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Analysis and Comparison of Calculation Methods for Physical Explosions of Compressed Gases

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Due to the complexity of the involved physical phenomena and to the lack of an adequate amount of reliable experimental data, a number of different models and calculation procedures for estimating the overpressure following the physical explosion of a compressed gas are presently reported in the literature. However, in many cases, only generic information about the main hypotheses adopted is provided and no guidelines about their accuracy, or range of applicability, are usually available.
In the present paper the physical explosion of a compressed gas, released after the catastrophic rupture of its containment system, is addressed. The analysis is carried out by means of two of the most commonly used calculation procedures, which have been applied to a number of study cases, characterized by different substances, volume, geometrical configuration, and operating conditions.
The obtained results are presented and compared. The analysis shows that, in all cases, the two methods give rise to different results, independently of the involved chemical, vessel size, and operating conditions. The dependence of the results on the main input parameters is highlighted in order to give a preliminary guideline in the selection of the proper calculation method for each specific study case.

1. Introduction

Different models and calculation procedures are presently available in the literature for estimating the peak overpressure and the other parameters of interest following the sudden explosion (expansion) of a compressed gas in air. This derives from the complexity of the physical phenomenon, the high number of parameters involved, the variability of the real geometrical configuration and of the physical conditions before the explosion, and so on. As a consequence, different simplifying hypotheses are often adopted, thus introducing some approximation and uncertainty of the results. Furthermore, in the field of risk analysis, a compromise is generally required between the accuracy of the models and their ease of use. This is often preferred, with respect to the use of a much more complex model, for the sake of simplicity and rapidity of application when a large number of simulations have to be carried out, or when a preliminary analysis of the system (a plant, activity, etc.) is only required.
In the following, the two probably most common models used in risk analysis to predict the pressure profiles generated by a gas explosion are adopted for estimating the overpressure profiles for a number of reference explosion scenarios. Their basic assumptions and calculation steps will be briefly recalled, while in the subsequent sections their results will be compared and critically discussed.

1.1 Baker's method

Baker et al. (1983) have developed a method for modeling pressure vessel bursts, either for ideal and non-ideal gases. Different versions of this model are reported in the literature (AIChE/CCPS, 1994; AIChE/CCPS, 1999) but the basic one will be adopted here.
In the Baker's method far and close range are treated differently; the energy of explosion is calculated by means of the Brode equation (Brode, 1959):

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$$E = \frac{(P_1 - P_0)V}{\gamma - 1} \quad (1)$$

where:
E = energy (J);
P_1 = initial pressure of the expanding gas (Pa);
P_0 = final (ambient) pressures of the expanding gas (Pa);
V = gas total volume (m^3);
γ = gas heat capacity ratio, C_p/C_v (-).

When the explosion occurs at ground level, the calculated value of the energy is generally multiplied by 2 to take into consideration ground effects, like the reflection of the shock wave, even if this is just an approximation, which does not properly represent the complexity of a real explosion.
The pressure profile is then obtained by using the Sachs scaling law (AIChE/CCPS, 1999), where the scaled distance, $\overline{R}$, is calculated as:

$$\overline{R} = r\left(\frac{P_o}{E}\right)^{1/3} \quad (2)$$

where;
E = energy (J);
P_0 = absolute pressure of ambient air (Pa);
r = distance (m);
$\overline{R}$ = scaled distance (-).

It is worth noting that the Brode equation is only a rough approximation of the reality, since it represents the energy required to compress an ideal gas, at constant volume, from P_0 to P_1. Of course, this is not the case in a real explosion, where the gas reaches an equilibrium condition after expansion from an initial volume at P_1 to a final volume at P_0. In addition, the expansion energy of the gas, even if properly calculated, still overestimates the actual explosion energy dissipated in the surrounding environment, because it would neglect several accompanying phenomena (like the energies required to rupture the vessel, to launch the fragments of the containment vessel, etc., which can amount up to 50 % of the total internal energy) as well as other aspects (such as the deformation of the vessel fragments, non-equilibrium effects, and so on).
Despite these considerations, the Brode equation is widely used and implemented in many models (AIChE/CCPS, 2000), and its approximation is counterbalanced by the introduction of some correction coefficients (Crowl and Louvar, 2002). Since in the proximity of the external surface of the exploding gas the method can calculate overpressures higher than the burst pressure, which is physically impossible, a modified procedure has been proposed for R < 2 (Baker et al., 1983): of course, it has been adopted also in the present work. However, adopting Baker's method a discontinuity will exist for $\overline{R}$ close to 2, where the two calculations procedures will give different overpressure values.

