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$DeNO_X$ Plants: a Prediction Method of the Overpressure Generated by an Ammonia Vapor Cloud Explosion

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Industrial fires and explosions are neither infrequent nor inconsequential. In consequence of the complexity of the phenomena, which are involved in an unconfined vapor cloud explosion (UVCE), a variety of prediction methods and calculation procedures is available to estimate the consequences (overpressure) of the flammable cloud explosion. These methodologies range from simplified methods, which relatively require few calculations, to complicated numerical models, that can involve millions of calculations. In the present paper an ammonia vapor cloud explosion is studied. The cloud is generated by an accidental release of aqueous ammonia (evaporation from pool) in a $DeNO_X$ plant, which is installed in a steam power plant. The analysis is carried out by a prediction method, that requires a specification of the chemical reactivity, congestion (obstacles density) and confinement in order to establish the maximum flame speed. The study has been focused on effects of area congestion on overpressure profile. In general for realistic plants geometries a high level of congestion results in higher turbulence and therefore higher flame speeds and overpressures. This parameter often is the most difficult element to assess in consequence of the plants complexities and has important effects on overpressure peak. In fact the definition of the congestion level requires meticulous and painstaking inspections of the plant areas. The results of the study are presented and compared. The goal of the paper is the illustration of a methodology, which can provide useful elements (an estimate of the plant congestion) to enrich the preliminary knowledge of the explosion consequences in order to improve the process safety during the operation of the $DeNO_X$ plants.

1. Introduction

In literature there are various prediction methods and calculation procedures, which can be used to estimate the overpressure peak, deriving from an UVCE. It depends on the complexity of the physical phenomenon (Bubbico and Mazzarotta, 2013) and the high number of parameters (fuel reactivity, confinement, plant congestion, turbulence, velocity gradients, etc.), which are involved. Simplified assumptions must be adopted, thus introducing uncertainty of the results. In this context a compromise is usually required between the methods accuracy and their ease of actualization. The paper focuses on a model, which belongs to the “blast curve methods”. These methodologies are based on UVCE specific blast curves, that were developed using numerical calculations. Blast curves were developed for a range of flame speeds from slow deflagrations to detonations. Blast curves methods are in widespread use in industry and in the risk analysis in order to predict the pressure profile, which can be generated by a gas explosion. In the following paragraphs the assumptions and calculation steps are illustrated.

1.1 Baker-Strehlow-Tang Method

A one-dimensional numerical study was performed by Strehlow et al. (1979) to predict blast waves, which were generated by constant speed and flames, propagating in a spherical geometry. Tang and Baker improved the blast curves with advanced numerical models. These new curves were called the “Baker-Strehlow-Tang” (BST) blast curves to distinguish them from the Strehlow’s curves. The BST method was

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developed for external UVCE. In the paper BST method is adopted in order to estimate the overpressure profile, which derives from an ammonia vapor cloud explosion in a DeNOx plant. BST curves are labelled by different flame speeds (M_f). The selection of the maximum flame speed depends on the combined effects of confinement, fuel reactivity and area congestion (AIChE/CCPS, 2010). Confinement is based on three symmetries (figure 1): point-symmetry (3-D), planar-symmetry (2-D) and line-symmetry (1-D).

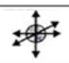
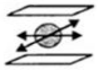
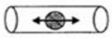
Type	Dimension	Description	Geometry
Point symmetry	3-D	Unconfined volume, almost completely free expansion	
Planar symmetry	2-D	Platforms carrying process equipment; space beneath cars; open sided multi-story buildings	
Line symmetry	1-D	Tunnels, corridors or sewage systems	

Figure 1: Confinement level

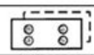
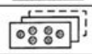
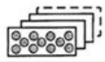
Type	Obstacle blockage ratio per plane	Pitch for obstacle layers	Geometry
Low	Less than 10%	One or two layers of obstacles	
Medium	Between 10% and 40%	Two or three layers of obstacles	
High	Greater than 40%	Three or more fairly closely spaced obstacle layers	

Figure 2: Congestion level for the BST Method

The fuel reactivity is a term, which is used to describe the propensity of a flame to accelerate in an UVCE. This parameter is classified as low, medium and high. Methane, carbon monoxide and ammonia are regarded as low reactivity. Congestion refers to the obstacles, that obstruct the passage of the flame front enough to create turbulence (Hjertager, 1984) and increase flame speed without preventing its expansion. Obstacles density (congestion) is classified as low, medium and high (figure 2) as a function of the area blockage ratio (ABR) and pitch. ABR is defined as the ratio of the area blocked by obstacles to the total cross-section area (Pierorazio et al., 2004). Low congestion is defined as ≤10 %ABR and pitch≥8D (D is the diameter of obstacles), medium congestion is defined between 10 and 40 %ABR and the pitch varies from 4D to 8D and high congestion is greater than 40 % ABR (the pitch is less than 4D). The pitch is defined as the distance between successive obstacles. The definition of the fuel reactivity, confinement and area congestion allows to define the maximum flame speed (M_f), that is expressed in Mach number (table 1).

