

Shock Waves from Explosions due to Boil-up of Superheated Liquids

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ABSTRACT

Boiling Liquid Expanding Vapor Explosions are energetic events following total or partial loss of containment, typical of high-pressure vessel bursts. The paper presents an approach to mathematical modeling of rapid expansion of a cloud of superheated liquid, generating pressure waves in the ambient atmosphere. The approach is based upon the assumption of thermodynamic equilibrium between the liquid and vapor phases in the two-phase mixture, with the coupled solution of equations of motion in the two-phase and single-phase zoned. The boundary between the zones is considered as a moving contact discontinuity. The model presented extends the approach developed earlier where the mass fraction of vapor was obtained under assumption that the mixture remains isentropic during its whole evolution. In the current model, on the contrary, the isentropic assumption is not made; rather, a total energy equation is considered in the two-phase zone. The advantages of the extended model are: i) entropy production in the shock waves in the two-phase mixture is taken into account, ii) the initial state can be set up without the all-liquid assumption inherent in the isentropic mode, allowing one to consider bursts of partially filled vessels. Example simulations of spherically symmetric cloud expansion and burst of partially filled vessel are presented.

KEYWORDS: BLEVE, shock wave, superheated liquid, hazards, numerical model.

NOMENCLATURE

e specific internal energy (J/kg)

E total energy density (J/m³)

\mathbf{H} vector of radial fluxes

h specific enthalpy (J/kg)

\mathbf{J} vector of vertical fluxes

L latent heat of evaporation (J/kg)

\mathbf{Q} vector of conservative variables

r radial coordinate (m)

\mathbf{S} vector of source terms

s specific entropy (J/(kg·K))

T temperature (K)

t time (s)

$\mathbf{U} = (u, w)$ velocity vector (m/s)

v specific volume (m³/kg)

x_v mass fraction of vapor (-)

z vertical coordinate (m)

Greek

ρ density (kg/m³)

Subscripts

a atmosphere

l liquid phase

m two-phase mixture

v vapor

0 storage (pre-burst) conditions

Superscripts

0 saturated

INTRODUCTION

Physical explosions, as opposed to conventional “chemical” explosions, are driven by rapid release of internal energy when a volume of high-pressure liquid becomes exposed to low-pressure environment due to loss of containment. Accidents of this type are known as Boiling Liquid Expanding Vapor Explosions (BLEVEs); they are encountered in transportation, storage and processing of substances existing in liquid state at high pressures.

Hazards of BLEVEs are generally attributed to shock waves generated in the air by rapid increase in the volume of boiling liquid in comparison with the initial single-phase state, as well as to projectile action of high-speed vessel fragments [1]. Physical explosions of BLEVE type can occur with various substances which must be in liquid state and at a high pressure in the pre-burst conditions. Such a state is achieved provided that the pre-burst temperature of the substance falls between the normal boiling point (so that the pre-burst pressure is above the atmospheric level) and the critical temperature (so that the substance can exist in liquid state). The most common such substances are pressure-liquefied hydrocarbons, however, BLEVEs can also occur with preheated water or carbon dioxide [2].

Engineering methods for assessment of BLEVE hazards mostly rely on the establishing the correlation for shock wave overpressure as a function of distance and matching these with high explosive (TNT) curves, see, e.g., [3–5].

BLEVE phenomenon is featured by a whole range of coupled physical, multiphase and gas-dynamical processes, including bubble nucleation and growth, existence of superheat limit, phase transitions, turbulence generation, mixing with the air etc. The reason for vessel failure can be related to dynamic processes and temperature stratification causing rapid growth of internal pressure [6, 7]. Due to high uncertainties in the initial conditions, vessel burst details (crack propagation, fragmentation of the container etc.) characteristic of accidents as uncontrolled and spontaneous events, start-to-end modeling with all details included in consideration does not seem to be straightforward. For example, a model for two-phase flow developed in [8] involves a number of parameters (most notably, the nucleation site concentration, flow regime boundaries etc.) poorly known in accident conditions. On the other hand, the idea of expansion-controlled evaporation [9] recognizes the large difference in the characteristic time scales for the relatively slow “external” (gas dynamics) flow and much faster processes in the boiling liquid at the scale of individual bubbles. In [9], however, only volume-averaged parameters were used in the two-phase zone.

