

MODELLING OF FORMATION AND COMBUSTION OF ACCIDENTALLY RELEASED FUEL CLOUDS

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Processes accompanying accidental releases of pressurised fuels into the atmosphere are considered from the pointview of their modelling for hazard evaluation. Models for the fuel cloud expansion in the case of total loss of containment (vessel bursts) are presented and applied to the analysis of boiling liquid expanding vapour explosions. Cloud expansion velocities, turbulent characteristics, parameters of pressure waves and fireballs occurring after fuel ignition are obtained and compared with the experimental data.

INTRODUCTION

Accidental release and ignition of flammable substances may have severe consequences[1,2], which requires development of predictive techniques for quantitative estimation of release characteristics and effects. One of the most dangerous types of accidents with pressure-liquefied hydrocarbons is the Boiling Liquid Expanding Vapour Explosion (BLEVE), a sequence of events involving burst of (usually pre-heated) storage vessel, boil-up and flash evaporation of liquefied substance generating blast wave in the atmosphere. BLEVEs are often followed by ignition of the fuel cloud and formation of a fireball in which large quantities of fuel burn over a short period (from several to about 10–20 seconds depending on fuel mass and pre-release conditions) emitting powerful heat fluxes endangering people and property[3].

Despite the evident recent progress in understanding and quantification of the main physical processes governing development and effects of industrial accidents involving flammable substances, there still remain areas where further progress is necessary. One such area is the formation and combustion of fuel clouds following bursts of pressure vessels. Experiments on BLEVEs, especially larger-scale ones, are difficult to conduct because the event is of short duration and accompanied by uncontrolled energy release, shock waves, projectiles etc. It is not surprising that each such experiment is unique, and the data reported is usually very scarce. Only a few theoretical approaches to this problem have been offered so far [4,5].

In this paper numerical modelling is applied to study the features and effects of accidental hydrocarbon releases into the atmosphere caused by loss of containment, formation and combustion of flammable clouds.

FUEL CLOUD EXPANSION

After a volume of pressure-liquefied gas has been exposed to low ambient pressure, as occurs after total loss of containment or massive damage to the pressure vessel, it starts to expand, mixes with the air, so that a fuel-air cloud builds up in the atmosphere. For a typical industrial accident, the internal energy released in this process if high enough to result in blast waves and missile effects of vessel fragments[3]. Note that, unlike conventional explosions, this energetic event occurs without involvement of any chemical reactions (so-called physical explosion), similar accidents can occur with non-combustible substances (e.g., high-pressure water).

Analysis of the available experimental data on visible cloud expansion velocities has shown that, in appropriately chosen non-dimensional variables, the visible cloud expansion velocity can be presented as a unified function of time in a wide range of superheated liquid masses, fuel properties (boiling temperature, heat of evaporation) and initial conditions (pre-release temperature and pressure)[6]. The length, velocity and time scales are defined as[7]

$$L_* = \left(\frac{MR_gT_a}{P_a}\right)^{1/3} \tag{1}$$

$$U_* = \{2(h_{l,0} - [(1 - x_v)h_{l,a} + x_v h_{v,a}])\}^{1/2} \tag{2}$$

$$t_* = \frac{L_*}{U_*} \tag{3}$$

where M is the fuel mass, R_g is the gas constant, T_a and P_a are the ambient temperature and pressure, h_l and h_v are the enthalpies of saturated liquid and vapour (subscripts 0 and a refer to the initial and ambient conditions respectively), x_v is the mass fraction of vapour after flash evaporation of superheated liquid determined from the isoentropic relationship

$$x_v = \frac{s_{l,0} - s_{l,a}}{s_{v,a} - s_{l,a}} \tag{4}$$

where $s_{l,0}$ is the entropy of the saturated liquid at the initial conditions, $s_{l,a}$ and $s_{v,a}$ are the entropies of saturated liquid and vapour at the ambient conditions.