Table 1: Flame speeds in Mach number (BST Method)

		Congestion		
Confinement	**Fuel reactivity**	Low	Medium	High
1-D	low	0.294	1.029	2.265
	medium	1.029	1.765	2.265
	high	5.2	5.2	5.2
2-D	low	0.079	0.47	0.66
	medium	0.47	0.66	1.6
	high	0.59	1.029	1.765
3-D	low	0.026	0.23	0.34
	medium	0.11	0.44	0.5
	high	0.36	DDT	DDT

Once the maximum flame speed is determined, figure 3 is used to determine the overpressure. The following equation is used to calculate the scaled distance (R_{SC}):

$$R_{SC} = R \cdot \left(\frac{p_{atm}}{E} \right)^{\frac{1}{3}} \tag{1}$$

Where R (m) is the distance from the explosion, p_{atm} (atm) is the atmospheric pressure and E is the energy term (J). This last parameter represents the heat, which is released by that portion of the cloud, contributing to the blast wave. In this case E is doubled to account for the ground reflection. Scaled pressure (p_{sc}) is defined as the ratio between the peak pressure (p_p) and p_{atm}. Scaled distance and pressure are adimensional parameters.

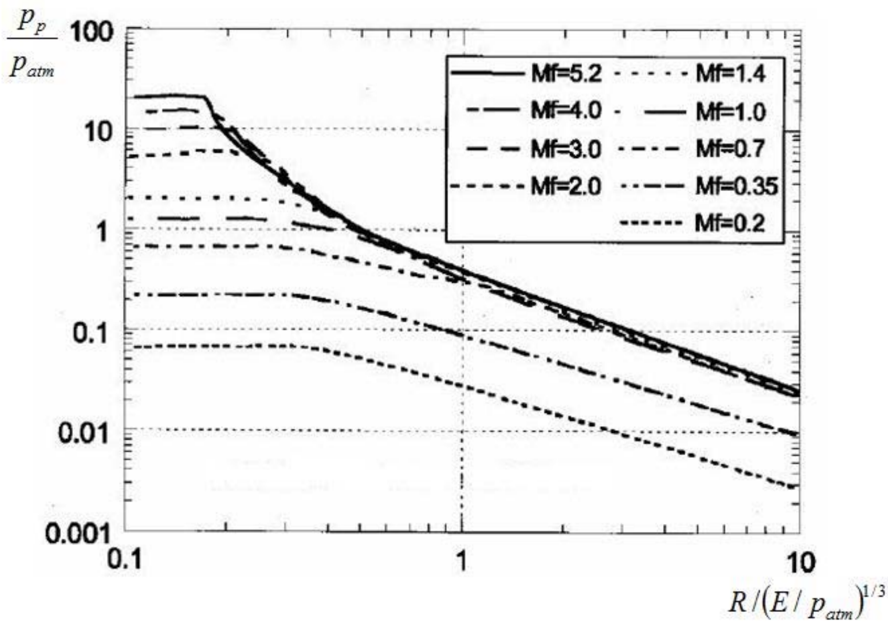


Figure 3: Overpressures for various flame speeds

2. Calculation procedure

The energy term (E) must be calculated in order to determine the scaled distance. E is expressed by the following equation:

$$E = 2 \cdot \eta \cdot n \cdot PM_{NH_3} \cdot H_{NH_3} \tag{2}$$

Where n represents the moles of ammonia in the combustion volume, PM_{NH3} is the molecular weight (17.03 kg/kmol) of ammonia, H_{NH3} (19.9 MJ/kg) is the heat of combustion and η indicates the stoichiometric concentration of the fuel (ammonia) and is defined by the ratio between fuel moles and fuel and air moles. This last parameter is calculated by the ammonia oxidation reaction (complete combustion):