In a recent paper [10], a model was developed in which the flow both in the two-phase (expanding boiling liquid) and single-phase (ambient gas) was described by gas dynamics equations (inviscid flow), with different equations of state on both sides of the moving contact discontinuity. In the two-phase zone, it was assumed that liquid and vapor phases are always located on the saturation curve of the respective phase diagram, following the variation of local pressure in the course of mixture expansion. In order to find the mass fraction of vapor in the mixture, an assumption of isentropic flow was invoked.

Detailed modeling of BLEVE-type events must take into account the multiphase processes and phase transition in the superheated liquid, as well as gas dynamics of gas flow in the atmosphere. In this paper, a recent model based on the assumption of thermodynamic equilibrium between the phases in the boiling liquid [10] is revised and applied to the analysis of bursts of high-pressure vessels filled partially with pressure-liquefied propane.

SCHEME OF THE PROCESS

In Fig. 1, the process of superheated liquid expansion into the atmosphere is sketched for an initially spherical volume of liquid substance at a high pressure P_0 , located above a flat horizontal surface. After instantaneous loss of containment, the high-pressure liquid becomes exposed to the atmosphere at a lower pressure $P_a < P_0$; boiling front propagates into the saturated liquid (SL) from periphery towards the center, and expanding boiling vapor/liquid mixture (BL), acting as a piston, generates pressure waves in the atmosphere.

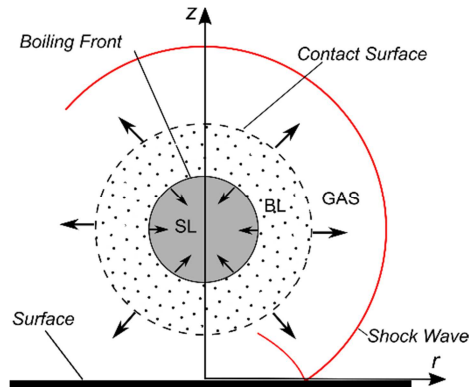


Fig. 1. Sketch of superheated liquid expansion into the atmosphere: BL is boiling liquid, SL is saturated liquid.

MODEL FOR TWO-PHASE MIXTURE

Mixture density model

The central point of the thermodynamically equilibrium model for two-phase mixture [10] is the assumption that both phases remain on the saturation line at any time, following the variation of local pressure. This implies that phase transition is very fast, in comparison with the fluid dynamics processes governing the expansion of two-phase mixture into the atmosphere. In addition, velocity slip between the phases is neglected, i.e., a single velocity U_m describes the mixture flow. The assumption of thermodynamic equilibrium allows one to avoid the consideration of fast non-equilibrium processes with liquid going into metastable state, followed by boil-up depending on such poorly known parameters as the concentration of nucleation sites in liquid substance. Infinitely fast boil-up of liquid provides the conservative estimate of the explosion effects, which is appropriate for accident hazard evaluation.

Under these assumptions, the mixture density is obtained from

$$\rho_m = (x_v v_v^0 + (1 - x_v) v_l^0)^{-1}, \quad (1)$$

where $v_i^0(P)$ is the specific volume of vapor ($i=v$) or liquid ($i=l$) on the saturation line, both quantities being single-valued functions of current pressure P .

Equation (1) involves the mass fraction of vapor in the mixture, x_v , which must be obtained from some energy considerations; in fact, it plays the role of a progress variable related to the process of liquid flash evaporation. In what follows, we consider two models for x_v : i) isentropic model used in the previous work [10], and ii) non-isentropic model proposed in the current work.

Isentropic model for flash fraction

A key point of the model [10] is the assumption that the mixture is isentropic during the whole its flow and phase transitions:

$$s_i^0(P_0) = x_v s_v^0 + (1 - x_v) s_l^0, \quad (2)$$

where s_i^0 is the specific entropy of i -th phase on the saturation line at the current pressure P , while on the left-hand side the entropy of liquid phase is taken at the storage pressure P_0 . The latter implies that initially all the substance was in liquid state.