1.2 Prugh's method

In Prugh's method, differently from Baker's one, the explosion energy is calculated assuming an isothermal expansion of the ideal gas, which also is not a correct hypothesis in the case under exam, and the following equation results:

$$E = \frac{V}{V_0} \cdot \frac{P_1}{P_0} \cdot \frac{T_0}{T_1} \cdot R \cdot T_1 \cdot \ln\left(\frac{P_1}{P_2}\right) \quad (3)$$

where:
E = energy (J);

P_0 = pressure of ambient air at standard conditions (101300 Pa);
P_1 = initial pressure of the expanding gas (Pa);
P_2 = final pressure of the expanding gas (Pa);
R = gas constant (8314 J/kmol K);
T_0 = ambient temperature at standard conditions (273 K);
V = volume of the compressed gas (m^3);
V_0 = volume of 1 kmol of gas at standard conditions (0.022414 m^3).

Differently from the Baker method, this method makes use of the TNT equivalency model to estimate the explosion energy, and the scaling method (Hopkinson's law) to evaluate the blast pressure profile as a function of the distance will also be different (AIChE/CCPS, 1994).
However, the procedure by Prugh (1988) has some similarities with that of Baker described in the previous paragraph since also in this case the maximum overpressure of the shock wave, i.e. the one at the contact surface between the expanding gas sphere and the air, has to be preliminarily evaluated. In this case the following equation is adopted:

$$P_b = P_s \left[1 - \frac{3.5(\gamma - 1)(P_s - 1)}{\sqrt{\left(\frac{\gamma T}{M}\right)(1 + 5.9 P_s)}} \right]^{-2\frac{\gamma}{\gamma - 1}} \qquad (4)$$

where:
M = molecular weight (kg/kmol);
P_b = blast pressure (Pa);
P_s = pressure at vessel surface Pa);
T = temperature (K);
γ = gas heat capacity ratio, C_p/C_v (-).

However, instead of using the same procedure of Baker's method, a virtual distance (Petes, 1971) is here introduced to fictitiously move the explosion centre "upwind" with respect to the surface of the expanding gas, making it possible to use the traditional TNT equivalency model from that point on. Specifically, the virtual distance is obtained by subtracting the geometrical distance between the centre and the external surface of the vessel (corresponding to the expanding gas initial surface), from the distance calculated by the TNT model to get the P_b overpressure. The value of the virtual distance thus obtained is than added to the actual distance, and properly divided by the explosion energy to get the scaled distance Z of TNT model (AIChE/CCPS, 2000), where the peak overpressure has to be determined. Therefore, the physical parameters are derived by those of an equivalent amount of TNT.

2. Results and discussion

In order to check the differences in the estimates obtained applying the two methods, a number of accidental scenarios have been simulated, calculating the overpressure profiles as a function of the distance from the centre of the explosion. The examined scenarios differ in terms of substance involved, total gas volume, operating conditions and geometrical configuration: in particular, a cylindrical and a spherical vessel have been considered, with volumes of 10, 100 m^3 (cylindrical) and 1,000 m^3 (spherical), respectively.

2.1 Ammonia

Storage tanks containing ammonia as liquefied gas under pressure at ambient temperature have been considered. As a consequence, liquid-vapour equilibrium conditions are established, and the initial (burst) pressures shown in Table 1 have been adopted.
Figure 1 shows the overpressure profiles as a function of the distance from the 10 m^3 tank centre, for the two models at different values of the burst pressure: since both models assume circular symmetry, the profiles are identical for any directions. It can be first observed from Figure 1 that, for a given model, the local overpressure varies remarkably with the burst pressure for relatively small distances from the centre of the explosion, while at

larger distances a much lower difference in the overpressure is experienced, so that the influence of the burst pressure is much more important in the proximity of the exploding vessel, rather than at larger distances.

