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Model for blast waves of Boiling Liquid Expanding Vapor Explosions

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ABSTRACT

A numerical model for boil-up of superheated liquid following loss of containment and expansion of two-phase mixture into the atmosphere is proposed and applied to evaluation of blast effects of Boiling Liquid Expanding Vapor Explosions (BLEVEs). The model assumes that the mixture in the two-phase cloud stays in thermodynamic equilibrium during expansion, whereas the air in the atmosphere obeys the ideal gas law with constant ratio of specific heats. The boundary between the two-phase cloud and ambient atmosphere is considered as a moving contact surface. The problem is solved numerically in the axisymmetric framework. Sample calculations of expansion of a spherical volume of superheated liquid are carried out for pressure-liquefied propane. Pressure profiles demonstrating propagation of depressurization wave into the cloud are presented together with mass fractions of vapor in the mixture. Solutions obtained for two-phase systems are compared with those for single-phase compressed gas. Scaling of overpressures in physical explosions is discussed. Validation of the model is carried out by comparison of simulations carried out in a wide range of cloud masses with experimental data. Two-dimensional simulations demonstrating BLEVE blast waves from a bursting near-surface vessel are presented.

1. Introduction

Accidental releases of pressurized or pressure-liquefied substances are one of major hazards in process industries, transportation or storage of flammable materials. Such releases can be caused by bursts of high-pressure vessels, pipeline rupture, processing equipment malfunction etc. [1]. Some striking examples of how destructive the explosions caused by accidental releases of flammable substances into the atmosphere can be are the accidents in Port Hudson (USA, 1970), Flixborough (UK, 1974), Mexico City (Mexico, 1984), Ufa (Russia, 1989), Xian (China, 1998), Nechapur (Iran, 2004), Buncefield (UK, 2005).

In the conventional explosions, rapid combustion or detonation of fuel yields the energy causing expansion of combustion products which act as a piston driving the ambient gas. However, there are different kinds of explosions, termed as "physical" (rather than chemical), which are driven by the internal energy accumulated in compressed gas or superheated liquid [2]. A well-known example of such an explosion is the burst of a vessel with pressure-liquefied substance, known as Boiling Liquid Expanding Vapor Explosion (BLEVE) [3,4]. BLEVE-type events, though occurring typically with pressure-liquefied hydrocarbons, can also occur with non-flammable substances, or even water, provided that preheating of vessel is high enough to bring the substance to the superheated state with respect to its thermodynamic equilibrium state at the ambient pressure.

It has been shown experimentally that parameters of shock waves from physical explosions differ substantially from those of TNT blasts [2,5,6]. Large and medium-scale tests on physical explosions and BLEVEs are quite rare [7–10]; laboratory-scale experiments [11,12,2,5,6] play an important role for understanding the features of shock waves generated by expanding superheated liquids, but there remains uncertainty on how to scale the results up to real accidents, keeping in mind multiple length and time scales present in the problem. Therefore, mathematical modeling is helpful in filling this gap.

Several BLEVE blast models have been proposed so far, differing in the assumptions and level of detail with which the complicated transient multiphase processes involved are tackled [13–20]. The approaches can be classified into the following broad categories: (i) empirical correlations aiming at comparing the BLEVE blast wave characteristics (overpressure, impulse) with those of high explosives (TNT equivalence approach) [18,19,10,20]; (ii) models focusing on the processes of liquid boil-up, superheat temperature limit, nucleation in superheated liquid, bubble growth etc. [21–24]; (iii) gas-dynamical models focusing on blast wave propagation in the atmosphere, while simplifying the description of boil-up processes by the assumption of expansion-controlled evaporation [16] or by approximating the expanding two-phase mixture by

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an equivalent gas [19]. The purpose of this work is to develop and validate a model "balanced" with respect to the details level of the "internal" or "external" problems.

The proposed model for expansion of a volume of superheated liquid is based upon the assumption that, as the pressure decreases, the liquid boils up and evaporates, this process being fast enough in comparison with the characteristic expansion time so that the vapor/liquid mixture reaches thermodynamic equilibrium. A similar model was applied to depressurization of ruptured pipes [25]; the difference is that an open atmosphere is considered, and no interaction with walls or flow choking occur. Another assumption is that no mixing occurs on the boundary between the expanding superheated liquid and ambient gas.

In what follows, mathematical model and its numerical implementation are presented, then spherical cloud expansion is considered, focusing on scaling of BLEVE overpressures with liquid mass and initial pressure. Finally, results of near-ground BLEVE simulations are validated against the experimental data.

2. Mathematical model

The assumed structure of superheated liquid expansion in the atmosphere is presented in Fig. 1. Two distinct zones are considered: (i) inner zone which includes the superheated liquid and thermodynamically equilibrium two-phase mixture emerging upon its boil-up, and (ii) ambient atmosphere in which shock waves can be generated by piston action of the expanding cloud.