In Figure 1 the data of small-scale experiments[8] (Freon-113, $M = 4 \cdot 10^{-3}$ kg), medium-scale tests[9] (propane, $M = 163$ kg) and larger-scale experiments[10] (propylene, $M = 15.6 - 452$ kg) are plotted in the logarithmic coordinates as the dependence of the

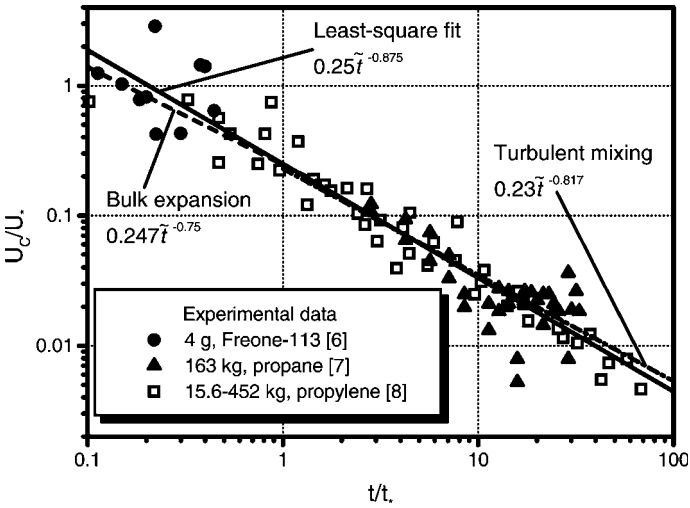

Figure 1. Summary of experimental data on expansion of two-phase clouds following total loss of containment (points); results of models for bulk expansion and turbulent mixing stages (lines)

non-dimensional visible cloud expansion velocity $\tilde{U}_C = U_C/U_*$ on the non-dimensional time $\tilde{t} = t/t_*$. It can be seen that, despite substantial differences in the masses and properties of the substances used, the data can be fitted by a single power-law approximation

$$\tilde{U}_C = 0.25\tilde{t}^{-0.875} \tag{5}$$

One of the first attempts to describe expansion characteristics of volumes of pressure-liquefied gases following partial loss of containment was undertaken by Hardee and Lee[11]. Their model implied momentum conservation during the development of a directional release into the atmosphere. By equating the momentum created by the source instant to the total momentum of the cloud at some instant, a relationship for the growth rate of the cloud was obtained. Isoentropic relationships (2), (4) were applied to estimate the initial velocity of two-phase mixture released by the source, i.e., the difference between the internal energies in the initial and final states was assumed to be equal to the mixture kinetic energy. The model[11] predicted only the size of the growing jet, but did not provide any means for estimating the spatial distribution of concentration in it.

As for the case of total loss of containment, where the superheated liquid expands radially in all directions and the cloud is almost spherical or hemi-spherical (for

near-ground vessel bursts), only a limited number of experimental studies detailed enough to quantify the cloud expansion characteristics has been carried out so far, and no physically grounded model predicting the cloud growth velocity existed until recently. For example, the model for fuel concentration in the expanding cloud[10], in which the cloud was assumed to consist of a constant-concentration core and the peripheral zone with exponentially decaying concentration, was just an approximation to the experimental data.

Development of pressurized fuel clouds following total loss of containment starts with pressure-driven bulk expansion of boiling liquid caused by rapid increase in its specific volume, followed by nearly isobaric cloud growth governed by turbulent mixing of vapour with the ambient air. While the first stage is featured by strong gas dynamics effects, shock wave formation etc., no significant radial velocities are observed during the second stage characterised by gradual dissipation of turbulence in the cloud.

