CHEMICAL ENGINEERING TRANSACTIONS
VOL. 48, 2016
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.aidic.it/cet
Guest Editors: Eddy de Rademaeker, Peter Schmelzer

ISBN 978-88-95608-39-6; **ISSN** 2283-9216
DOI: 10.3303/CET1648034

CFD Modelling of Blast Waves from BLEVEs

Olav R. Hansen, Malte T. Kjellander*

Lloyd's Register Consulting – Energy, Fjøsangerveien 50B, 5059 Bergen, Norway
Malte.Kjellander@lr.org

Boiling Liquid Expanding Vapour Explosions (BLEVEs) are among the major hazard scenarios to be considered in siting studies as well as transportation safety assessments. The main hazards from BLEVEs consist of blast waves and projectiles, and radiation for flammable and toxicity for toxic substances. Well established relations exist to predict consequences for BLEVEs in the open. With increasing confinement, due to tanks being inside or surrounded by buildings, or tunnels for transport scenarios, the consequences from blast waves become more severe, while the empirical relations can no longer be used to predict the consequences. Blast waves from BLEVEs are partly caused by expansion of pressurized vapour head, partly by the rapid phase change of the boiling liquid, and further pressure waves may be generated by pressure oscillations and combustion. Which mechanism that will dominate the blast generation will depend on the vapour head volume and pressure and the degree of superheat of the liquid. FLACS, a computational fluid dynamics (CFD) model has been applied to model blast waves from BLEVEs. The modelling of the different contributions to blast waves has been validated against experiments. For accurate results, both directional effects due to shape of tank and the cooling during the rapid phase change must be included in the modelling. With the validated modeling approach the CFD model can be applied to predict partially confined BLEVE scenarios, including tunnel scenarios. We consider our modelling approach to be more accurate than similar work published in the past.

1. Introduction

BLEVEs might occur when vessels storing a liquid above its normal boiling point loose containment catastrophically. If the breach is not catastrophic, that is, if it is limited or slow, the result will be a flashing liquid or gaseous jet leak. For a BLEVE to occur it is necessary that the vessel ruptures entirely and instantaneously. The liquid will quickly be depressurized and suddenly be far above its boiling point, resulting in violent flashing. The appearing vapour will push away the surrounding air and if the process is fast enough, generate shock waves. If the gas is flammable it may ignite and cause further damage as large fireballs are formed, causing thermal radiation. Many common liquids are stored at such conditions, e.g. hydrocarbons, chlorine, carbon dioxide, ammonia and other refrigerants. Certain liquids with boiling points normally above ambient conditions may be heated and thereby reaching conditions where a BLEVE might occur, for example water in an overheated steam boiler.

The consequences of a BLEVE are often severe and excluding escalation effects these can be divided in three sources: pressures waves, projectiles and – if the liquid is flammable – fireball radiation. Empirical methods exist to estimate the pressure and fireball effects in the open, and especially the radiation from the fireball have shown good agreement with experiment. The present study is concerned only with the pressure waves. The blast overpressure can be predicted with an analogue of the TNT-equivalence method, where the energy of the explosion is estimated from the available expansion energy in the vapour and/or liquid. Different authors suggest methods for estimating the energy to be used as input: usually assuming isentropic or irreversible expansion of the vapour and/or liquid to ambient conditions, and then selecting an empirically determined fraction of that energy. Some, if not all of these methods seem to over-predict the strength of the blast waves however, and they naturally may only be used in unrestricted geometries.

There seem to be no complete consensus on the exact source of the blast overpressures. Reid (1976, 1979) stated that a BLEVE may only happen if the pressure and temperature is around or above the superheat limit temperature, so that spontaneous homogenous nucleation occurs. However, experiments have shown that

Please cite this article as: Hansen O., Kjellander M., 2016, Cfd modelling of blast waves from bleves, Chemical Engineering Transactions, 48, 199-204 DOI:10.3303/CET1648034

strong pressure waves might be generated even though the temperature is well below this limit. Typically the vessel will not be completely filled with liquid: it also contains a vapour head. At tank rupture, this pressurized and overheated gas will cause a shock wave to form as it rapidly expands – Birk (2007) states that this vapour space is may be the main source of the blast wave and that the liquid evaporation may be too slow to contribute to far-field blasts – but might have significant effects in the near-field or propel projectiles consisting of pieces of the vessel. Birk also suggests there might be a scaling effect and that liquid flashing might produce shock waves in larger scale BLEVEs.