The mathematical model describing the inner zone includes the continuity and momentum equations for boiling liquid–vapor mixture:

$$\frac{\partial \rho_m}{\partial t} + \nabla \rho_m U_m = 0, \tag{1}$$

$$\frac{\partial \rho_m U_m}{\partial t} + \nabla \rho_m U_m \otimes U_m = -\nabla P. \tag{2}$$

The mixture density, ρ_m, is obtained from specific volumes of liquid (subscript l) and vapor (subscript v), and mass fraction of vapor x_v:

$$\rho_m = \frac{1}{(1-x_v)v_l^0 + x_v v_v^0}. \tag{3}$$

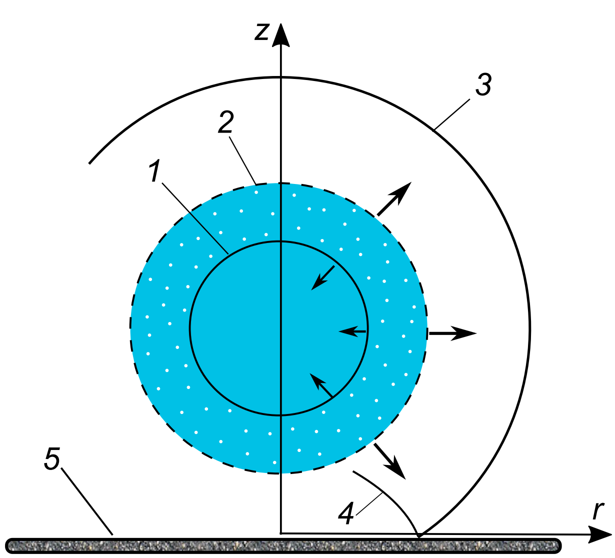

Fig. 1. Sketch of a superheated liquid cloud expanding into the atmosphere: 1 — boiling front, 2 — outer boundary of expanding two-phase cloud, 3 — atmospheric blast wave, 4 — reflected shock, 5 — ground surface.

The specific volumes of both phases, $v_{l,v}^0$, are taken on the saturation line at the local pressure P, while x_v is evaluated from the isoentropic relation

$$s_l^0(P_0) = (1-x_v)s_l^0(P) + x_v s_v^0(P), \tag{4}$$

with the liquid and vapor entropies, $s_{l,v}^0$, also taken on the saturation line. The mixture equation of state (3) is barotropic (ρ_m is a unique function of P). However, since s_l^0 depends on the initial pressure P_0 (see Eq. (4)), the mass fraction of vapor depends on both P and P_0:

$$x_v(P, P_0) = \frac{s_l^0(P_0) - s_l^0(P)}{s_v^0(P) - s_l^0(P)}. \tag{5}$$

Therefore, the mixture density also depends on P_0 parametrically: $\rho_m = \rho_m(P, P_0)$.

The equation of state for two-phase mixture, Eqs. (3) and (4), is only valid for $P \leqslant P_0$, which is generally sufficient for the description of the initial stage of two-phase mixture expansion into lower-pressure atmosphere. However, it will be shown later on that converging shock waves can be formed in the mixture leading to implosion causing short-duration peak pressures at the cloud center exceeding P_0. Therefore, the equation of state must be extended to pressures $P > P_0$ where the single-phase liquid becomes subcooled with respect to its saturation temperature at the local pressure. It was assumed that compression of single-phase liquid is isothermal (proceeding at the saturation temperature corresponding to P_0), and the pressure-density relationship is described by the modified Tait equation [26]

$$P = P_0 + B\left(\left(\frac{\rho_m}{\rho_0}\right)^n - 1\right), \tag{6}$$

where ρ_0 is the density of saturated liquid at $P = P_0$. In the subcooled liquid, we set $x_v(P, P_0) = 0$, so that the mixture density and mass fraction of vapor are continuous on the saturation line dividing the saturated mixture and subcooled compressed liquid. However, the speed of sound is discontinuous; in the subcooled liquid it is calculated from (6) as

$$C_s = \left(\frac{\partial P}{\partial \rho_m}\right)_s^{1/2} = \left(\frac{nB\left(\frac{\rho_m}{\rho_0}\right)^n}{\rho_m}\right)^{1/2}. \tag{7}$$

Eq. (6) is also barotropic, so that the same numerical procedure can be applied for solving the mixture continuity and momentum equations in the whole two-phase zone. The Tait Eq. (6) describes compression of liquid from its saturated state, i.e., the reference density $\rho_0 = \rho_{sat}(P_0)$ and parameters B, n depend on P_0 (increase in P_0 means increase in the saturation temperature T_0, decrease in ρ_0, and increase in liquid compressibility).

In the ambient atmosphere, the Euler equations are solved, with the air considered as an ideal gas with the ratio of specific heats $\gamma = 1.4$. The boundary between the zones is a contact surface moving with time. The pressure and normal velocity component are continuous across the contact surface, whose shape and position are obtained in the course of the solution. A similar model was applied earlier to spherically symmetric expansion of superheated liquids [13–15]. Here, the model is extended to multidimensional problems, so that it is applicable to near-ground vessel explosions.

3. Numerical method

The complex problem requiring solution of different equation sets in different domains divided by a sharp contact interface is tackled by the Ghost Fluid Method (GFM) [27] in which the cells neighboring the interface are alternatively filled with "ghost" fluid of the same type as current, enabling solution of equations across