methodologies are said to be valid for K_G ≤ 550 bar·m·s^{-1}, which represents the normalised rate of pressure rise for hydrogen, as measured at the time of the development of the Bartknecht formula. Using the current EN 13673 standard (2003) for the determination of explosion properties, the reported K_G of hydrogen is approximately 850 bar·m·s^{-1}. This trend is also true for methane and propane, which at the time of the development of the Bartknecht formula had K_G values of 55 and 100 bar·m·s^{-1} respectively, but according to current standards have K_G values of 64 and 120 bar·m·s^{-1}

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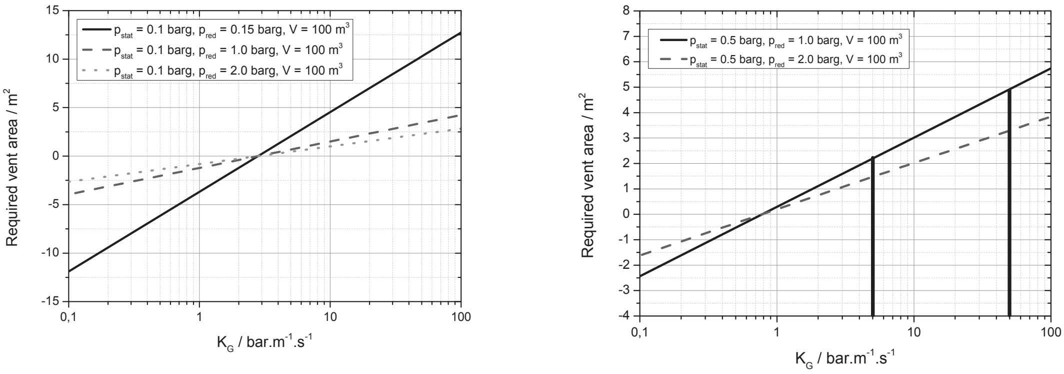
respectively. In the first instance this leads to the conclusion that, if using the Bartknecht formula for gases with K_G values determined using the latest standards, a conservative result will be obtained. Another criticism is the relevance of this upper limit, as due to the propensity of gases with high K_G values to undergo the transition to detonative modes of burning, in many cases it is impractical to employ explosion venting for all but the simplest of systems (i.e. without any potential turbulence enhancing elements).

Although there is no lower limit it is thought unlikely that the EN 14994 and NFPA 68 methodologies have been comprehensively validated against gases with low K_G values ($\leq$ 50 bar·m·s^{-1}), proof of this can be seen in Figure 1 (a), which shows the predicted venting areas, using the Bartknecht formula, as a function of K_G. Below K_G values of approximately 3 bar·m·s^{-1} the formula yields negative results. Whilst gases with K_G values as low as 3 bar·m·s^{-1} are unlikely to be used in practice it should not be the case that the formula can yield negative venting area, and if so then a lower boundary for the applicability of the formula must be given.



(a) (b)

Figure 1: Required venting area as predicted by the EN 14994 and NFPA 68 methodologies as a function of the K_G value for (a) reduced pressures of between 0.15 and 2 barg, and (b) reduced pressures of between 1 and 2 barg, horizontal lines mark the K_G values of 5 and 50 bar·m·s^{-1}.

Another seemingly strange result is obtained when comparing the venting requirements of gases with 5 and 50 bar·m·s^{-1}, as shown in Figure 1 (b). The resulting required venting area for the gas with a K_G value of 50 bar·m·s^{-1} is only twice the required venting area for a gas with a K_G value of 5 bar·m·s^{-1}, despite the rate of pressure rise being ten times higher. Several other criticisms have been directed at the Bartknecht formula recently, suggesting that for the EN 14994 and NFPA 68 methodologies the disparity between predicted and measured reduced pressures is much larger than that obtained with other simple methodologies. Due to these shortcomings it was realised that there was a need for an improved, but still easy to apply, methodology capable of reliably predicting venting requirements for gases with low K_G values, based not just on simple empirical formulae, but also on first principles.