Equation (2) defines the mass fraction of vapor x_v :

$$x_v = \frac{s_l^0(P_0) - s_l^0(P)}{s_v^0(P) - s_l^0(P)} = \frac{T_s(P)(s_l^0(P_0) - s_l^0(P))}{h_v^0(P) - h_l^0(P)} \quad (3)$$

(note that the denominator in the rightmost formula (3) is the latent heat of evaporation $L = h_v^0 - h_l^0$ at the current pressure). Equation (3) shows that the mass fraction of vapor is a single-valued function of pressure P , although it depends parametrically on the initial (pre-burst) pressure P_0 .

With the initial conditions fixed, it follows from (1)–(3) that mixture density depends on pressure only, therefore, the flow of this mixture is barotropic and can be described by the continuity and momentum equations only. The energy conservation is taken into account implicitly, via the conditions (2), (3).

Non-isentropic model for flash fraction

In the current work, the model for mass fraction of vapor x_v was modified by omitting the isentropic condition in its form (2). As a result, the flow can no longer be considered barotropic, and mixture energy equation must be solved together with the mass and momentum conservation equations. When introducing the mixture energy, we still assume thermodynamic equilibrium between the phases, i.e., properties of both liquid and vapor phases follow the variation of local pressure along the saturation curve for the current substance.

Introduce the specific internal energy of mixture

$$e_m = x_v e_v^0 + (1 - x_v) e_l^0, \quad (4)$$

where the specific internal energies of both phases e_i^0 are taken on the saturation line, i.e., they are single-valued functions of pressure P .

In this approach, the mixture density $\rho_m(P, x_v)$ and specific internal energy $e_m(P, x_v)$ are primary variables obtained by solving the equations of motion to be considered below. Having in hand the pressure dependencies of saturated properties $v_i^0(P)$ and $e_i^0(P)$ in an analytical or tabular form, we can determine the pressure P and mass fraction of vapor x_v by solving a system of two non-linear equations to obtain $P(\rho_m, e_m)$ and $x_v(\rho_m, e_m)$.

Two advantages of the non-isentropic model are evident. Firstly, since Eq. (2) is no longer considered, we do not have to assume that the whole pressure-liquefied substance exists initially in the state of single-phase saturated liquid (see the left-hand side of Eq. (2)). Spatially non-uniform

initial conditions can now be set for ρ_m and e_m in the two-phase zone, allowing one to model bursts of partially filled vessels, with single-phase liquid and saturated vapor separated in the lower and upper parts of vessel due to gravity stratification. Secondly, it was shown in [10] that in the two-phase zone, quite a complex flow develops, with mixture overexpansion, followed by propagation of converging shock (implosion), its reflection from the origin and generation of the secondary pressure wave travelling behind the primary one. It is well known from classical gas dynamics that entropy increases across the shock wave, reflecting the irreversible energy conversion to heat. Since the current model no longer relies on the assumption of constant entropy (2), such irreversible energy losses are taken into account.

EQUATIONS OF MOTION

General formulation

We consider the problem as axisymmetric in the cylindrical coordinates (r, z) shown in Fig. 1. Both in the two-phase (boiling liquid) and single-phase (ambient air) zones, flow is described by the system of Euler equations, however, with different fluid properties and equations of state. The general form of Euler equations is

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{H}}{\partial r} + \frac{\partial \mathbf{J}}{\partial z} + \frac{\mathbf{S}}{r} = 0, \quad (5)$$

where \mathbf{Q} is the vector of conservative variables, \mathbf{H} and \mathbf{J} are flux vectors in radial and vertical directions, respectively, the source term \mathbf{S} arises due to curvilinear (cylindrical) coordinates.

Two-phase zone (isentropic model)

In the isentropic model [10], only the continuity and momentum equations need to be solved, due to barotropic nature of flow:

$$\mathbf{Q} = \begin{pmatrix} \rho_m \\ \rho_m u \\ \rho_m w \end{pmatrix}, \quad \mathbf{H} = \begin{pmatrix} \rho_m u \\ \rho_m u^2 + P \\ \rho_m u w \end{pmatrix}, \quad \mathbf{J} = \begin{pmatrix} \rho_m w \\ \rho_m u w \\ \rho_m w^2 + P \end{pmatrix}, \quad \mathbf{S} = \begin{pmatrix} \rho_m u \\ \rho_m u^2 \\ \rho_m u w \end{pmatrix}, \quad P = P(\rho_m). \quad (6)$$

Pressure P is found from mixture density ρ_m by inverting the equation of state (1), (3).