Table 1: Set of initial (burst) pressures for ammonia cases

Temperature (°C)	Internal pressure (bar)
30	11.40
25	9.84
20	8.42
10	6.00
0	4.30

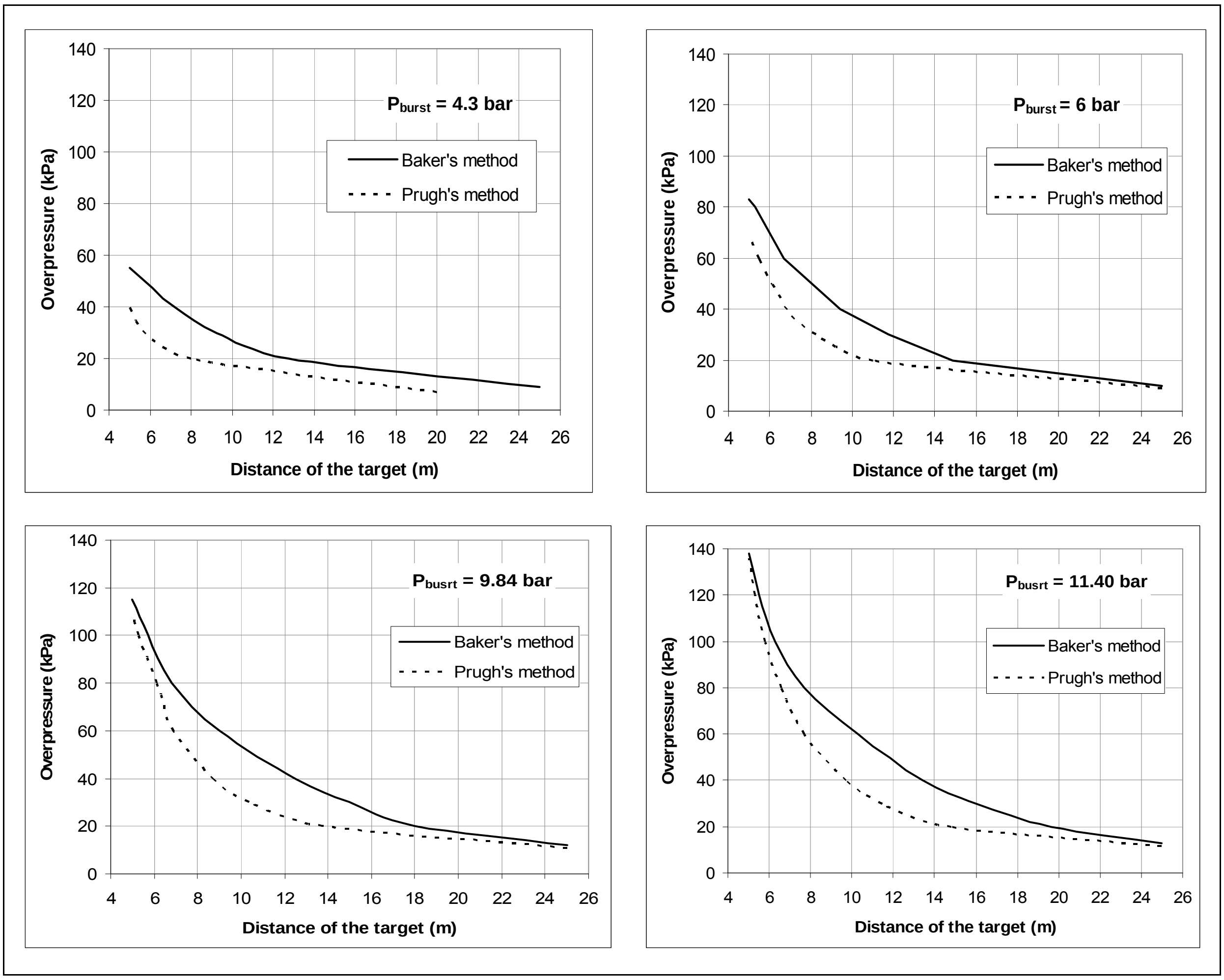

Figure 1: Comparison of the models for a 10 m^3 cylindrical ammonia vessel

Secondly, at any given initial tank pressure, if the results of the two models at a given distance are compared, it can be noticed that Baker's model always provides larger values of the overpressure, turning out to be more conservative than Prugh's. However, by increasing the distance from the centre of the explosion, the difference between the models becomes progressively smaller: from a given distance on (about 22 m in this case), the curves get very close, also due to the low absolute values of the overpressure.
The value of 30 kPa is usually assumed as the overpressure threshold giving rise to immediately lethal effects on humans, and to domino effects for structures. Therefore, the intersections of the pressure profiles with the

horizontal line at 30 kPa will give an approximate safety distance, beyond which significant physical injuries and/or destructive damages to structures are not expected. This is, obviously, an abrupt approximation of the actual effects caused by a shock wave, and it is used only as a benchmark value for models comparison, since no significant variation in the conclusions is expected for different values.