3. Prediction of venting requirements using the efflux function for gases

In order to determine the size of rupture disks for mixtures with low K_G values, the efflux function for gases was utilized. Firstly the expansion of the hot reaction gases during an explosion, which causes the pressure rise in the closed vessel, was simulated by the generation of new gas (i.e. gas is added to the vessel at a rate based on the maximum rate of pressure rise). The rate at which gas is lost through a vent opening was then determined using the efflux function, enabling a description of the pressure in the vessel as a function of time. This method contains some simplifying and empirically based assumptions in order to easily enable sizing of explosion venting based on the explosion properties of a gas mixture and the vessel dimensions, as the goal of this work is not exact quantification of the pressure-time history of a vented deflagration but an easily applicable desk-top engineering tool.

The simulated rate at which new gas is generated inside the vessel is determined using the equation of state for ideal gases, which with the addition of a term for the mean molar mass, $\overline{M}_w$ (kg·mol^{-1}), can be rearranged to yield:

$$\frac{dm}{dt} = \frac{d}{dt}\left(\frac{\overline{M}_w pV}{RT}\right) = \frac{\overline{M}_w V}{RT} \cdot \frac{dp}{dt} \tag{2}$$

where p is the absolute pressure bar, R is the universal gas constant (R = 8.314 J·mol^{-1}·K^{-1}) and T is the absolute temperature (K). The rate of pressure rate can then be quantitatively determined from the K_G value according to:

$$\frac{dp}{dt}_{max} = K_G \cdot V^{-\frac{1}{3}} \cdot A_T \tag{3}$$

where A_T is a factor which is used to account for the turbulence generation developed during venting which increases the rate of pressure rise, this value is currently empirically determined and is described in further detail in Section 4.

It is assumed that the rate of pressure rise is constant over the course of the explosion which in reality will not be the case, however until a more accurate prediction of the pressure rise over time in a vessel during venting is possible this method should be used as it returns a conservative result.

The decrease in mass and hence pressure over time resulting from the gas flow through the venting surface is described using the efflux function, as shown in Equation 4.

$$\frac{-dm}{dt} = \alpha \cdot F \cdot \Psi \cdot p_1 \cdot \sqrt{\frac{2\overline{M}_w}{RT_E}} \tag{4}$$

where F is the venting area (m^2), Ψ is the efflux function, p_1 is the pressure inside the vessel (same units as the later determined dp), α accounts for the effective fraction of the area, F, through which gases are able to escape (i.e. α=1 signifies that the entire surface, F, is available for venting) and T_E is the temperature of the efflux gases which is also empirically determined as described in Section 4. The efflux function for ideal gases is defined for either supercritical or subcritical efflux depending on the ratio between the pressure inside the vessel and the pressure outside the vessel (Stephan and Mayinger, 1998).

Equations 2 and 4 can be combined to yield a term for the required venting area, however, this assumes that the rate of pressure rise is constant over an infinite time, an assumption which produces very conservative results (Heinrich, 1969). It is possible to estimate the time over which combustion (and hence pressure rise) takes place, t_c, when assuming that the rate of pressure rise is constant over a finite time, the combustion time is then the time required to achieve the maximum explosion pressure (as measured in a closed spherical vessel), and can be determined from the maximum explosion pressure, p_{max}, and the initial gas pressure, p_{ini} according to (it should be noted that due to many vessels not being spherical, this calculation also introduces a certain conservatism to the determined venting area (Drahme, 2010)):