It is interesting to note that a simple extension of the model[11], developed for the directional outflows, to the case of symmetric cloud expansion following total loss of containment, gives quite a good agreement with the experimental data presented in Figure 1. The main difference in deriving the model relationships is that, because of spherical symmetry, the momentum conservation should be applied to the flow contained within some given solid angle, rather than to all the flow generated by the source. Assuming frontal capture of the ambient air by the expanding cloud, the following result for the bulk expansion stage was obtained in[4]:

$$\tilde{U}_C = \frac{3^{1/4}}{4\pi^{1/4}}\tilde{t}^{-3/4} \approx 0.247\tilde{t}^{-0.75} \tag{6}$$

This relationship is plotted in Figure 1 by the dashed line.

For the second (turbulent mixing-governed) stage of cloud growth a different model has to be applied because the main assumptions used in deriving (6) are no longer valid. At this stage, since the average velocity is very low due to spherical symmetry and isobaric conditions, no significant shear stresses exist and, hence, generation of turbulent energy can be neglected. The cloud turbulence generated during its bulk expansion decays gradually due to viscous dissipation and entrainment into the cloud of the non-turbulent ambient air. Thus, the cloud can be approximated by a variable-size spherical volume with some volume-averaged levels of turbulent kinetic energy k and its dissipation rate ε, the cloud growth is governed by turbulent diffusion at its envelope which depends on the current turbulent characteristics of the cloud. This approach was followed in[4], where ordinary differential equations for the volume-averaged cloud characteristics were derived from the well-known $k-\varepsilon$ model of turbulence with the turbulence generation terms omitted. Power-law solutions were found for the non-dimensional expansion velocity $\tilde{U}_C$, turbulent kinetic energy $\tilde{k} = k/U_*^2$ and its dissipation rate $\tilde{\varepsilon} = \varepsilon L_*/U_*^3$:

$$\tilde{U}_C = A\tilde{t}^{\alpha-1}, \quad \tilde{k} = B\tilde{t}^{2(\alpha-1)}, \quad \tilde{\varepsilon} = E\tilde{t}^{2\alpha-3}, \quad \alpha = \frac{2C_2-5}{5(C_2-1)} \approx 0.183 \tag{7}$$

Here $C_2 = 1.92$ is the empirical constant of the $k - \varepsilon$ turbulence model. The constant A was found from the best fit of the expansion velocity (7) to the experiments in Figure 1 (see the dash-dotted line), the B and E constants were then calculated from the consistency relationships naturally emerging in the model. This results in

$$\tilde{U}_C = 0.23\tilde{t}^{-0.817}, \quad \tilde{k} = 0.46\tilde{t}^{-1.634}, \quad \tilde{\varepsilon} = 0.50\tilde{t}^{-2.634} \tag{8}$$

It can be seen from Figure 1 that both models agree quite well with the experimental data, the intersection of lines corresponding to bulk expansion (6) and turbulent mixing (8) stages occurs at $\tilde{t} \approx 1$, so that the change of the cloud expansion mechanism can be expected at this instant. This conclusion seems physically grounded because the time scale t_* (see (1)–(3)) is defined in terms of the characteristic cloud size and the expansion velocity caused by the internal energy release. Unfortunately, the experimental data is too noisy to substantiate the exact instant at which the change of expansion regimes occurs.

An insight into the dynamics, structure and characteristics of expanding volume of superheated liquid or pressure-liquefied gas following total loss of containment may be obtained from the differential model[7]. One-dimensional spherically symmetrical statement of the problem is used, the following zones presented schematically in Figure 2 are considered: saturated liquid, liquid-bubble mixture, vapour-air-droplet mixture and ambient air. Multiphase fluid dynamics equations are used, different sub-models are applied to the liquid/bubble and vapour/droplet flows, they are matched at the interface corresponding to some prescribed volume fraction of the vapour phase (typically, 70%). Special treatment is given to the modelling of turbulence generation in a radially expanding cloud