According with the previous observations, i.e. with the more conservative approach of the Baker's method, the threshold distances calculated by this procedure always provide larger distances with respect to the Prugh's ones, by a 40 % average (see Table 2)
If the same analysis is carried out for the larger vessels (100 m^3 cylindrical and 1,000 m^3 spherical), it can be found that the above considerations apply as well, the differences between the two approaches being even more apparent, since the overpressures calculated by the Baker's method are always higher than Prugh's ones, independently on the initial pressure and in the whole range of distance analyzed.
Also for the threshold distances, the difference is more evident for the large vessels than for the small one, since the values provided by the Baker's method are more than double those calculated by Prugh's one (Table 2) for the 100 m^3 cylindrical tank and about 80 % in the case of the 1,000 m^3 spherical one.

Table 2: Distance to 30 kPa for the two models for ammonia vessels.

Initial pressure (bar)	10 m^3 cylindrical vessel		100 m^3 cylindrical vessel		1000 m^3 spherical vessel	
	Baker (m)	Prugh (m)	Baker (m)	Prugh (m)	Baker (m)	Prugh (m)
11.40	16.00	11.50	51.5	23.5	80.5	45.0
9.84	15.00	10.40	49.5	22.0	76.2	42.0
8.42	14.00	9.70	46.5	20.5	72.0	39.0
6.00	11.75	8.25	41.0	18.0	61.0	32.5
4.30	9.25	5.80	35.5	15.6	49.5	28.0

Figure 2 shows the trend of the threshold distance as a function of the initial (burst) pressure.