Detailed CFD (computational fluid dynamics) simulations accounting for the multi-phase nature of the problem, including nucleation and evaporation of the subsequently expanding vapour have been carried out in 1D, but are currently not practical in a real three-dimensional setting. Van den Berg (2004, 2006) carried out single-phase 2D CFD studies where the BLEVE was modelled as a pseudo-source through a boundary-condition where the evaporation-rate was driven by inertial forces. Simulating the flashing liquid is computationally expensive and currently not practical to use in industrial-scale risk analysis. The present study aims to create a source-model that can be used in three-dimensional simulations with readily available commercial softwares.

The approach presented considers both the vapour and liquid sources of pressure waves. The vapour is modelled in a straightforward manner while a pseudo-source models the liquid. The liquid energy is represented by an overpressure region containing expansion energy equal to the energy available for flashing and expansion in the liquid space, with the flashed gas cooled to ambient boiling point of the liquid. The models are used in a regular Navier-Stokes solver.

2. Experiments

Our simulations are mainly based on the experiments conducted by British Gas (Johnson et al., 1991) and Birk et al. (2007). The British Gas experiments centered on a base case of a 5.7 m^3 tank filled with 2 metric tonnes of butane. Blast overpressures, projectiles, fireball size and resulting radiation were measured and documented. A parametric study was made varying tank size, fuel mass, pressure and gas. The fuel was heated using electrical heaters inside the tanks until desired temperature and pressure. Shaped charges placed along the top of the tanks were used to initiate catastrophic failure. The method of heating and rupture produced repeatable results with the tanks failing in similar manner. The scale and repeatability makes the experiments suitable for the purpose of developing methods to predict the effects of the BLEVE and will serve as benchmark tests for the present study.

Birk et al. presents a number of BLEVE experiments conducted over a decade. The tanks were heated until they ruptured: this is realistic but for our purposes the opening is less controlled and the repeatability is limited. They distinguished between what they designate one-step and two-step BLEVEs. The one-step process was described to be a single continuous opening of the tank that is too fast for the flashing of the liquid to do any work on the tank, and the vapour space is therefore partly depleted while doing work to rupture the tank. In the two-step BLEVE the opening temporarily stops or slows down as the pressure of the vapour space is depleted, and a second opening stage occurs when flashing from the liquid quickly replenishes the vapour space. When the tank eventually ruptures there is more energy available in the vapour, which causes stronger blast waves. It is likely that the opening is re-accelerated before the pressure reaches the pressure of the initial of rupture and a conservative choice of vapour pressure at the time of final and catastrophic failure is the pressure at the initial rupture. Although the model is benchmarked against the British gas experiments, a comparison with one of the worst cases from Birk's experiments will also be offered as a realistic test of the method: case 01-2 which was described as a two-step process.

3. Problem formulation

At the time of rupture it is assumed that the tank is filled to some level of liquefied gas. Above the liquid there is a gas head at the same pressure but possibly with another temperature. Assuming an ideal opening, i.e. one where the tank ruptures instantly and completely, a shock wave will be formed at the interface between atmosphere and vapour space. This is a 2- or 3D equivalence of a shock tube problem, which has a well-known solution and most relevant CFD tools are validated for this problem. Simultaneously the liquid space is quickly depressurized. Suddenly having a temperature far above the saturation temperature, the liquid starts to boil violently. The processes involved are not nearly as well-known as with those in the vapour space, as described previously. The evaporation rate for this process is not known, and shock waves will only be formed if this rate is rapid enough. Depending on the circumstances, the remaining liquid might burn in a pool fire or continue to evaporate. The released gas will disperse or, if the gas is flammable, it may ignite and result in a fireball. Delayed ignition with flash fires or vapour cloud explosions is also possible. The change in pressure experienced by a point in the far field due to these events may be summarized as:

1. An initial overpressure peak caused by the expansion of the vapour space and/or the flashing of the liquid
2. A negative phase due to overexpansion
3. A second pressure peak due to the reflection of the expansion wave, or oscillation of the expanded gas cloud.
4. Overpressure generated by combustion if the gas is flammable and ignited