Two-phase zone (non-isentropic model)

For non-isentropic model, energy equation is solved in the two-phase zone together with the continuity and momentum equations:

$$\mathbf{Q} = \begin{pmatrix} \rho_m \\ \rho_m u \\ \rho_m w \\ E_m \end{pmatrix}, \quad \mathbf{H} = \begin{pmatrix} \rho_m u \\ \rho_m u^2 + P \\ \rho_m u w \\ (E_m + P)u \end{pmatrix}, \quad \mathbf{J} = \begin{pmatrix} \rho_m w \\ \rho_m u w \\ \rho_m w^2 + P \\ (E_m + P)w \end{pmatrix}, \quad \mathbf{S} = \begin{pmatrix} \rho_m u \\ \rho_m u^2 \\ \rho_m u w \\ (E_m + P)u \end{pmatrix}, \quad (7)$$

$$e_m = E_m - \rho_m \frac{u^2 + w^2}{2}, \quad P = P(\rho_m, e_m).$$

Equations (7) are Euler equations, with all specific features for two-phase mixture condensed in the with equation of state in which substance properties on the saturation line are embedded. Pressure in

(7) is found by inverting equations (1) and (4). Note that in both cases (6) and (7) the mass fraction of vapor x_v is obtained in the course of solution.

Single-phase gas

In the ambient atmosphere, conventional Euler equations apply, with the air considered as an ideal gas with a constant ratio of specific heats $\gamma = 1.4$:

$$\mathbf{Q} = \begin{pmatrix} \rho \\ \rho u \\ \rho w \\ E \end{pmatrix}, \quad \mathbf{H} = \begin{pmatrix} \rho u \\ \rho u^2 + P \\ \rho uw \\ (E + P)u \end{pmatrix}, \quad \mathbf{J} = \begin{pmatrix} \rho w \\ \rho uw \\ \rho w^2 + P \\ (E + P)w \end{pmatrix}, \quad \mathbf{S} = \begin{pmatrix} \rho u \\ \rho u^2 \\ \rho uw \\ (E + P)u \end{pmatrix}, \quad (8)$$

$$P = (\gamma - 1) \left(E - \rho \frac{u^2 + w^2}{2} \right).$$

NUMERICAL IMPLEMENTATION

In each zone, equations (5) were solved by an explicit second order-accurate numerical scheme [11]. Tracking of the interface between zones and matching the solutions was performed by the Ghost Fluid Method [12] which can successfully handle contact discontinuities between different materials (for example, in the isentropic model not only equations of state are different, but the number of equations to be solved is different too across the interface). Properties of substances on the saturation line were taken from NIST database [13] in tabular form; inversion of equation of state necessary for finding the pressure (see (6) and (7)) was performed by iterative procedure.

RESULTS

Spherical cloud expansion

The model developed in [10] was validated against large-scale experiments [14, 15] where bursts of vessels filled completely with propylene were studied. Good agreement of the calculated overpressure-distance curves with measured data was demonstrated. What is important, the model does not involve any tweakable parameters, therefore it is quite robust in application.

In this work, we present further simulations carried out in the spherically symmetric case. As the base case for validation, the experiment on burst of 1.9 m³ vessel reported in [5, 16] was selected. BLEVE happened after the reservoir failure at 1.9 MPa; at the burst instant, the reservoir was filled about half with saturated propane liquid and half with saturated vapor at the instant of failure.

When performing comparison of spherically symmetric simulations with field test data, it must be taken into account that for neat-surface vessel bursts (and conventional explosions as well) energy is released into half-space; this effectively doubles the explosion yield. Therefore, in the simulations presented below, it was assumed that the vessel was filled completely. With the density of saturated propane at $P_0 = 1.9$ MPa and temperature $T_0 = 328$ K (55 C) being equal to $\rho_0 = 439.2$ kg/m³, we obtain that the mass of pressure-liquefied propane participating in BLEVE is evaluated as $M = 840$ kg, and the energy yield evaluated from thermodynamics (see details in [10]) is about 39 MJ (9.3 kg TNT).

In Fig. 2, pressure profiles are shown at several instants, revealing the wave nature of two-phase flow in the boiling liquid, and generation of shock waves in the atmosphere. The sequence of events includes initial rapid expansion of vapor generating the primary air shock, propagation of boiling

wave through the saturated liquid, reaching the origin by the time 22.5 ms, followed by overexpansion of two-phase zone with significant drop in pressure (see the pressure curves at times 25-39 ms). A secondary inward-facing shock propagates towards the origin, its reflection (implosion) occurs at about 39.5 ms, it results in the generation of a secondary shock travelling in the atmosphere behind the primary one.