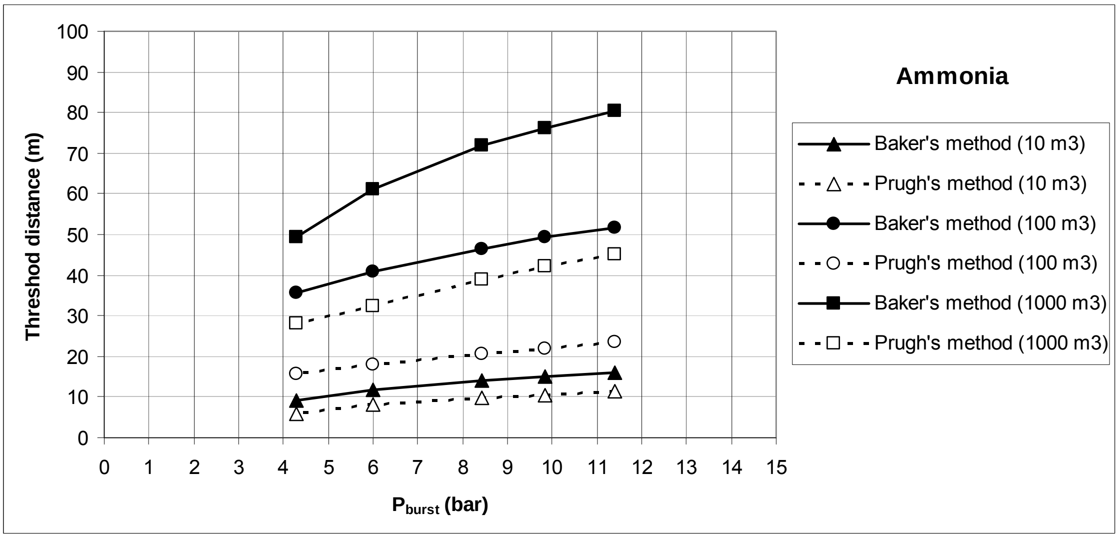

Figure 2: Threshold distance vs. burst pressure for ammonia cases

Finally, it has to be pointed out that the predictions of the overpressure according to Baker's method present a discontinuity for $\overline{R}$ approaching the value of 2: for example, this discontinuity is shown in Figure 3, with reference to the 100 m^3 vessel, for values of the burst pressure ranging from 8.42 to 11.4 bar. The discontinuity is more evident as the burst pressure increases, and for larger vessels.

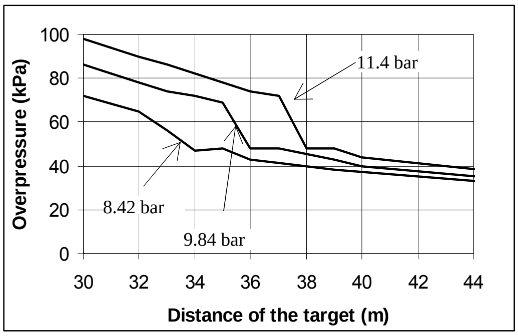

Figure 3: Discontinuity of the Baker's method for the 100 m^3 cylindrical ammonia vessel

2.2 Chlorine

The same storage tanks considered for the ammonia cases were then assumed to contain chlorine, analyzing 5 explosion scenarios, with the burst pressures up to 100 bar, in order to compare the predictions of the two methods in a different (wider) range of operating conditions. Also for this product, the Baker's method is always more conservative than the Prugh's one, giving higher values of the overpressure at any distance: the differences increase at higher burst pressures. Accordingly, the threshold distances are remarkably higher for Baker's method (see Table 3): the ratio between the distances calculated according to the two methods decreases with increasing the initial pressure, which, in absolute terms, correspond to a decreasing difference at greater distances from the explosion centre.

Table 3: Distance to 30 kPa for the two models for chlorine vessels

Initial pressure (bar)	10 m^3 cylindrical vessel		100 m^3 cylindrical vessel		1000 m^3 spherical vessel	
	Baker (m)	Prugh (m)	Baker (m)	Prugh (m)	Baker (m)	Prugh (m)
100	49.5	24	107	52	178.5	112
50	39.5	17.5	84.5	38	131.5	82.5
25	31	13	68	28	99.5	61
10	23	8.5	48.5	18.5	63	40
5	17	6.5	37	14.5	43	29.5

Figure 4 shows the trend of the threshold distance as a function of the initial (burst) pressure.