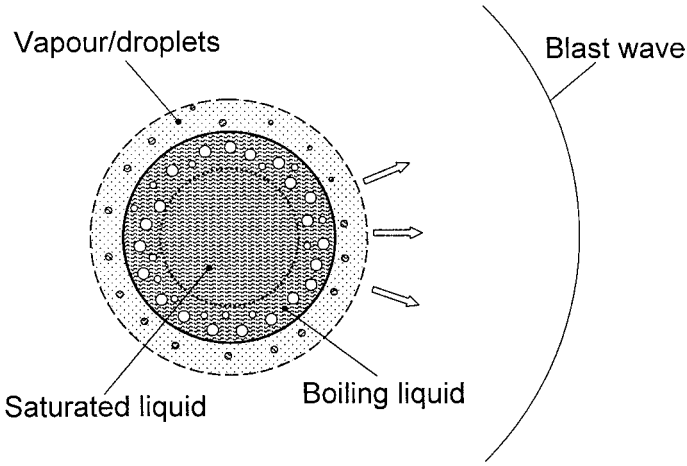

Figure 2. Main zones of expanding two-phase cloud considered in differential model [5]

where the shear stresses due to average velocity gradients are very low. To account for the intensive cloud turbulisation observed in the experiments within the framework of one-dimensional spherically symmetric statement of the problem, the turbulence generation terms were modelled by assuming similarity of the turbulent structure of expanding cloud and of an imaginary set of turbulent jets originating from the cloud centre. Calculations were performed using adaptive grids to ensure high resolution of gas-dynamic discontinuities and of steep gradients of flow variables. The model gives the characteristics of the expanding flow (spatial and temporal distributions of fuel vapour and droplets, turbulent characteristics, pressure distributions) which cannot be obtained from the theory of Hardy and Lee. The equations may also be solved using the single-phase state relationships, which allows the bursts of vessels with compressed gases to be analyzed. Below application of the differential model[7] to the analysis of BLEVE blast effects is presented.

PRESSURE WAVES GENERATED BY EXPANDING CLOUDS

Consider first the radial pressure distributions demonstrating the dynamics of pressure-liquefied fuel cloud expansion following total loss of containment. Calculations were carried out for pressure-liquefied propane at different pre-release conditions summarised in Table 1. The total energy E released during the cloud expansion was estimated as the difference between the enthalpies of liquid and vapour-liquid mixture in the initial and final states determined from thermodynamics (see Eqs. (2), (4)):

$$E = M(h_{l,0} - [(1 - x_v)h_{l,a} + x_v h_{v,a}]) = \frac{MU_*^2}{2}$$

In Figure 3a,b the radial pressure profiles are shown at several instants after burst of a vessel filled with $M = 100$ kg of propane at the initial temperature of $T_0 = 300$ K (the initial pressure $P_0 = 10$ bar, the length, velocity and time scales (1)–(3) are $L_* = 3.8$ m, $U_* = 177$ m/s, $t_* = 13$ ms, the initial diameter of the liquid volume is 0.73 m). The pressure P, bar, is plotted against the non-dimensional radial coordinate r/L_*.

Table 1. Parameters of calculations of pressure-liquefied propane cloud expansion

Run No.	M, [kg]	T_0, [K]	E, [MJ]	r_{eff}/r_*	Explosion efficienty χ, [%]
1	1	300	0.0157	3.5	2.3
2	10	300	0.157	3.5	2.3
3	100	300	1.57	3.7	2.0
4	1000	300	15.7	3.7	2.0
5	10	315	0.306	2.8	4.6
6	2000	315	61.2	2.8	4.6
7	10	350	0.84	2.5	6.4