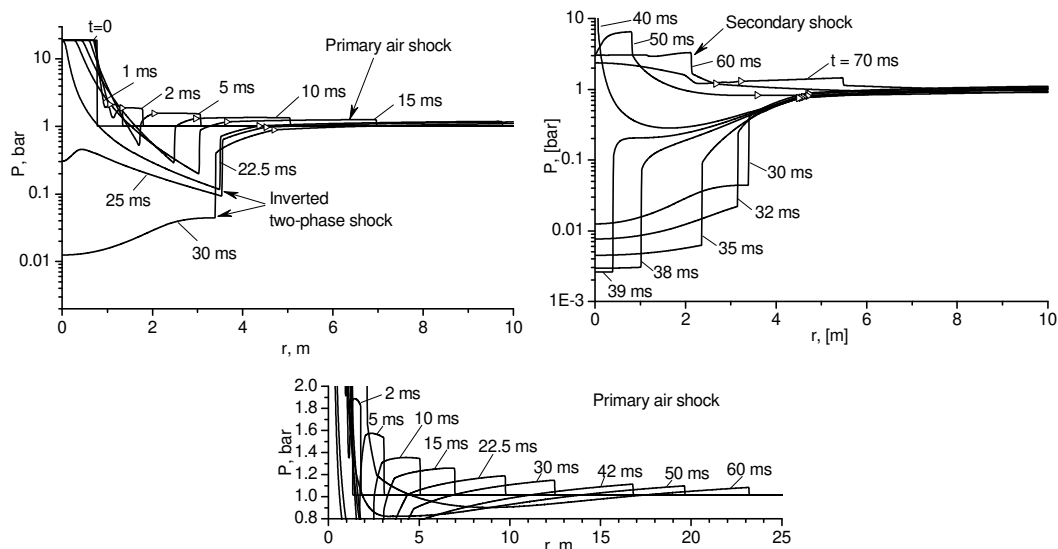


Fig. 2. Pressure profiles at different instants in spherically symmetric expansion of 1.9 m³ propane at initial pressure 1.9 MPa (triangles denote the position of contact surface).

By the triangular symbols, the position of contact discontinuity (boundary between the two-phase zone and air) is shown on each curve of Fig. 2. It can be seen that the expanding cloud reaches its maximum radius of about 4.7 m by the time 32 ms, after which the outer boundary halts until implosion occurs, and only after that the cloud shrinks to its minimum radius of about 2.5 m, then weaker secondary expansion follows etc. As a result of these wave processes with periodic overexpansion and implosions, a sequence of pressure pulses is generated in the atmosphere.

Validation against the experimental data [5, 16] was carried out by comparing the properties of the primary shock, namely, the arrival time t_s and peak pressure value P_{max} in the primary shock. Comparisons were carried out at three distances for which both experimental and simulation data were available. Results are summarized in Table 1; note that the experimental values were picked up from graphs in [5] and must be considered as indicative only.

Table 1. Comparison of calculated primary shock values with experiments [5, 16]

Distance, m	t_s , ms (Calc./Exp.)	P_{max} , kPa (Calc./Exp)
10	23/30	16.9/14.9
20	52/65	8.3/8.9
30	80/90	5.3/6.0

Generally, reasonable agreement between the pressure peak values obtained in simulations and

measured experimentally is observed; the arrival times in simulations are smaller by an offset of about 10 ms, which might indicate differences in the initial instant on the experimental graphs. More detailed comparison of the pressure-time profiles will be carried out in the future work.

Bursts of partially filled vessel

To reveal the dynamic processes accompanying BLEVEs of partially filled vessels, the revised (non-isentropic) model presented in this work was applied to simulation of propane vessel burst at the same initial conditions as in the experiments [14, 15] and in the previous section (1D spherically symmetric expansion). Simulations were carried out in the 2D (axisymmetric) formulation, therefore, doubling of liquid mass which was necessary in the spherically symmetric simulation presented above, was not applied here. It should be kept in mind that in the experiments [14, 15], commercial gas tanks were mounted horizontally near the surface, and measurements were carried out in two directions (on side and end of the vessel). In the axisymmetric framework, such a setup is not possible; therefore, the vessel was arbitrarily set as a vertical cylinder of diameter 1.2 m and height 1.68 m. The lower half of the vessel was filled with saturated liquid, the top half was filled with saturated vapor at the same pressure of 1.9 MPa. Simulations were performed in the domain 10×10 m (in the radial and vertical directions) on the grid containing 300×30 cells.