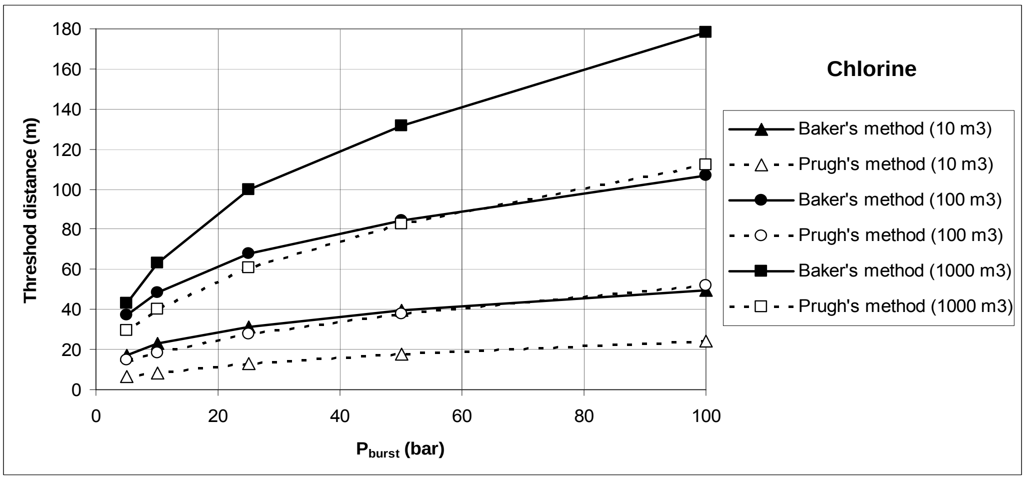

Figure 4: Threshold distance vs. burst pressure for chlorine cases

Of course, also for this substance the discontinuity in the predictions of the overpressure according to Baker's method for $\overline{R}$ approaching the value of 2 exist: the discontinuity is proportionally more important when the internal pressure increases, since it depends on the scaled $\overline{R}$.

2.3 Comparison of different substances

Figures 5 and 6 compare the obtained trends of the threshold distance as a function of the burst pressure for the two substances adopted for the study cases, limiting the scale to 12 bar, for the sake of clarity.

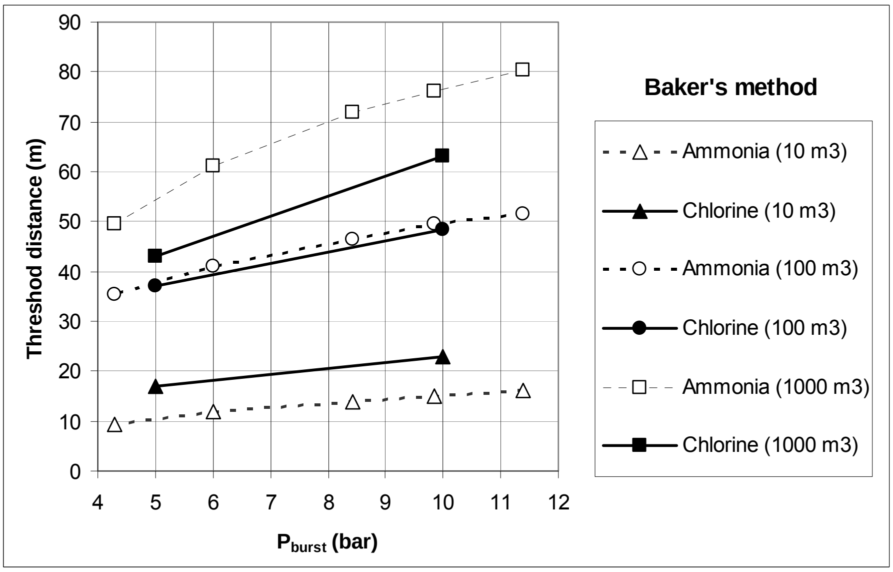

Figure 5: Threshold distance vs. burst pressure for ammonia and chlorine, according to Baker's method