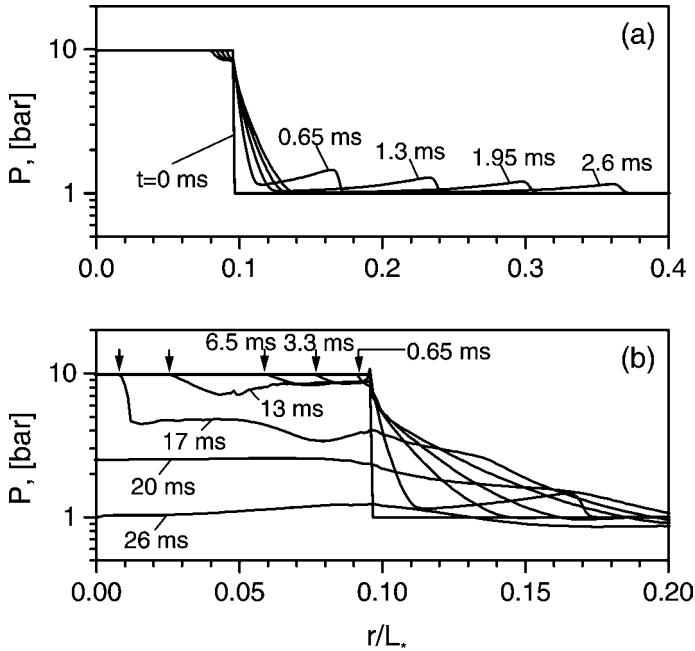

Figure 3. Radial pressure profiles after burst of vessel filled with 100 kg of propane at $T_0 = 300$ K: a) formation of pressure wave in the air caused by cloud expansion; b) propagation of boiling wave (shown by arrows) through the volume of superheated liquid

Break-up of the pressure discontinuity existing initially at the liquid-air boundary causes formation of a pressure wave travelling outwards in the ambient air (Figure 3,a). At the same time, a pressure relief wave propagates through the initially saturated liquefied gas towards the centre. Behind the converging boil-up front (i.e., in the zone between the boil-up front and outer boundary of the liquid-bubble mixture, see Figure 2) the liquid is in equilibrium with vapour at the saturation conditions corresponding to the local pressure. The boil-up front velocity is much lower than the velocity of the outward pressure wave because the speed of sound in the saturated liquid-bubble mixture is very low (of the order of 10 m/s) in comparison with the speed of sound in the saturated liquid and in the air[12]. Therefore, the energy release rate is limited by this slow propagation of boiling wave, which is in sharp contrast with high explosives, vapour cloud explosions and bursts of vessels filled with compressed non-condensable gases, where fast energy release and its efficient conversion into the energy of blast wave occurs.

More details about the pressure relief and boil-up wave propagation through the initially saturated liquid following total loss of containment are given in Figure 3b,

where pressure profiles are shown for the same initial parameters as in Figure 3a, from an early instant t = 0.65 ms, up to the time t = 26 ms when the pressure in all the cloud nearly drops to the ambient level. The positions of the boil-up front, corresponding to the points of sharp decrease in the pressure, are denoted by arrows. The converging boiling front reaches the cloud centre in about 18 ms, which corresponds to the time when all high-pressure saturated liquid starts to boil and the internal zone in Figure 2 disappears. Afterwards the radial flow generated results in some overexpansion (the pressure falls below the ambient level in some limited area near the origin), this overexpansion, however, is much weaker than that observed in the case of bursts of vessels filled with compressed single-phase gases[15].

An important issue in estimating BLEVE hazards is the quantification of the parameters of blast waves generated by the expanding superheated liquid. Here the results of numerical calculations carried out for the parameters listed in Table 1 are used to assess the efficiency of energy conversion into the blast wave in comparison with high explosives. Firstly, for each run the maximum relative overpressure ΔP_s was determined at each numerical grid point and the energy-based radius r_* was calculated from the total internal energy E:

$$\Delta P_s = \frac{P - P_a}{P_a}, \quad r_* = \left(\frac{E}{P_a}\right)^{1/3} \tag{9}$$

The dependencies of the relative overpressure on the non-dimensional radius are plotted for each run in Figure 4a. The dashed line represents the Waren formula[14] valid for high explosives (trinitrotoluene, TNT):

$$\Delta P_s^{TNT} = 0.6\left(\frac{r_*}{r}\right)^{4/3} \tag{10}$$

It can be seen that because the energy release rate is limited by the slow boiling process, the overpressures generated are 5–8 times lower than those from high explosives. This estimate is consistent with the experimental observations[10,15].

