Calculating overpressure from BLEVE explosions

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Abstract

Although a certain number of authors have analyzed the prediction of boiling liquid expanding vapour explosion (BLEVE) and fireball effects, only very few of them have proposed methodologies for predicting the overpressure from such explosions. In this paper, the methods previously published are discussed and shown to introduce a significant overestimation due to the erroneous thermodynamic assumptions—ideal gas behaviour and isentropic vapour expansion—on which they are based (in fact, they give the maximum value of overpressure which can be caused by a BLEVE). A new approach is proposed, based on the—more realistic—assumption of an adiabatic and irreversible expansion process; the real properties of the substance involved in the explosion are used. The two methods are compared through the application to a given case.
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1. Introduction

Among the diverse major accidents which can occur in process industries, in energy installations and in the transportation of dangerous materials, boiling liquid expanding vapour explosions or BLEVEs are especially important due to their severity and the fact that they involve simultaneously diverse effects which can cover large areas: overpressure, thermal radiation and missile ejection.

Although BLEVEs occur with a certain frequency, and unfortunately will continue to occur in the future (both the substances which can give rise to them—butane, propane, vinyl chloride, etc.—and the equipment in which they usually happen—tanks and tank cars—are relatively common), they are not yet sufficiently well-known.

The knowledge of this type of accident involves two aspects: the mechanism by which the accident takes place, and the main features of its physical effects.

Concerning the mechanism by which a BLEVE occurs, several authors have analyzed it and proposed theoretical treatments (Birk, 1995; Casal, Arnaldos, Montiel, Planas-Cuchi, & Vílchez, 2001; Reid, 1976, 1979); this aspect will therefore not be dealt with here.

With respect to the physical effects caused by these explosions, the following point must be taken into account: although a BLEVE is an explosion which takes place in a superheated liquid and—strictly speaking—can happen in a water tank, BLEVEs are usually associated with the explosion of tanks containing flammable liquids (for example, hydrocarbons). Therefore, to the effects of the BLEVE, one must add those corresponding to the fireball often occurring immediately after the explosion. On the whole, then, the physical effects from this type of explosion are usually thermal radiation, overpressure (blast) and the ejection of fragments (missiles).

Amongst these effects, thermal radiation has been widely studied (see, for example, Satyanarayana, Borah, & Rao, 1991), as has the behaviour of the fragments ejected by the explosion (Baum, 1988, 1999; Birk, 1995, 1996; Holden & Reeves, 1985). However, the overpressure generated by the explosion has been analyzed only by a few authors and is still difficult to predict. In this paper, the methodologies published up to now are discussed, and a new one that is more accurate from the thermodynamical point of view is proposed.

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Nomenclature

C_p	specific heat at constant pressure (J kg^{-1} K^{-1})
d	distance from the centre of the vessel to the point at which the overpressure must be calculated (m)
d_n	normalized or scaled distance (m kg$^{-1/3}$)
E_v	energy released in the vapour expansion (kJ)
f	vapourization factor (–)
H_v	enthalpy of vapourization (kJ kg^{-1})
m	mass of vapour existing initially (kg)
m_T	overall mass in the vessel (kg)
P	vapour pressure (bar)
P_a	atmospheric pressure (bar)
P_c	critical pressure (atm)
P_o	pressure just after the explosion (usually P_a) (MPa)
P_{sat}	liquid saturation pressure (bar)
S	entropy (kJ kg^{-1} K^{-1})
T	temperature (K)
T_c	critical temperature (K)
T_b	boiling temperature (K)
T_o	temperature of the substance at the moment of the explosion (K)
T_s	saturation temperature corresponding to atmospheric pressure (K)
u	internal energy of the vapour (kJ kg^{-1})
U_i	overall internal energy of the system just before the explosion (MJ)
u_L	internal energy of the liquid at the final state of the irreversible process (MJ kg^{-1})
u_G	internal energy of the vapour at the final state of the irreversible process (MJ kg^{-1})
ΔU	variation in the internal energy of the vessel content (kJ kg^{-1})
V	volume of vapour in the vessel (m^3)
ΔV	volume variation of the whole vessel content (m^3)
V_i	volume of the vessel (m^3)
V_r	volume of the spherical vessel (m^3)
V_l	volume of liquid in the vessel just before the explosion (m^3)
v_L	specific volume of the liquid at the final state of the irreversible process (m^3 kg^{-1})
v_G	specific volume of vapour at the final state of the irreversible process (m^3 kg^{-1})
W_{TNT}	equivalent mass of TNT (kg)
x	vapour fraction at the final state of the irreversible process (–)
β	fraction of the energy released converted into a pressure wave (–)
γ	ratio of specific heats, C_p/C_v (–)
ρ	density (kg m^{-3})
ρ_l	liquid density (kg m^{-3})
ρ_v	vapour density (kg m^{-3})