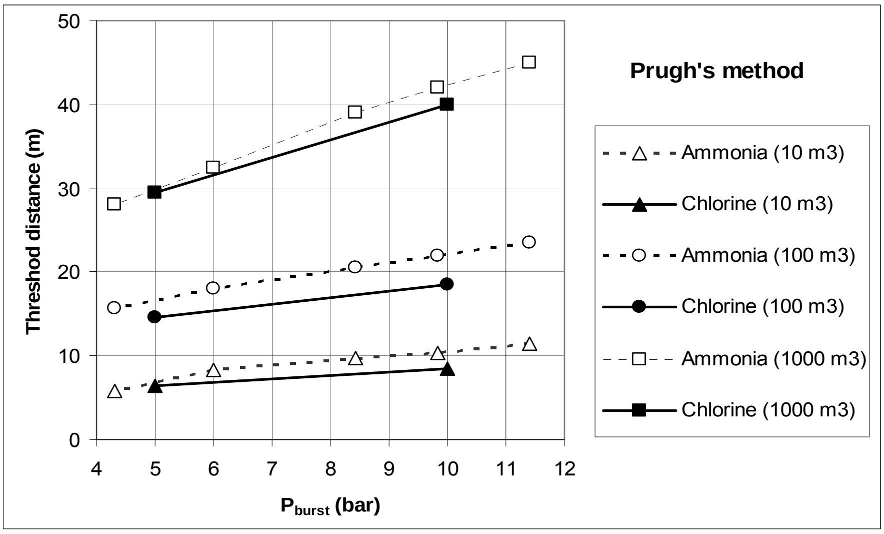

Figure 6: Threshold distance vs. burst pressure for ammonia and chlorine, according to Prugh's method

It can be noticed that, at a given burst pressure, different threshold distances are obtained for the examined substances. In particular, the predictions obtained according to Baker's method (Figure 5), show that the percent differences among the threshold distances calculated for ammonia and chlorine depend on the vessel size: the values are closer for the 100 m^3 vessel , and more distant for the 1000 m^3 and the 10 m^3 vessels, in this order. Moreover, there is no general sequence, since the lower values are associated to ammonia, for the 10 m^3 vessel and to chlorine for the 100 and 1000 m^3 ones.

As far as the predictions of Prugh's method are concerned (Figure 6), the threshold distance values calculated for the two substances are remarkably closer than using Baker's method, the values of ammonia being slightly higher than those of chlorine, independently of the vessel size.

2.4 Discussion

The substances analysed in this study present different physical properties: Table 4 summarizes some data of interest.

Table 4: Physical properties of the substances

Physical properties	Ammonia	Chlorine
Molecular weight, M (kg/kmol)	17.0	70.9
Heat capacity ratio (at 15°C and 1 atm), γ (-)	1.310	1.355
γ/M ratio (kmol/kg)	0.077	0.019
Normal boiling point (K)	239.9	238.2
Vapour pressure at 20°C (bar)	8.379	6.899

In order to compare the different results obtained using Baker's and Prugh's methods, the energy of explosion for the different cases were compared. According to both expressions (eq.1 and eq.3) the energy is a linear function of the vessel volume: Figures 7 and 8 show its trend vs. the burst pressure for the 100 m^3 cylindrical vessel, calculated according to Baker's and Prugh's methods, respectively, limiting the scale to 12 bar, for the sake of clarity.

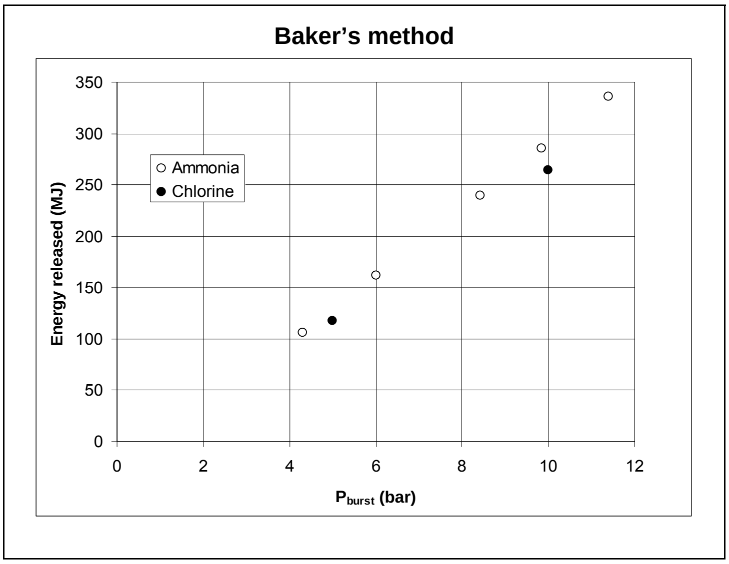

Figure 7: Energy released in the explosion vs. burst pressure for ammonia and chlorine (100 m^3 cylindrical vessel) according to Baker's method