To estimate the effective energy yield E_{eff} and the explosion efficiency $\chi = \mathrm{E_{eff}/E}$, an effective radius r_{eff} was determined first for each set of parameters which, when used instead of r_* (see (9)), would provide best agreement of $\Delta P_s(r/r_{eff})$ with the Warren formula (10) for TNT.

In Figure 4b the relative overpressures are plotted against the non-dimensional radius r/r_{eff} together with the Warren relationship (10), it can be seen that a good agreement of all curves is achieved. The ratio of the effective and real energy-based radii r_{eff}/r_* is presented for each run in Table 1. It shows that, for the same energy yield, the same overpressure levels from bursting vessels are attained at distances 2.5–3.8 times closer to the explosion point than in the case of high explosives. By using the definition of characteristic radius in terms of the energy yield (9), the explosion efficiency factor χ may be

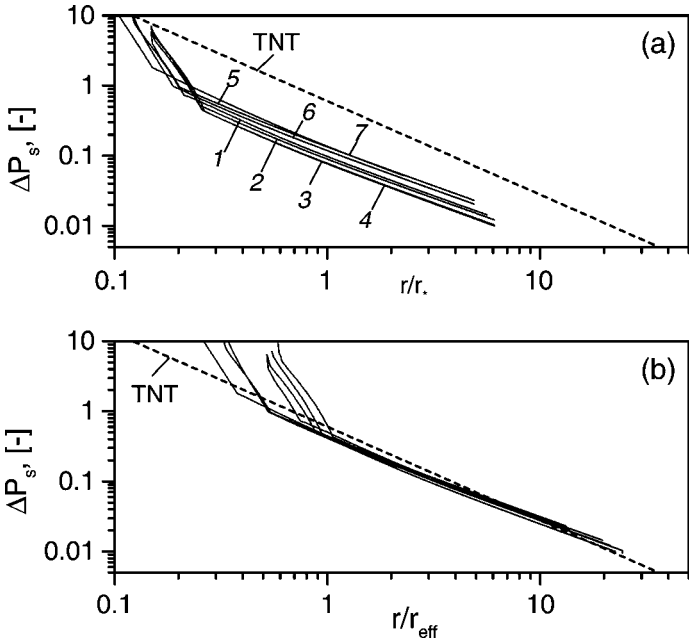

Figure 4. Overpressure-distance graph represented in energy-based coordinates (curves are numbered according to run numbers in Table 1): a) original calculation results; b) results represented in terms of efficient energy-based length scale

found:

$$\chi = \frac{E_{eff}}{E} = \left(\frac{r_*}{r_{eff}}\right)^3$$

The explosion efficiencies calculated in this way are also given in Table 1. It can be seen that the values of χ are quite low, about 2–6%, and the explosion efficiency increases with the increase in the pre-explosion heating of liquefied gas.

MODELLING OF FIREBALLS

Ignition of fuel clouds, which often accompanies BLEVEs, results in development of a burning cloud, or fireball. Vertical short-duration fuel releases and instantaneous formation of spherical or hemispherical cloud are representative scenarios of partial and total loss of containment respectively.

The numerical model used for calculation of fireballs is presented in detail in[16,17]. The model is based on axisymmetric Navier-Stokes equations in the small Mach number approximation, it is closed by the $k-\varepsilon$ turbulence model and eddy break-up turbulent combustion model. Lagrangian approach is used for description of the dispersed droplets. Radiative heat transfer is taken into account using the weighted-sum-of-grey-gases model, Monte Carlo approach is used for calculation of heat fluxes from the burning cloud.