In the British Gas experiments a second peak immediately after the first sometimes occurred, but the nature of this peak was not thoroughly explained. It was suggested that the overpressure pulse from the vapour expansion sometimes merges with pressure waves emanating from the flashing of the liquid and subsequent expansion, while sometimes they come separated. Assuming that this is correct we have used the following approach:

I. Modelling only the vapour space neglecting flashing entirely. First investigate whether the overpressure from the vapour space can be adequately modeled. Compare with the experiments: if the assumption above is correct, in the cases where the liquid and vapour peaks are separated this should give good predictions.
II. Vapour and liquid. Unfortunately no large-scale experiments with only liquid were available - instead, the vapour and liquid spaces are modeled simultaneously and comparisons made with experiments. The liquid space will be modeled by a pseudo-source as described below.

The vapour space is straightforward to model. Assuming an ideal opening, which is a reasonable model for the British gas experiments where explosives were used to break the tank evenly and instantaneously, this can be modelled directly as a volume of high pressure gas. The liquid space on the other hand is modelled by a pseudo-source: a second high pressure volume, but the pressure and mass are determined so that the irreversible expansion energy of the pseudo-source corresponds to the energy calculated from the real liquid source. Different methods to estimate this energy were tested, the one selected for the calculations estimated the mass of flashed gas and added this as a high pressure volume next to the vapour space. The temperature of the liquid source is set to the boiling point of the liquid as it is assumed the gas cools as it flashes. Initial tests showed that immediate and complete flashing resulted in overestimation of pressure peaks of an order of magnitude. This is not surprising as it has previously been pointed out that the evaporation may not be fast enough to produce pressure waves coalescing into shock waves, and e.g. Genova (2008) suggests using only 7% of the available thermal energy when applying energy-equivalent methods. The pressure was therefore reduced to an empirical fraction of 20% of the initial pressure. Descriptions of these processes may be found in e.g. Reid (1976) and Casal, J. et al. (2002).

4. Simulations

The numerical computations were performed with the commercial 3D RANS-solver FLACS. A square domain with grid size 0.1 m in the vicinity of the tank was used. The pressure was monitored at the same locations as in the experiments: however the slightly inclining ground in the experiments was replaced with a completely flat surface. The monitor points in the simulations were located at the same height above the ground as the real pressure sensors and not at the height relative to the tank. Table 1 shows an overview of the test cases, five from the British Gas tests and one from Birk (2007).

Table 1: Overview of the test cases

Experiment	Mass (t)	Pressure (barg)	Gas	Vessel size (m^3)	Liquid fill (-)	Liquid temp (°C)	Vapour temp (°C)
British gas experiments:							
1R	2	15.1	Butane	5.7	77%	95	83
2	2	15.2	Butane	5.7	39%	101	90
3	1	7.7	Butane	5.7	68%	50	12
4	2	15.1	Butane	10.8	40%	82	90
5	2	15.2	Propane	5.7	80%	35	34
Birk 02—1		18	Propane	1.9	51%	57	61

Figure 1 shows the pressure histories for various distances from the tank. The typical appearance of the BLEVE pressure wave is well reproduced and the values are either reasonably accurate or conservative. Peak values for all cases are tabulated in Table 2, for comparison with experiments. Figure 2 shows the pressure contours along the perpendicular axis and at a horizontal plane 1 m above the ground. The 3-dimensional effects as a result of the elongated tank shape are clearly seen, with shock waves being stronger in the perpendicular direction. Reflection against the ground shows a stronger wave close to the ground.

For most cases the simulations considering only the vapour space give pressures as high as the experiments. Only in some cases the pressures were lower than the experimental. Especially BLEVE 1R with the smallest vapour head resulted in pressure 30-40% lower than the measured. This is likely a combination of a small vapour head and a large degree of superheat: BG BLEVEs 3-5 have relatively low temperatures compared to the superheat limit. The vapour head simulations are performed by direct simulation of the vapour head the results show that the overpressure generation might very well be mainly due to the vapour in the tank. However, when the tank is mostly filled with liquid or the degree of superheat is large, also the liquid flashing must be taken into consideration.