2. BLEVEs: a brief description

BLEVEs occur when a tank containing a pressurized liquid is heated, for example, due to a fire. As pressure increases, a condition is reached at which the walls of the container (whose temperature has been increasing, especially in the upper part where the liquid is not in contact with them) can no longer withstand the pressure and the vessel bursts. At the moment of failure, due to the instantaneous depressurization, the temperature of the liquid will be higher than that which would correspond to it according to the saturation curve on the P–T diagram: the liquid will be superheated. If the liquid temperature in the instant of the depressurization is higher than the "superheat temperature limit" (which is different for each substance), a violent and instantaneous flash of a fraction of the liquid will occur and a superheated liquid vapour explosion will take place.

The rapid and significant increase in the liquid's volume when it vapourizes plus the expansion of the previously existing vapour will give rise to a strong pressure wave, as well as to the breaking of the container into several pieces which will be propelled considerable distances (Stawczyk, 2003). Furthermore, if the substance involved is combustible, the mixture of

the liquid/gas released by the explosion will probably ignite, giving rise to a turbulent fireball. Due to the entrance of air and the heating of the mixture, the whole mass increases in volume turbulently, evolving towards an approximately spherical shape which rises, leaving a wake of considerable diameter. The radiation of such a fireball is very intense and covers large areas.

It is practically impossible to establish the exact instant at which the explosion will take place. In fact, once the conditions that can lead to a BLEVE are reached, the explosion can happen at any moment. Therefore, only preventive measures can be taken and evacuation is the best option in such circumstances.

However, to establish safety distances and to estimate the possible consequences of these accidents, the prediction of their physical effects is required.

3. Energy released and overpressure

The mechanical energy contained inside a vessel is suddenly released if it bursts in a BLEVE explosion. The substance contained in the vessel instantaneously increases in volume due to the expansion of the vapour already existing in the vessel at the moment of the explosion and to the partial vapourization—practically instantaneous (flash)—which the superheated liquid undergoes. This expansion will give rise to a pressure wave (blast) with an extraordinary destructive power. In the following sections, the methods proposed for estimating it are discussed.

3.1. Previous work

The energy released in the expansion of the vapour in the vessel (from the breaking pressure in the vessel up to the atmospheric pressure) is:

$$E_v = m(u_1 - u_2) \tag{1}$$

where E_v is the energy released in the expansion of the vapour (kJ), m is the mass of vapour already existing in the vessel at the moment of the failure (kg), u_1 is the internal energy of the vapour under the conditions at which the vessel bursts (kJ kg^{-1}), and u_2 is the internal energy of the vapour immediately after the expansion up to atmospheric pressure (kJ kg^{-1}).

Assuming that the vapour behaves as an ideal gas and that the expansion is adiabatic and reversible (isentropic), Prugh (1991) calculated this energy as:

$$E_v = \int P \, dV \tag{2}$$

integrating and introducing the relationship $P \cdot V^\gamma =$ constant (γ being the ratio of specific heats):

$$E_v = 10^2 \cdot \left(\frac{P \cdot V}{\gamma - 1} \right) \left(1 - \left(\frac{P_a}{P} \right)^{(\gamma-1)/\gamma} \right) \tag{3}$$

where E_v is the energy released (in kJ), P_a is the atmospheric pressure (bar), V is the initial volume of vapour (m^3), and P is the pressure (bar) in the vessel just before the explosion.