In[16,17] the model was applied to simulation of fireballs resulting from short-duration vertical releases of hydrocarbons ranging from propane to octane. Such releases may occur after partial loss of containment, pipeline bursts etc, featured by the directional outflow of fuel into the atmosphere with flowrates rapidly decaying because of the decrease in the internal pressure. Flashing and non-flashing releases were considered in a wide range of fuel masses. It was shown that predicted integral characteristics of fireballs (size, lifetime, maximum height) agree well with the experimental data. Also, the radiative energy fractions obtained (20–30%) are in agreement with the values measured for large-scale hydrocarbon flames.

Recently the model[16,17] was extended to calculation of fireballs following total loss of containment (BLEVE scenario). The main difference with the case of partial loss of containment is in posing the initial conditions, including those for turbulent parameters of the fuel cloud. Preliminary calculations have revealed that simulation of combustion of an initially quiescent hemispherical cloud is much more sensitive to the method of posing the initial values than in the case of vertically directed outflow. In the latter case, a mixing layer develops at the boundary of the starting fuel jet where additional turbulence is generated overshadowing to some extent the turbulent characteristics posed in the source orifice and, thus, making predictions relatively insensitive to the initial and boundary values of the turbulent parameters (some dependence on these still exists, but reasonable turbulent parameters can be posed, e.g., by matching the growth law of a starting fuel jet to the experimental data).

Unlike this, development of an initially quiescent (i.e. having zero average velocity) fuel cloud is mainly governed by the turbulence which initially exists inside it. This turbulence is created on the initial short-duration stage featured by gas dynamics effects, which can not be described by the two-dimensional model[16,17]. By arbitrary setting the intensity and scale of turbulence in the cloud, large discrepancies between the predictions and experiments, and even unphysical flowfields or combustion patterns can be easily obtained.

This difficulty could only be overcome by applying the models described above to relate the pre-ignition state of the fuel cloud with the initial conditions (fuel mass, temperature, thermophysical properties etc.). One of the ways for setting the initial size and turbulent characteristics of the cloud is to calculate the characteristic scales (1)–(4) from the initial thermodynamic state of pressure-liquefied gas (note that any fuel pre-heating can be taken into account at this stage), then choosing some instant $t > t_*$ and calculating the cloud expansion velocity $\tilde{U}_C$ and turbulent characteristics $\tilde{k}_0$ and $\tilde{\varepsilon}_0$ from (8). The non-dimensional size of turbulent cloud is found by integrating $\tilde{U}_C(\tilde{t})$ with respect to

time: $\tilde{R}_C = 1.26\tilde{t}^{0.183}$. Finally, the average fuel concentration in the cloud can be found by dividing the fuel mass by the cloud volume. The dimensional cloud characteristics are then found using the calculated scales. As for the choice of the initial instant, it was found in practical calculations advantageous to take some instant, assign the initial conditions and