$4\ NH_3 + 5\ O_2 + 18.8\ N_2 \rightarrow 4\ NO + 6\ H_2O + 18.8\ N_2$ (3)

$$\eta = \frac{4}{4 + 23.8} = 0.144 \tag{4}$$

Equation of ideal gases is used in order to determine the moles (n) of gas in the combustion volume, assuming that the entire congested volume is filled with a stoichiometric mixture of ammonia and air:

$$n = \frac{p \cdot V}{R \cdot T} \tag{5}$$

In the previous equation p (ambient pressure), R (the universal gas constant) and T (ambient temperature) are known, while V (the volume of ammonia cloud) depends on the amount of ammonia, which evaporates from the pool. In Italy in the $DeNO_X$ plants aqueous ammonia is usually stored in horizontal and cylindrical tanks, which are surrounded by a containment basin and an accidental release generates a pool, which is composed by water and ammonia. NH_3 is more volatile ($T_{boiling_{NH_3}}$ =-33 °C) than water and its evaporation primarily depends on the thermal exchange between basin and pool (its boiling temperature is lower than ambient temperature), but when the basin surface cools, the solar radiation becomes important and has to be considered in order to calculate more accurately the amount of ammonia, that evaporates. The mass flow (m_{NH_3}) of ammonia, which evaporates from the pool per square meter, is calculated by the following equation:

$$m_{NH_3} = \frac{q_B}{\lambda_{VAP_{NH_3}}(T_{eb_{NH_3}})} + \frac{q_{irr}}{\lambda_{VAP_{NH_3}}(T_{eb_{NH_3}})} = \frac{k_b \cdot (T_b - T_{eb_{NH_3}})}{\lambda_{VAP_{NH_3}} \sqrt{\pi \cdot \alpha_b \cdot t}} + \frac{q_{irr}}{\lambda_{VAP_{NH_3}}} \tag{6}$$

Where:

- q_B is the thermal flow, which is transmitted by the basin surface (W/m^2);
- q_{irr} indicates the contribution of the solar radiation (W/m^2);
- $\lambda_{VAP_{NH_3}}(T_{eb_{NH_3}})$ represents the latent heat of vaporization of ammonia= 13.7 · 10^5 J/kg;
- k_b is the thermal conductivity of the basin (cement) = 0.92 W/m°C;
- T_b is the basin temperature = 20 °C;
- $T_{eb_{NH_3}}$ is the boiling temperature (at atmospheric pressure) of ammonia = -33°C;
- α_b represents the thermal diffusivity of the basin (cement) = $4.16 \cdot 10^{-7}$ m^2/s;
- t is the time after the release= 600 s. This value has been estimated considering the leakage detection time and the operation time of the safety device (foam system), which can interrupt the ammonia evaporation.

m_{NH_3} is expressed in kg/s · m^2. Once m_{NH_3} is determined, the volume (m^3) of ammonia cloud is calculated by the following equation:

$$V = \frac{m_{NH_3} \cdot t \cdot A_{pool(NH_3)}}{\rho_{NH_3}} \qquad (7)$$

$A_{pool_{NH_3}}$ (m^2) indicates the pool area, which is occupied by ammonia, and ρ_{NH_3} (kg/m^3) is the ammonia density. In this application a concentration of 25 % (by weight of NH_3) ammonia in water has been considered. At this point n and E can be calculated.

3. Results and discussion

In order to evaluate the consequences of the ammonia vapor cloud explosion different scenarios have been considered and for every case the overpressure profile as a function of the distance from the centre of the explosion has been reported and compared. The analyzed accidental scenario is an UVCE, which is the result of the ignition of an ammonia cloud, that is generated by a release of aqueous ammonia in the containment basin (evaporation from pool). These scenarios differ in terms of pool area (different radiuses have been examined) and congestion level (low, medium and high congestion). Nine explosion scenarios have been analyzed in order to compare the overpressure profiles and estimate the potential damages. In particular a circular pool has been considered, because its dimension is really known when the released volume covers the entire area of the basin. The ammonia reactivity is low and a 3-D confinement has been assumed, because ammonia density is lower than air density at 20 °C. Three pool radiuses have been chosen (0.5, 1 and 1.5 m) and for every scenario the examined distances from the centre of the explosion are 10, 15, 20, 25, 30 and 35 m. The considered $DeNO_X$ plant is located in Apulia (q_{irr}= 481 W/m^2) (Cogliani et al., 2000). The results of the study are shown in Table 2 and in Figure 4, that shows the trends of the overpressures at the established distances (the overpressures, which are related to low congestions, haven't been reported, because they are not remarkable). High congestion causes the greatest overpressures and damages, because the flame acceleration mechanism due to turbulence and flow velocity gradients increases. The calculated overpressures (high congestion) are over 0.1 atm (the maximum value is 0.22 atm) except for the distances, which are included between 30 and 35 m (r_{pool}=1 m) and 20 and 35 m (r_{pool}=0.5 m). It can be noticed that the three scenarios of low congestion don't cause significant effects on the structures and mankind safety (Table 3). More considerable overpressures are related to the medium congestion, but only at short distances from the centre of the explosion. In this case the maximum overpressure is 0.091 atm and this value is fairly close to the threshold (0.1 atm), which could cause a partial demolition of buildings. The scenario, which determines the biggest pressure (p_p=0.22 atm), is related to the high congestion and biggest radius (r_{pool}=1.5 m). In fact when the pool radius assumes growing values (a failure of the leakages detection system or the safety devices could occur), the volume of ammonia cloud increases (in Eq 7 m_{NH_3}, t and ammonia density don't vary). The direct consequence is the increase of the energy term (in equation 5 n only depends on the volume) and therefore the value of the scaled distance decreases.