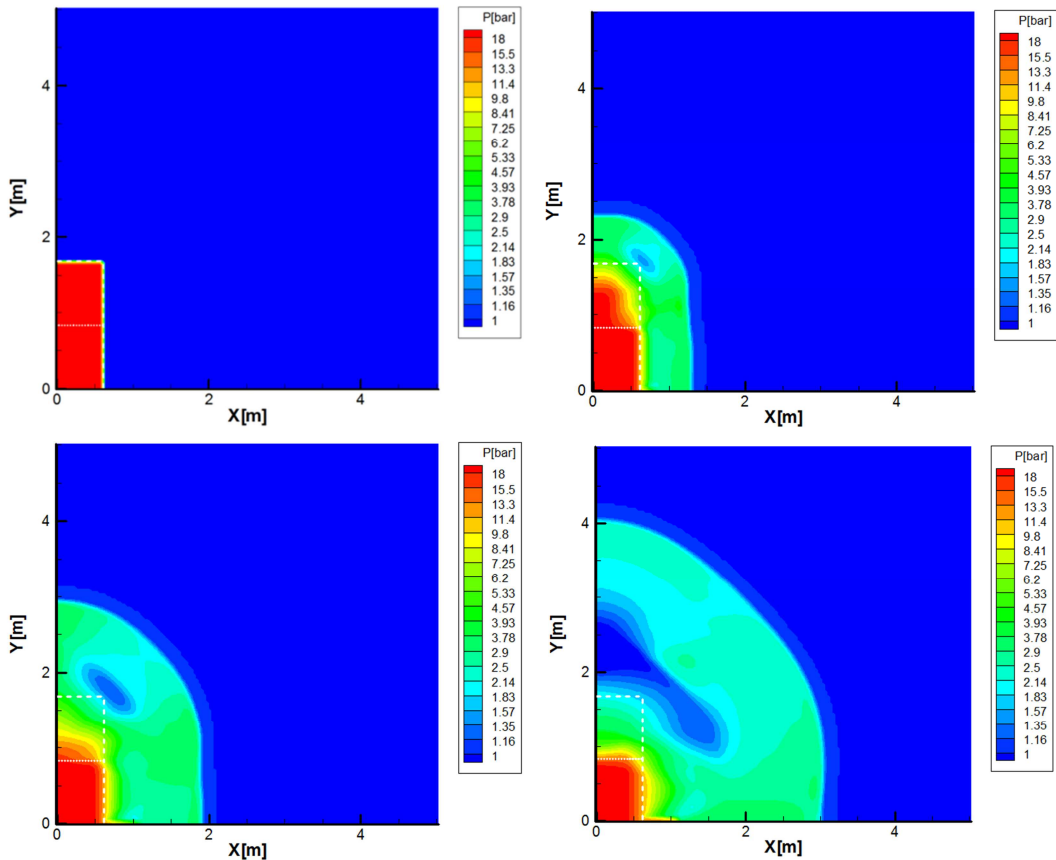


Fig. 3. Pressure fields at times 0, 1, 2, and 4 ms for burst of a cylindrical 1.9 m^3 propane vessel at initial pressure 1.9 MPa (initial two-phase zone shown by dashed lines).

In Fig. 3, pressure fields are plotted at four consecutive times, demonstrating the initial development of pressure wave in the atmosphere. By the dashed line, the initial boundaries of the saturated

substance in the vessel in outlined; the horizontal dashed line denotes the initial liquid level. It can be seen that pressure relief wave propagates through the upper (vapor) space much faster than in the lower saturated liquid) half of the vessel: by the time 4 ms, high pressure in the vapor space disappears, where the lower half of the vessel is still at the initial pressure. The difference is attributed to different speed of sound in single-phase and two-phase zones, as is discussed in [10].