$$t_c = \frac{p_{max} - p_{ini}}{K_G \cdot V^{-1/3} \cdot A_T} \tag{5}$$

An example of the output from this methodology is shown in Figure 2, for a gas having a K_G of 30 bar·m·s^{-1} and a p_{max} of 5, as measured in a closed spherical vessel at the required initial conditions. The vented vessel in this case has a normal working pressure, p_{ini}, of 1.2 bara, a p_{stat} of 1.4 bara, a volume of 100 m^3 and a venting area of 2 m^2, also in this example the temperature of the efflux gases is conservatively assumed to be equal to the normal working temperature of 200 °C and turbulence during venting is assumed to increase the rate of pressure rise by a factor of three. The black line displays the conservatively simulated rate of pressure rise, i.e. 3 x K_G·$V^{-1/3}$, which occurs over a time necessary to achieve a pressure of 5 bara. After a pressure of 1.4 bara, i.e. p_{stat}, is achieved, venting commences and the pressure in the vessel is determined from Equations 3 and 4. These calculations were carried out using a time-step of one millisecond, with the pressure from the previous time-step being used in Equation 4 to determine the efflux rate and hence the pressure for the next time step. The validity of using this time-step for this case was proven by the fact that further decreasing the time-step by a factor of 10 had no significant influence on the resulting simulated pressure-time curve. After t_c is reached the simulated generation of new gas is turned off and the pressure in the vessel is determined solely by the efflux equation (Equation 4). The result of the calculation is a p_{red}, dependent on the venting surface area which can be compared to the design pressure. The required venting area (with a suitable safety margin) can then be determined by varying F until p_{red} equals the design pressure.

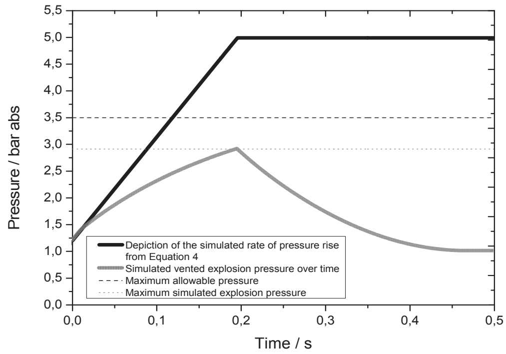


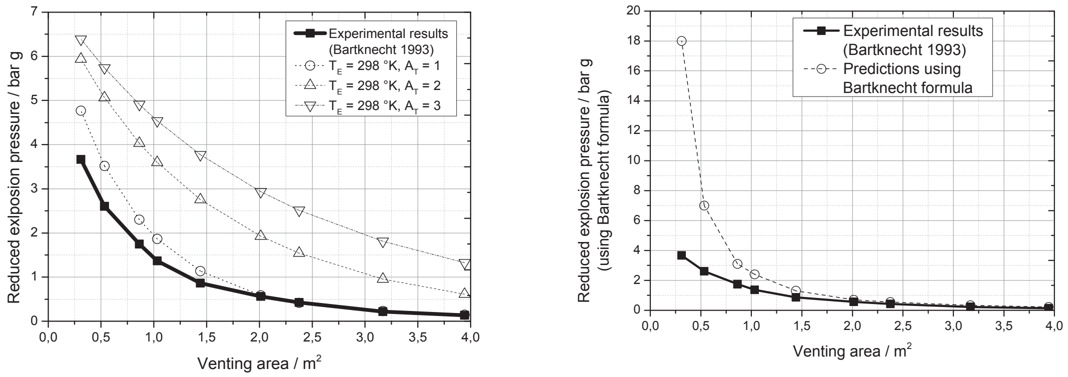
Figure 2: Example of a simulated pressure-time trace for a vented explosion as determined using the efflux method.

4. Comparison of the results from the efflux method with experimental data

In order to determine the validity of this methodology the maximum simulated pressure attained during venting was compared to experimental observations (Bartknecht, 1993). However, before applying this method several issues exist which first need to be resolved, including to what extent the rate of pressure rise is enhanced by turbulence and how to treat the temperature of the efflux gases over the course of the explosion. As no comprehensive data-set could be found describing the reduced explosion pressure for gases with low K_G values (≤ 50 bar·m·s^{-1}) for industrially relevant vessel sizes, data from stoichiometric methane-air mixtures at ambient conditions ignited inside a 30 m^3 vessel (p_{stat} = 0.1 barg) were used initially to develop empirically based assumptions concerning turbulence enhancement during venting and the temperature of the efflux gases. Obviously these two factors will change during the course of the explosion, however, in order to aid the ease of application they are considered to be constant.