This energy can be expressed as TNT equivalent mass by using the appropriate energy conversion factor (approximately 4680 J/g of TNT),

$$W_{TNT} = \left(\frac{0.021 \cdot P \cdot V}{\gamma - 1} \right) \left(1 - \left(\frac{P_a}{P} \right)^{(\gamma-1)/\gamma} \right) \tag{4}$$

where W_{TNT} is the equivalent mass of TNT (kg).

Furthermore, if the vessel contained superheated liquid—as is the case in a BLEVE explosion—the released energy can be estimated approximately by using the same method. In this case, it must be taken into account that the mass of liquid will partly vapourize suddenly when it reaches atmospheric pressure. The volume of this vapour at the pressure in the vessel just before the explosion must then be calculated; adding this fictitious volume to the real one, the equivalent mass of TNT will then be (Prugh, 1991):

$$W_{TNT} = \left(\frac{0.021 \cdot P \cdot V^*}{\gamma - 1} \right) \left(1 - \left(\frac{P_a}{P} \right)^{(\gamma-1/)\gamma} \right) \tag{5}$$

where V^* is the volume of vapour in the vessel plus the volume (at the pressure inside the vessel) of the vapour generated in the instantaneous vapourization, in m^3:

$$V^* = V + V_1 \cdot f \cdot \left(\frac{\rho_l}{\rho_v} \right) \tag{6}$$

V is the volume of vapour inside the vessel before the explosion, V_1 is the volume of liquid in the vessel before the explosion (m^3), and f is the vapourization fraction (flash), i.e. the fraction of liquid which vapourizes in the depressurization. The value of f can be calculated by applying the mass and energy balances to a differential mass of liquid which vapourizes adiabatically. By introducing the adequate equations to take into account the approximate variation of H_v and $C_{p(liquid)}$ as a function of temperature, the following expression (Prugh, 1991) is obtained:

$$f = 1 - e^{-2.63 \cdot (C_p/H_v)(T_c - T_b)(1 - ((T_c - T_o)/(T_c - T_b))^{0.38})} \tag{7}$$

where T_c is the critical temperature of the substance (K), T_b is the boiling temperature (K) of the substance at atmospheric pressure, T_o is the temperature of the substance in the moment of the explosion (K). H_v and C_p are, respectively, the enthalpy of vapourization of the substance (kJ kg^{-1}) and the specific heat (kJ kg^{-1} K^{-1}) of the liquid at boiling temperature.

Once W_{TNT} is known, the pressure wave generated by the explosion can be estimated from the classical plot of overpressure vs. scaled distance (d_n) (Van den Berg & Lannoy, 1993).

However, in practice, the energy released when a vessel bursts in a BLEVE explosion is distributed among the following phenomena:

– the energy of the pressure wave,
– the kinetic energy of the projectiles,
– the potential energy of the fragments (the plastic deformation energy absorbed by the fragments), and
– the heating of the environment.

The way in which the energy is distributed among these different factors depends on the particular conditions of the explosion. An important aspect is the type of failure (fragile or ductile) (Casal et al., 2001). It has been suggested that in a fragile failure of a vessel, 80% of the energy released contributes to the creation of the pressure wave. On the other hand, in the case of a ductile failure—in which large fragments of the vessel are propelled—the energy in the pressure wave is only 40%. In both cases, the rest of the energy becomes kinetic energy of the fragments, as the fourth factor (heating of the environment) is negligible. In practice, most vessels are constructed with materials that are ductile in the operating conditions and BLEVE explosions usually involve ductile failure.