Pressure distributions at later instants are shown in Fig.4 (note that a larger domain is shown in these pictures). The high-pressure zone near the surface is shrinking as the boiling front propagates through the saturated liquid. The nearly-spherical leading shock front is expanding into the atmosphere, while behind the shock the structure on pressure field is quite complex due to reflections and interactions of pressure waves from expanding liquid.

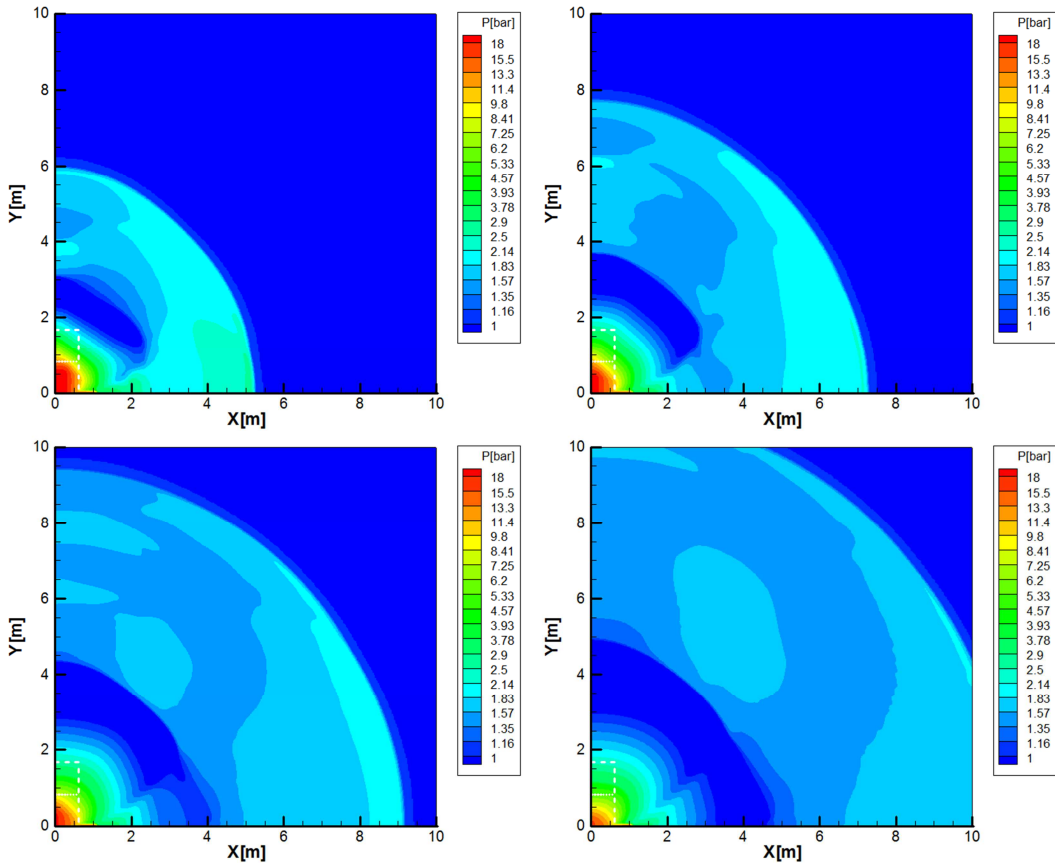


Fig. 4. Pressure fields at times 8, 12, 16, and 20 ms for burst of a cylindrical 1.9 m^3 propane vessel at initial pressure 1.9 MPa (initial two-phase zone shown by dashed lines).

CONCLUSIONS

Thus, the model developed in this work provides adequate description of the gas dynamic processes accompanying BLEVE-type events. The model allows one to describe boil-up of high-pressure liquid and evaluate the shock effects of BLEVEs. Initial validation of the model performed in this work has to be continued with more detailed comparisons of pressure records (pulse shape, peak value, impulse and duration) at different distances from the bursting vessel. In particular, it is necessary to validate the model against experimental data on BLEVEs with different fill levels of

vessel in order to evaluate the predictive capabilities of the proposed approach in terms of the expansion effects of the pressure-liquefied substance and of the vapor contained in the vessel above it. Another validation direction is to compare the BLEVE shock effects on the side and on the axis of cylindrical vessels of different aspect ratio, which is important from the hazard evaluation point of view.

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