In Figure 3 the reduced explosion pressure determined using the efflux method and the Bartknecht formula is plotted alongside the experimental results from the aforementioned scenario for venting areas of between 0.5 and 4.0 m^2, a K_G of 63.7 bar·m·s^{-1} and a p_{max} of 8.5 bara. It is well known that turbulence caused by the flow of gases through a vent opening can increase the rate of pressure rise, which can also account for the observation that in some cases the reduced pressure decreases with increasing vent size (Daubitz, Schmidt et al, 2001). However, as can be seen in Figure 3(a), using an A_T factor of 1, i.e. no enhancement of the rate of pressure rise due to the venting, produces the best fit to the experimental results (assuming a constant efflux gas temperature of 298 K, the temperature of the efflux gas also has an effect on the venting required which is discussed further in the following text.). It could be the case that buoyancy driven combustion plays a significant role, which would be expected to increase as the K_G value of a gas mixture decreases further, and is actually decreasing the rate of pressure rise as compared to that seen in a relatively small vessel (e.g. a 20 l sphere), in this case a turbulence factor of < 1 would be required, however in order to prove this and to be able to fit an appropriate turbulence enhancement/reduction factor experimental observations at appropriate scales would need to be taken into consideration. Furthermore, any turbulence enhancement by elements inside the vessel should be taken into account by choosing a suitable value for A_T. The reduced explosion pressures predicted using the Bartknecht formula for the same scenarios are shown in Figure 3(b). In the range of validity of the Bartknecht formula (i.e. < 2 barg) it shows a good agreement with the experimental results, however, as the venting area decreases below 1.5 m^2, approaching scales more likely to be encountered in many industrial applications, predicted explosion overpressures become inconceivably large.

The aforementioned calculations were carried out using the conservative assumption that the temperature of the efflux gases was constant during the venting process and equal to the initial temperature. In reality it is not always possible to predict exactly where ignition will take place relative to venting devices and so during the course of an explosion the value of T_E can vary from between the initial gas temperature to the adiabatic flame temperature. Considering ignition at the furthest point from the explosion venting, the worst case for efflux will occur as cold un-reacted gas will be vented, i.e. using the initial temperature of the efflux gas yields the biggest required venting surface area. However, due to the relatively smaller amount of gas taking part in an explosive reaction inside the vessel the overpressure and rate of pressure rise seen by the vessel could be less severe. The other extreme considered is when ignition takes place at the explosion vent, in this case all of the gas inside the vented vessel will undergo combustion, however, in this scenario the hot reaction products will be vented and therefore require a relatively smaller venting area. In the experiments used for this validation the mixture was ignited centrally, therefore, it would initially be expected that “cold” gas would be expelled through the vent opening followed by “hot” gas as the flame front approached the boundaries of the vessel. Shown in Figure 4 are the experimental and simulated results for the aforementioned scenario for 3 efflux temperatures: the initial gas temperature, the adiabatic flame temperature and the average of the two. Assuming that slight enhancement of rate of pressure rise relative to that recorded in a closed vessel is observed during these vented explosions (i.e. A_T = 2) the best fit for the simulated results is found when the temperature of the efflux gases are assumed to be equal to the adiabatic flame temperature (i.e. T_E = 1950 °C).



(a) (b)

Figure 3: Comparison of experimental and calculated results for (a) the reduced explosion pressure as a function of venting area and turbulence enhancement for stoichiometric methane-air explosions in a vessel with a volume of 30 m^3 and a p_{stat} of 0.1 barg, and (b) the predicted reduced explosion pressure for the same scenarios using the Bartknecht formula.