Therefore, to find the value of d_n, the fact that only a fraction of the mechanical energy released contributes to overpressure must be taken into account (Casal, Montiel, Planas, & Vílchez, 1999):

$$d_n = \frac{d}{(\beta \cdot W_{TNT})^{1/3}} \tag{8}$$

where d_n is the scaled distance (m kg$^{-1/3}$), β is the fraction of the energy released converted into pressure wave, and d is the real distance (from the centre of the explosion) at which the overpressure must be estimated (m).

The methodology explained above assumes ideal gas behaviour and a reversible adiabatic (isentropic) process, and involves the use of average properties for γ, C_p and H_v to calculate the energy released and the theoretical state that will be reached. However, these assumptions are far removed from the real phenomenon. Although in the sudden expansion associated with an explosion, the condition of an adiabatic process can be assumed due to the velocity of the phenomenon, it will never be a reversible process but rather a highly irreversible one. In fact, as the work associated with an isentropic process is the maximum of all the possible works that can be obtained from an adiabatic process, a considerable overestimation is introduced, the overpressure calculated being really the maximum possible value.

This is what spurred us to look for another method to establish the energy released if a—more realistic—adiabatic and irreversible expansion process is assumed and the real properties of the substance involved in the explosion are used.

3.2. A new approach

In this new methodology, the real expansion work ranges between two extreme values: the work corresponding to the isentropic expansion mentioned above, and the expansion work obtained when one assumes that the expansion is adiabatic but so irreversible that the only work performed is that associated with the variation in volume (ΔV) that takes place when the contents of the vessel changes from the conditions at explosion to the point of reaching atmospheric pressure ($P_o = 0.1013$ MPa). As in the isentropic approach, the hypothesis that immediately after the explosion there is liquid–vapour equilibrium at atmospheric pressure and the corresponding saturation temperature is also assumed; however, the state (entropy) will be different.

The real expansion work is $-P_o \cdot \Delta V$, ΔV being the variation in volume of the whole content of the vessel when it changes from the explosion state to the hypothetical final state. On the other hand, for an adiabatic process, this work must be equal to the variation in internal energy of the vessel content, ΔU:

$$-P_o \cdot \Delta V = \Delta U \tag{9}$$

This equation can be solved graphically. Fig. 1 shows the variation in U (for the whole content of the vessel) from the explosion situation to that of different conditions, defined by a common pressure of 0.1013 MPa and different liquid–vapour equilibrium conditions corresponding to different vapour fraction values. For both situations (just before the explosion and the final state), the whole mass of liquid plus vapour contained in the vessel was considered. In the same figure, the variation in $-P_o \cdot \Delta V$ was also plotted against the
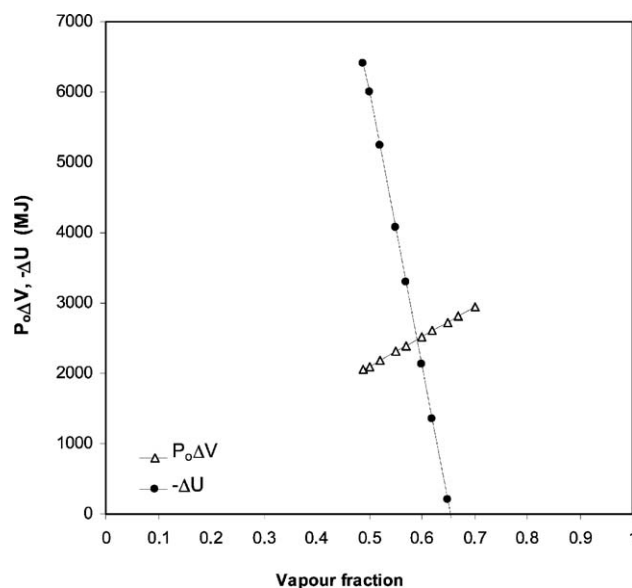

Fig. 1. Variation in U and $P_o \cdot \Delta V$ as a function of the vapour fraction of the theoretical final condition (see Example of application).

vapour fraction corresponding to the theoretical final condition. The intersection of both straight lines corresponds to the condition imposed by Eq. (9). The ordinate at this point represents both the variation in U and the energy released by the explosion.