Adopting Baker's method, the calculated values of energy released in the explosion are very similar for ammonia and chlorine, based on their quite similar values of the heat capacity ratio γ: however, the heat capacity ratio of chlorine is slightly higher than that of ammonia, thus resulting in slightly lower energy values, as calculated from eq.(1). On the contrary, Prugh's method, based on the assumption of isothermal expansion of the gas, eq.(4), predicts that the explosion will release an amount of energy which is independent of the involved substance. However, independently of the fact that the released energy for ammonia is greater (Baker's method) or equal

(Prugh's method) to that of chlorine, for the 100 m^3 vessel, both methods predict higher safety distances for ammonia than for chlorine (see Figs. 5 and 6).

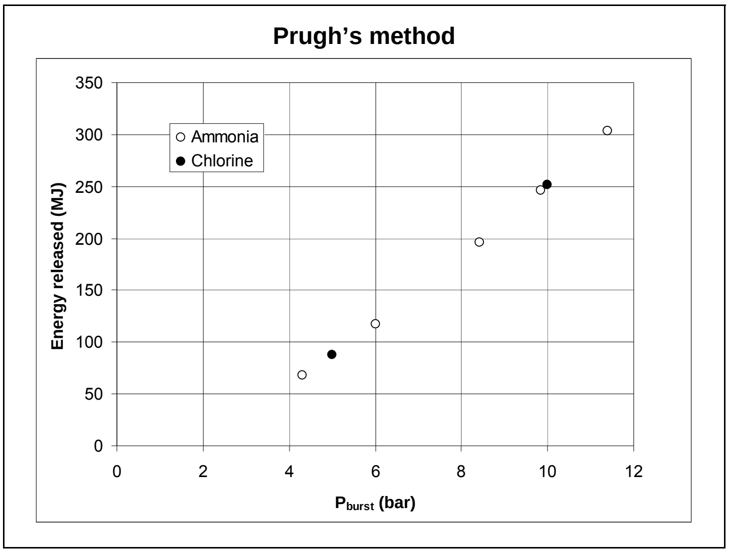

Figure 8: Energy released in the explosion vs. burst pressure for ammonia and chlorine (100 m^3 cylindrical vessel) according to Prugh's method

Besides using different equations to estimate the explosion energy, Baker's and Prugh's methods finally make use of different routes to predict the resulting overpressure based on such energy and, other factors, associated to the physical properties of the substances, have also to be taken into account. For example, according to eq. (4), different virtual distances are calculated for the considered substances, depending on the values assumed by the heat capacity ratio, but also by the molecular weight: the values of the γ/M ratios are much higher for ammonia than for chlorine (Table 4).

2.5 Conclusions

The study cases demonstrate that the two most used simplified methods for estimating the trend of overpressure vs. distance in case of gas explosions give rise to rather different profiles in the near field, which become closer in the far field, where the absolute overpressure values are lower. From this point of view, the obtained results are particularly interesting at distances in the range of the usual equipment spacing.

Baker's method estimates are invariantly more conservative for both the chemicals investigated: in absolute terms the observed differences are also function of the initial pressure, of the vessel size and of the substance under exam. On the other hand, the two methods make use of different assumptions to estimate the energy released in the explosion, based on the expansion of the compressed gas, as well as of different procedures to derive the overpressure profiles starting from those values.

The predictions of both methods, for the same vessel size and burst pressure, give different results for the two investigated substances, indicating that the physical properties of the chemicals, namely the heat capacity ratio, and the molecular weight, play a significant role. However, the size of the vessel also exhibit some influence on the results obtained using Baker's method, since the examined cases show that the highest safety distance may be associated to ammonia or to chlorine depending on the volume of the gas.

It can be concluded that both models can be used to estimate the overpressure field at a certain distance from the explosion centre, where no significant differences are found, while they behave differently in the close proximity of the explosion source. In such region, Baker's method turns out to be more conservative, and thus more reliable from a prevention point of view; however, where more accurate data are needed, more sophisticated and time-requiring techniques (such as CFD) should be used.

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