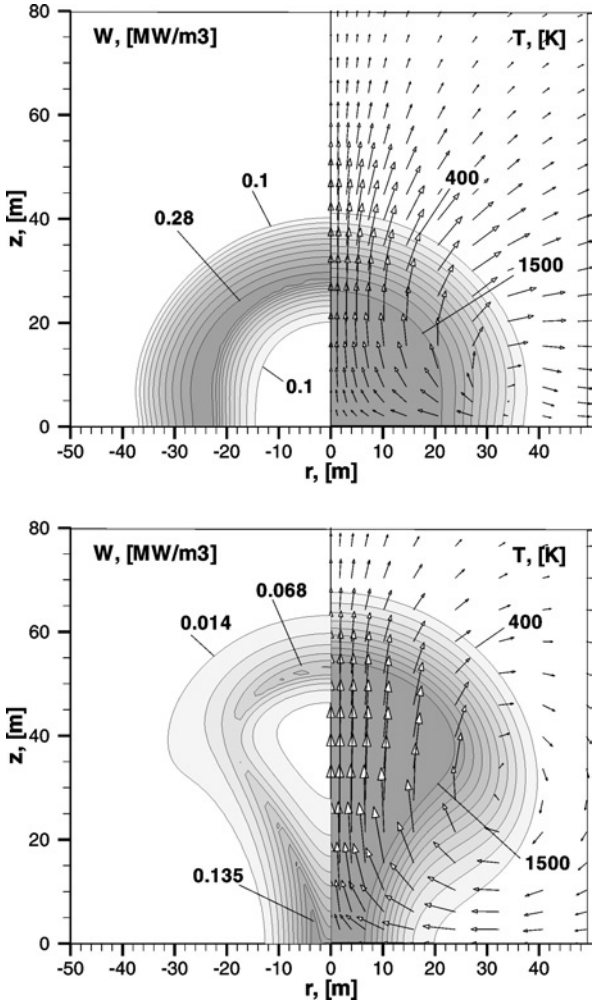

Figure 5. Structure of butane fireball with fuel mass of 2000 kg at $t = 2$ s (top) and 4 s (bottom) after vessel burst. Left: volumetric heat release rate; right: temperature contours

run the code for some time to make all fields adjust to each other, and only after that ignite the cloud. While this approach can be considered as the "first approximation", more detailed distributions (including the concentration field and fuel droplets) can be obtained by interpolating onto the numerical grid the profiles obtained from the differential model of fuel cloud expansion.

As an example, calculation of a BLEVE fireball following burst of a 2000 kg vessel with butane preheated to $T_0 = 373$ K ($P_0 = 15$ bar) is presented in Figure 5. The parameters and initial conditions correspond to field test[16]. Monodispersed droplets with the initial diameter of 10^{-4} m were considered, which resulted in complete involvement of all fuel released in fireball combustion (although the Lagrangian model used for the dispersed phase allows more detailed droplet size distributions to be specified and, in particular, account for partial rain-out of larger-size droplets). Temperature fields (right) are shown together with heat release rate fields (left) at two consecutive instants $t = 2$ and 4 s after vessel burst. The reaction was initiated by a small hot kernel on the axis of symmetry near the ground level. Since initially the cloud in fuel-rich, a nearly-spherical premixed flame propagates outwards through the cloud, while the remaining fuel burns afterwards mixing with the on the cloud boundary, where the heat release rate is the highest. Buoyancy of hot combustion products generates the vortex ring which rolls up the cloud into a well-defined fireball detaching it from the ground.

The predicted integral parameters of the burning cloud agree reasonably with the measurements[18]. The maximum diameter determined from the 500 K temperature contour is equal 80 m (74 m in the experiments), the maximum height of the fireball is also equal 80 m (85 m in the experiments). The burning and lift-off times are equal 6 and 3 s, while close values of 6.5 and 3.6 s were measured experimentally.

Comparison of the fireball characteristics for the same initial conditions, but for different release types (vertical release vs total loss of containment) has shown that BLEVE fireballs pose more hazards because they burn faster and at lower elevations: in the numerical calculations[7] it was found that a butane fireball with the above parameters but released vertically would burn over about 10 s and its elevation would reach 150 m.

CONCLUSIONS

The paper demonstrated an approach to "start-to-finish" modelling of boiling liquid expanding vapour explosions (BLEVEs), including blast effects of expanding volumes of superheated liquid and fireballs following ignition of the fuel cloud. In accordance with the physical processes involved, different types of models are necessary to describe the initial stage of fuel cloud formation featured by large pressure differences, high flow velocities etc, and its further isobaric evolution governed by turbulent mixing with the ambient air. Although the first stage is of short duration, it must be considered because during this stage the initial conditions (e.g., pre-heating, liquid fill level) and fuel thermodynamic properties affect the initial turbulisation of the cloud, which, in turn, determines the dynamics of further evolution and combustion of fuel cloud.

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