Eq. (9) can also be solved analytically. Taking into account the mass and energy balances, the equations of the two straight lines plotted in Fig. 1 are:

$$-\Delta U = (u_L - u_G) \cdot m_T \cdot x - m_T \cdot u_L + U_i \quad (10)$$

$$P_o \cdot \Delta V = P_o \cdot [(v_G - v_L) \cdot m_T \cdot x + m_T \cdot v_L - V_i] \quad (11)$$

From these two equations, the intersection point can be found:

$$x = \frac{m_T \cdot P_o \cdot v_L - V_i \cdot P_o + m_T \cdot u_L - U_i}{[(u_L - u_G) - (v_G - v_L) \cdot P_o] \cdot m_T} \quad (12)$$

By substituting the value of x in Eq. (10) or (11), ΔU is found.

The TNT equivalent mass is therefore

$$W_{TNT} = \beta \cdot 0.214 \cdot \Delta U \quad (13)$$

(0.214 is the conversion factor (0.2136 kg MJ^{-1}); if this factor is used, units of ΔU must be bar m^3). The overpressure at a given distance can be found as mentioned before.

Although this approach leads to a lower theoretical value of the energy released, the real overpressure will be usually lower due to the drag and other practical aspects.

3.3. Example of application

To compare the values obtained using this new method with those obtained using the previous one, they were applied to a given case (Casal et al., 1999): a tank with a volume of 250 m^3, filled to 80% capacity with propane (stored as a pressurized liquid at room temperature), is heated by fire up to 55 $^\circ$C (19 bar) and bursts; the pressure wave must be estimated at a distance of 180 m from the location of the vessel.

The calculations were solved using real data for propane (Tillner-Roth, 1998); thus, the hypothesis of ideal gas must not be applied and it is not necessary to use average values of the propane properties. Table 1 shows all the values that define the initial state of propane (first column): temperature, pressure, specific volume of saturated liquid and vapour, internal energy and specific entropy corresponding to the saturation states, mass and volume of vapour and liquid, and internal energy of each phase and of the whole mass. It has been assumed that the volume of the tank does not vary and that no mass is lost (the safety valve is closed). Therefore, the vessel evolves at constant volume until it reaches the explosion temperature of 55 $^\circ$C. All data corresponding to this state can be seen in the second column of Table 1. The states and processes considered have been plotted schematically in the T–s diagram for propane (Fig. 2).

Table 1
Propane properties used in the example

	Initial state[a]	Explosion state[b]	Hypothetic final state (isentropic process model)[c]	Hypothetic final state (adiabatic process model and $W = -P_o \Delta V$)[d]
Pressure [kPa]	834.4	1901	101.3	101.3
Temperature [$^\circ$C]	20	55	−42.02	−42.02
Total mass [kg]	100 956	100 956	100 956	100 956
Mass of liquid [kg]	100 054	100 007	51 508	41 288
Mass of vapour [kg]	902	949.1	49 448	59 668
Vapour specific volume [m^3 kg^{-1}]	0.05539	0.02293	0.4136	0.4136
Liquid specific volume [m^3 kg^{-1}]	0.001999	0.002282	0.001721	0.001721
System specific volume [m^3 kg^{-1}]	0.002476	0.002476	0.2035	0.2452
Total vapour volume [m^3]	50	21.8	20 454	24 681
Total liquid volume [m^3]	200	228.2	89	71
Total volume [m^3]	250	250	20 543	24 752
Vapour fraction	0.008941	0.009401	0.4898	0.591
Vapour specific internal energy [kJ kg^{-1}]	549.7	582	483.7	483.7
Liquid specific internal energy [kJ kg^{-1}]	250.3	349.2	100.1	100.1
System specific internal energy [kJ kg^{-1}]	253.0	351.4	288	326.8
Total vapour internal energy [MJ]	500	560	23 920	28 860
Total liquid internal energy [MJ]	25 040	34 920	5150	4133
Total internal energy [MJ]	25 540	35 480	29 070	32 990
Vapour specific entropy [kJ kg^{-1} K^{-1}]	2.355	2.33	2.448	2.448
Liquid specific entropy [kJ kg^{-1} K^{-1}]	1.181	1.501	0.6068	0.6068
System specific entropy [kJ kg^{-1} K^{-1}]	1.192	1.508	1.508	1.695