Table 2:Results

	High congestion (M_f=0.34) r_{pool}=0.5 m	Medium congestion (M_f=0.23) r_{pool}=0.5 m	Low congestion (M_f=0.026) r_{pool}=0.5 m	High congestion (M_f=0.34) r_{pool}=1 m	Medium congestion (M_f=0.23) r_{pool}=1 m	Low congestion (M_f=0.026) r_{pool}= 1 m	High congestion (M_f=0.34) r_{pool}=1.5 m	Medium congestion (M_f=0.23) r_{pool}=1.5 m	Low congestion (M_f=0.026) r_{pool}=1.5 m
Distance (m)	$p_{sc}=p_p$ (atm)	$p_{sc}=p_p$ (atm)	$p_{sc}=p_p$ (atm)	$p_{sc}=p_p$ (atm)	$p_{sc}=p_p$ (atm)	$p_{sc}=p_p$ (atm)	$p_{sc}=p_p$ (atm)	$p_{sc}=p_p$ (atm)	$p_{sc}=p_p$ (atm)
10	0.19	0.072	0.015	0.21	0.09	0.016	0.22	0.091	0.019
15	0.15	0.054	0.0075	0.19	0.08	0.013	0.2	0.085	0.017
20	0.1	0.04	0.006	0.15	0.06	0.01	0.18	0.07	0.015
25	0.08	0.033	0.0057	0.12	0.05	0.0085	0.16	0.057	0.012
30	0.069	0.028	0.0052	0.1	0.042	0.0079	0.12	0.05	0.01
35	0.056	0.023	0.0048	0.089	0.031	0.0067	0.109	0.041	0.007