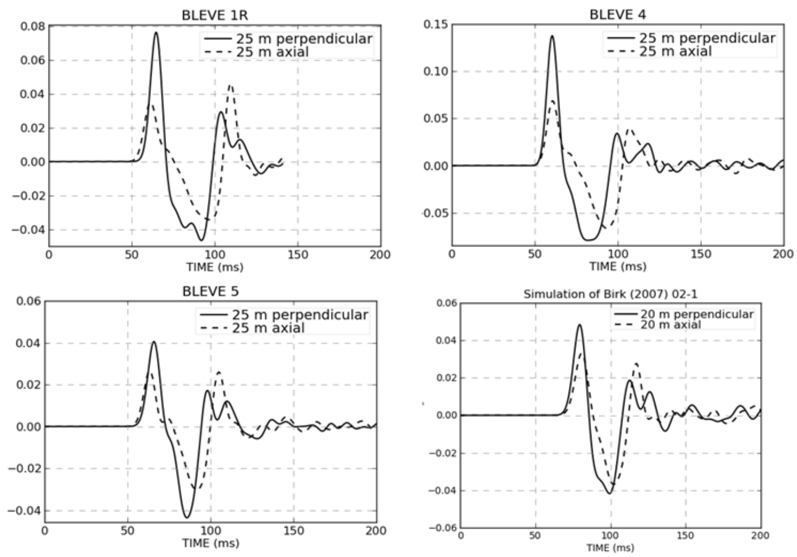

Figure 1: Pressure histories from sensors 1 (25 m perpendicular to axis) and 2 (25 m along axis) from BLEVE 1R, 4, 5 and Birk 02-1 (at 20m) are shown. The typical two-peak behaviour is clearly captured by the simulations.

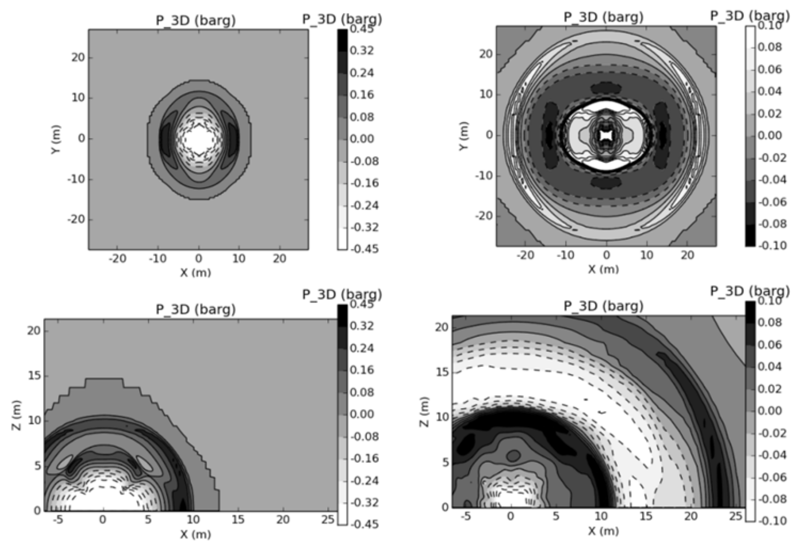

Figure 2: Pressure contours of BLEVE 1R at 20 ms (left) at 60 ms (right) after rupture. Upper pictures show a horizontal plane 2 m above the surface, while the lower show the perpendicular cross-section.

Table 2: Overview result. BG refers to the British Gas experiments. All values in mbarg.

Case	Mass (t)	Simulations vapour only	Simulations Vapour&liquid	Experiments
BG 1R	25 m W	45	76	63
	50 m W	18	26	39
	25 m N	15	35	18
	50 m N	6	14	10
BG 2	25 m W	89	96	50
	50 m W	35	40	28
	25 m N	40	45	16
	50 m N	16	20	11
BG 3	25 m W	30	76	10
	50 m W	12	24	5
	25 m N	10	37	4.5
	50 m N	4	14	-
BG 4	25 m W	110	138	82
	50 m W	42	47	34
	25 m N	30	68	9
	50 m N	19	27	8
BG 5	25 m W	35	40	23
	50 m W	10	13	12
	25 m N	12	26	11
	50 m N	5	9	6
Birk 02-1	10 m	155	300	130
	20 m	65	95	90
	30 m	36	43	60

5. Conclusions

A new method for simulating the pressure effects from BLEVEs in 3D has been developed. Although the simulations were performed with the Navier-Stokes equations, they could be even faster using the Euler equations without much loss of accuracy. The method enables detailed studies of actual incidents or risk analysis with realistic geometries, such as tunnels and process or storage facilities.