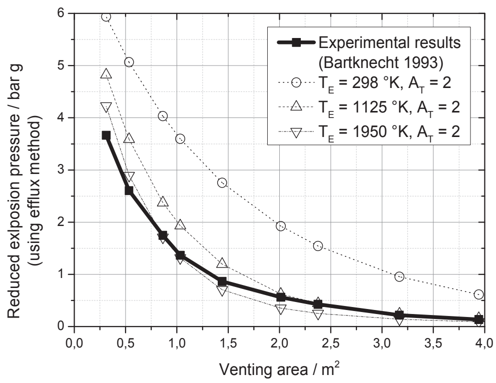
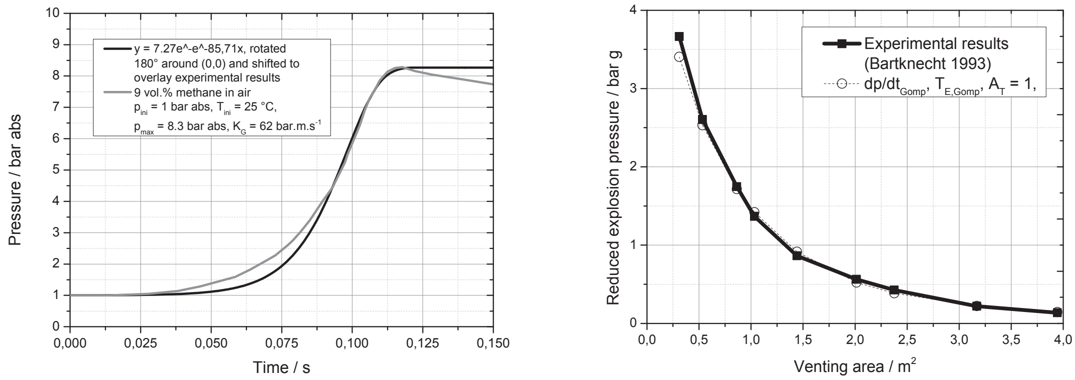


Figure 4: Comparison of experimental and simulated results for the reduced explosion pressure as a function of venting area and the temperature of the efflux gases for stoichiometric methane-air explosions in a vessel with a volume of 30 m^3 and a p_{stat} of 0.1 barg.

There is also still potential for the refinement of the efflux method, by, for example, developing a better description of the predicted vented pressure-time profile. Some promising results have already been obtained using Gompertz curves to define non-linear rates of pressure rise based on those measured in closed vessels, as shown in Figure 5(a), where the Gompertz curve has the same maximum and maximum gradient as the experimental results. This simulated pressure-time profile, adjusted for volume effects, was then used in place of the constant rate of pressure rise attained from Equation 5 in determining the simulated reduced overpressure as a function of venting area for the aforementioned experimental scenarios, as shown in Figure 5(b). Also included in this calculation is a non-linear description of the temperature of the efflux gases as a function of time which follows the same form as the Gompertz curve from T_{ini} = 298 °K to T_{max} = 1950 °K. The best fit was obtained to the experimental results when no net increase or decrease in the rate of pressure rise relative to that seen in a closed vessel was employed (i.e. A_T = 1).



(a) (b)

Figure 5: (a) Experimental results from the explosion of a 9 vol.% methane-air mixture in a 20 l sphere and a Gompertz sigmoidal curve of the form y=Ae^Be^Cx , rotated 180° around (0,0) and shifted to overlay the experimental results, where A = 7.27, B = -1 and C = -85.71, these three factors where iteratively adjusted until the p_{max} and dp/dt_{max} of the sigmoidal curve matched those of the experiment, and (b) comparison of experimental and simulated results for the reduced explosion pressure as a function of venting area for stoichiometric methane-air explosions in a vessel with a volume of 30 m^3 and a p_{stat} of 0.1 barg, using a Gompertz curve to describe the rate of pressure rise and the temperature of the efflux gas.

5. Conclusions

Using this simple example, the efflux method for determining the reduced explosion pressure and hence the required venting area for stoichiometric methane-air explosions in large vessels shows a good fit to experimental results by assuming that during venting there is no net effect (enhancement or reduction) on the rate of pressure rise during venting, as compared to an explosion in a closed spherical vessel. However in order to promote further confidence in the efflux method, especially with gases having lower K_G values than that of stoichiometric methane-air, in large vessels, further experimental validation needs to be carried out, which is currently difficult due to the lack of relevant data in the open literature. Of particular interest to this further development, regarding gases with low K_G values, will be the description of the rate of pressure rise for scenarios where combustion tends to being buoyancy driven. Furthermore, the efflux method can be refined with further empirical observations in order to take into account the effects arising from the vessel geometry, the measured temperature of efflux gases, a better description of turbulence enhancement during venting, the effect of the efflux direction and efflux of non-ideal gases, all of which require well-designed experimental campaigns at relevant scales.

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