[a] This and all the other states are supposed to be in thermodynamic equilibrium. There are not temperature or pressure gradients.
[b] This state is supposed to be reached because the tank does not change its volume and no mass is lost.
[c] This hypothetic state is specified by $P_o = 101.3$ kPa and a specific entropy equal to the tank specific entropy just before the explosion.
[d] This hypothetical state is specified by $P_o = 101.3$ kPa and the condition: $\Delta U = -P_o \cdot \Delta V$.
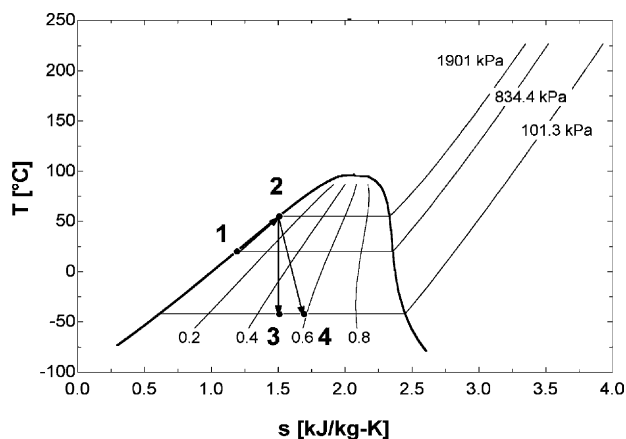
Fig. 2. Diagram temperature–entropy for propane. 1–2: heating of the tank; 2–3: isentropic (adiabatic and reversible) process; 2–4: adiabatic irreversible process.

Table 2
Variation in the internal energy and work for the two models

| | From explosion conditions to final conditions | |
	Isentropic	Irreversible
ΔU (MJ)	−6410	−2490
Work (MJ)	−6410	−2490

The third column of Table 1 shows the results obtained assuming an isentropic process: the final state is established by the pressure ($P_o = 0.1013$ MPa) and the entropy, which has the same value as the entropy just before the explosion.

Finally, the fourth column shows the results obtained assuming an adiabatic and irreversible expansion. The variation in the internal energy was obtained from the intersection of the two straight lines of Fig. 1.

Table 2 shows the variation in internal energy, heat and expansion work for the two models analyzed. It can be observed that in the case of an adiabatic irreversible expansion the energy released by the explosion is 2.5 times smaller than the energy obtained when an isentropic process is assumed.

Using the equivalence of 4680 J/g of TNT and assuming ductile failure of the vessel, an equivalent mass of TNT of 548 kg is obtained for isentropic expansion and 212 kg for adiabatic irreversible expansion. For the distance of 180 m, the plot of overpressure vs. scaled distance for TNT gives the values of overpressure of 5.3 and 4.0 kPa, respectively.

4. Conclusions

It is very difficult to predict accurately the overpressure generated by a BLEVE explosion in a given case, as it will depend on the specific circumstances.

The method proposed by Prugh (1991) and slightly modified by Casal et al. (2001)—which considers isentropic vapour expansion and ideal gas behaviour (approximate correlations are used to take into account the variation of properties as a function of temperature)—is far from the real phenomenon and in fact gives the maximum value of the overpressure that could be reached.

The new approach proposed here uses the real properties of the substance involved in the explosion; this is not a problem actually thanks to the existence of databases of thermophysical properties (NIST, JANAF, etc.) and avoids the use of approximate correlations. Furthermore, it considers adiabatic and irreversible expansion (an assumption which is more correct from the thermodynamic point of view) and thus gives a value of the pressure wave much closer to the real situation and allows less conservative and more realistic estimations of blast effects.

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