The shock caused by the vapour head is simulated by assuming a pressure jump with instantaneous opening. Comparison with experiments shows that in many cases it is entirely possible for the vapour head to cause the measured maximum pressures without direct contribution from the liquid flashing. The liquid would in this case contribute indirectly by creating boiling before and during the vessel failure to build up or replenish the pressure, as described by Birk.

The liquid space was modelled using a pseudo-source with a high-pressure region contained expansion energy corresponding to that of the liquid space in the tank. Using the entire energy severely overestimates the resulting pressure waves and there is a need to determine the fraction of energy that contributes to blast waves. This is analogous to the energy-equivalent methods using an empirical fraction of the energy.

Some simulations underestimated the pressure when only vapour was used, and since the vapour setup is idealized with a perfect opening, this indicates that liquid contribution should be considered. It is worth noticing that, consistent with the conclusion, this happened for the cases with the largest degree of superheat and largest amount of liquid fill.

The pressure histories from experiments show a distinct pattern with two or more sharp peaks. The second pressure wave is clearly affected by the evaporation of the liquid even if the first peak would be mainly due to vapour. If only vapour is present, the second peak is due to the reflection of the expansion wave and is not nearly as distinct, and comes much closer behind the first. Evaporation would clearly interfere with this process and temperature drop causes a delay of the second peak compared to when only vapour head is simulated. It is expected that finite evaporation rates would affect this, but this is out of the scope of this study.

The largest advantage of being able to use CFD is that 3D effects and complicated geometries ca be represented which enables realistic situations to be modelled. The effect of tank shape is also captured: the pressure is higher in the direction perpendicular to the tank axis. In all scenarios the pressure is either similar to the experiments or slightly conservative.

References

Birk A.M., Davison C., Cunningham M., 2007, Blast overpressures from medium scale BLEVE tests, Journal of Loss Prevention in the Process Industries 20, 194-206, doi:10.1016/j.jlp.2007.03.001

Casal J., Arnaldos J., Montiel H., Planas-Cuchi E., Ichez J. A. V., 2002, Modeling and understanding BLEVEs, chapter 22 The Handbook of Hazardous Materials Spills Technology, McGraw-Hill, New York, USA

Genova B., Silvestrini M., Trujillo F.J.L., 2008, Evaluation of the blast-wave overpressure and fragments initial velocity for a BLEVE event via empirical correlations derived by a simplified model of released energy, Journal of Loss Prevention in the Process Industries 21(1), 110-117, DOI:10.1016/j.jlp.2007.11.004

Hemmatian B., Planas-Cuchi E., Casal J., 2014, Analysis of methodologies and uncertainties in the prediction of BLEVE blast, Chemical Engineering Transactions, 36, 541-546, DOI: 10.3303/CET1436091

Johnson D.M., Pritchard M.J., Wickens M.J., 1991, A large scale experimental study of BLEVEs, British Gas Report No I536, the United Kingdom

Johnson D.M. & Pritchard M.J., 1991, Large scale experimental study of boiling liquid expanding vapour explosions
(BLEVEs), Gastech 90: The 14th Int. LNG/LPG Conference And Exhibition, 1-30.

Laboureur D., 2012, Experimental characterization and modelling of hazards: BLEVE and boilover, PhD Thesis from the von Karman Institute / Université Libre de Bruxelles, ISBN 978-2-87516-055-3

Reid, R. C. 1976, Superheated Liquids, American Scientist 64, 146–156

Reid, R. C. 1979, Possible Mechanism for Pressurized-Liquid Tank Explosions or BLEVEs, Science 203, 1263–1265.

van den Berg A.C., Van der Voort, M.M., Weerheijm, J., Versloot, N. H. A., 2004, Expansion-controlled evaporation—A safe approach to BLEVE blast, Journal of Loss Prevention in the Process Industries 17, 397-405, Doi:10.1016/j.jlp.2004.07.002

van den Berg A.C., Weerheijm, J., 2006, Blast phenomena in urban tunnel systems, Journal of Loss Prevention in the Process Industries 19, 598-603, DOI: 10.1016/j.jlp.2006.03.001