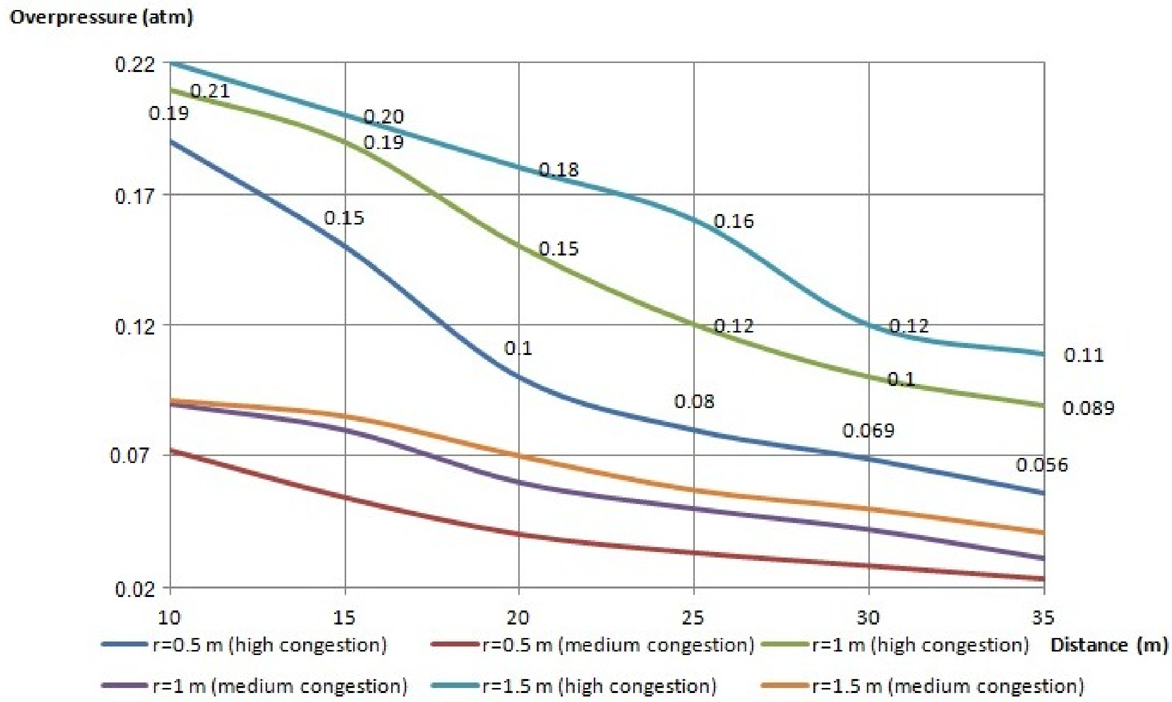


Figure 4: Trends of the overpressures

In this way the intersection of the blast curve with the vertical lines, which are related to the calculated scaled distances, provides growing values of pressure. All the scenarios are related to deflagrations (flame speeds are subsonic) and the overpressures are included between 0.0048 and 0.22 atm (collapse of metallic and concrete structures). Table 3 is used to estimate the potential damages of the calculated overpressures. It can be noticed that the high congestion (radius is constant) determines a bigger increase of the overpressure than the growth of the pool radius (high congestion). In fact the overpressure increase due to the radius growth is averagely 66.3 % than the value, that is related to the smallest radius, while the passage from low congestion to high congestion determines final pressures, which averagely are fourteen times the initial pressures.

4. Conclusions

Various prediction methods are available for an UVCE. They range from simplified methodologies, which require few calculations, to complex numerical models. Of course there are tradeoffs among the different methods. For example the BST method is more accurate than TNO Multi-Energy method and TNT method.

Table 3: Damage estimate (explosions)

Pressure (atm)	Damage
0.001	Annoying noise (137 dB)
0.01	Glasses breakage
0.03	Limited structural damages
0.1	Partial demolition of buildings
0.2	Collapse of metallic and concrete structures
0.3	Possible eradication of steelworks
0.5	Complete destruction of buildings
1	Damages to mankind (pneumonic hemorrhage)

In fact in the TNO Multi-Energy method the choice of the class number is left to the user discretion and it is less guided. On the contrary in the BST method the choice of the maximum flame speed (M_f) is highly guided. In fact it depends on the combined effects of confinement, fuel reactivity and congestion. In particular this last parameter plays an important role in order to estimate the overpressure peak, because it strongly influences the mechanisms of flame acceleration. The BST method provides a practical and quick mean of evaluation of the plant congestion. This aspect is very important in the risk analysis, because physical layout of a process area has a direct effect on the outcomes of UVCE. The calculated overpressures are significant for the scenarios of high congestion (it depends on the confinement and low fuel reactivity), but the pool radius reduction determines a decrease of their values and dangerousness, which is limited to a potential and partial demolition of buildings (this damage could only occur at short distances from the explosion). It can be concluded that BST method can be initially used such as a reasonable and useful tool for a preliminary risk analysis, but a higher accuracy level can be only reached by computational fluid dynamics (CFD) models, which are able to provide a more detailed description of an explosion over a wider range of conditions and geometries.

References

AIChE/CCPS, 2010, Guidelines for vapor cloud explosion, pressure vessel burst, bleve and flash fire hazards, 2nd Edition. American Institute of Chemical Engineers, New Jersey, USA.

Bubbico R., Mazzarotta B., 2013, Analysis and comparison of calculation methods for physical explosions of compressed gases, Chemical Engineering Transactions, 32, 133-138, DOI: 10.3303/CET1332023.

Cogliani E., Petrarca S., Spinelli F., 2000, The global solar radiation over Italy (La radiazione solare globale al suolo in Italia). ENEA, Italia.

Hjertager B.H., 1984, Influence of turbulence on gas explosions. Journal of Hazardous Materials. Elsevier, 315-346.

Pierorazio A.J., Thomas J.K., Baker Q.A., Ketchum D.E., 2004, An update to the Baker-Strehlow-Tang vapor cloud explosion prediction methodology flame speed table, 38th Annual Loss Prevention Symposium, AIChE Spring National Meeting, April 26-29, New Orleans, USA.