Wave phenomena upon interaction between water and high-temperature melt

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Abstract. A multiphase model for steam explosion is considered, with assumption of mechanical equilibrium between water and vapor phases in the mixture, but with non-equilibrium drag and heat exchange with high-temperature melt droplets taken into account. Governing equations are formulated and solved numerically. Simulations of pressure waves following thermal interaction of hot melt and water-vapor mixture are presented, the structure of steam explosion wave is discussed.

1. Introduction
In many scientific fields, problems of interaction between cold and hot fluids are encountered. Of particular interest are energetic interactions occurring when the fluids possess significantly different boiling temperatures, and the initial temperature of hot fluid is well above the boiling point of the cold fluid. In this case, coexistence of the two substances is only possible if a vapor film of more volatile substance is formed, preventing thus the substances from direct interaction. However, if vapor film instability develops for some reason, direct contact between the liquids can occur, leading to rapid boil-up and expansion of volatile liquid. Phenomena of this type are encountered in nuclear power energy in the case of severe accidents, when the core melt (corium) having the temperature of about 3000 K penetrates into water coolant. Pressure waves developing upon such interaction can be quite destructive; the energetic fuel-coolant interaction termed as steam (or vapor) explosion [1,2]. In recent experiments [3] it was shown that energetic melt-water interaction is possible not only in the classical case of melt jet penetrating into a deep water pool, but also in stratified configuration, when melt is poured in a shallow pool, spreading over the bottom plate. Explosion initiation is caused by collapse of vapor film separating the spreading melt from water above it, resulting in direct contact of water and melt.

Propagating pressure wave in three-phase (water, vapor, hot dispersed melt) system resembles features of chemical detonation wave propagating in combustible mixture. The feedback mechanism providing energy to the propagating wave is rapid boil-up of water behind the front caused by vapor film collapse, resulting in vapor generation being the source of mechanical energy.

Numerous approaches to the description of steam explosions were proposed in the literature. For modeling steam explosions of melt jet in a big volume of coolant, specialized computer codes were developed: PM-ALPHA and ESPROSE (USA), TEXAS-V (USA), IDEMO (Germany), MC3D (France), JASMINE (Japan, South Korea), VAPEX (Russia). Analysis of modern
multiphase flow averaging based models (that played the foremost role in 70s-90s) and their implementation leads to the conclusion that success in application to particular problems is mostly determined by availability and adequacy of closure correlations.

In this work, we attempt to develop a simple model for steam explosion wave, and demonstrate relative significance of the main physical mechanisms governing different aspects of pressure wave formation and self-sustained propagation. The simplified model allows one to focus attention on the principal phenomena, rather than numerous details.

2. Model

2.1. Governing equations

Three phases (water, vapor, melt) are considered in the Eulerian framework, with the respective volume fractions \( \varphi_w, \varphi_v, \) and \( \varphi_s \) satisfying the condition \( \sum \varphi_i = 1 \). It is assumed that vapor exists as dispersed bubbles, therefore, mechanical equilibrium between the liquid water and vapor is implied; both phases possess the same velocity. Under this assumption, we can consider the water-vapor mixture as an effective compressible fluid. The volume fraction of mixture is then \( \varphi_m = \varphi_w + \varphi_v \) (so that \( \varphi_m + \varphi_s = 1 \)), its velocity is \( \mathbf{V}_m \); the velocity of melt particles is \( \mathbf{V}_s \).

The system of governing equations takes the following form:

\[
\frac{\partial \rho_m \varphi_m}{\partial t} + \nabla (\rho_m \varphi_m \mathbf{V}_m) = 0 \tag{1}
\]

\[
\frac{\partial \rho_m \varphi_m \mathbf{V}_m}{\partial t} + \nabla (\rho_m \varphi_m \mathbf{V}_m \mathbf{V}_m) = -\varphi_m \nabla P - \mathbf{F} \tag{2}
\]

\[
\rho_m \varphi_m \left( \frac{\partial x_v}{\partial t} + (\mathbf{V}_m \nabla) x_v \right) = \Gamma \tag{3}
\]

\[
\frac{\partial \rho_s \varphi_s}{\partial t} + \nabla (\rho_s \varphi_s \mathbf{V}_s) = 0 \tag{4}
\]

\[
\rho_s \varphi_s \left( \frac{\partial \mathbf{V}_s}{\partial t} + (\mathbf{V}_s \nabla) \mathbf{V}_s \right) = -\varphi_s \nabla P + \mathbf{F} \tag{5}
\]

Here, \( x_v \) is the mass fraction of vapor in the water-vapor mixture, \( \mathbf{F} \) is the drag between solid particles and water-vapor mixture, \( \Gamma \) is the evaporation rate per unit mass of water-vapor mixture.

2.2. Closures

The equation of state for homogeneous water-vapor mixture is expressed as

\[
\frac{1}{\rho_m} = \frac{x_v}{\rho_v} + \frac{1-x_v}{\rho_w} \tag{6}
\]

For the liquid phase, the Tait equation of state is used in the form

\[
P = P_0 + K_0 \frac{n}{n} \left( \left( \frac{\rho_w}{\rho_l} \right)^n - 1 \right) \tag{7}
\]

whereas for the vapor a polytropic equation of state is assumed

\[
\rho_v = \rho_v^0 \left( \frac{P}{P_0} \right)^k \tag{8}
\]

with \( 1 \leq k \leq \gamma \), where \( \gamma = c_p/c_v \) is the ratio of specific heats; \( k = 1 \) corresponds to isothermal compression, \( k = \gamma \) to adiabatic. Generally, in the presence of vapor liquid water compressibility
plays a minor role, however, it becomes important in a single-phase fluid \((x_v = 0)\). As a result of (7) and (8), we obtain barotropic equation of state (6). The density of melt, \(\rho_s\), is assumed constant.

The drag force \(\mathbf{F} = nf\), where \(n\) is the melt droplet concentration, while \(f\) is the force acting on a single melt droplet which depends upon the relative velocity \(\mathbf{V}_r = \mathbf{V}_m - \mathbf{V}_s\). Expressing \(n\) in terms of volume fraction \(\varphi_s\) and taking into account melt interaction with liquid water only through multiplication by the corresponding volume fraction, obtain the drag force

\[
\mathbf{F} = \varphi_s \varphi_w \frac{3C_D \rho_w |\mathbf{V}_r|}{4d} \mathbf{V}_r
\]

with the drag coefficient described by the standard expression

\[
C_D = \frac{24}{Re} \left( 1 + 0.179 Re^{1/2} + 0.013 Re \right)
\]

where \(Re = \rho_w |\mathbf{V}_r| d/\mu_w\) is the Reynolds number, \(\mu_w\) is water viscosity.

Water evaporation rate per unit volume is defined by \(\Gamma = 6 \varphi_s \varphi_w \gamma/\pi d^3\), where \(\gamma\) is the evaporation rate per melt droplet. For the latter quantity, the balance between the heat flux and energy consumed for liquid heating to the boiling point and evaporation is expressed by

\[
\gamma = \frac{h(T_s - T_b) S_p}{c_w (T_b - T_w) + \Lambda_w}
\]

where \(h\) is the heat transfer coefficient between a melt particle and water, \(S_p = \pi d^2\) is the particle surface area, \(c_w\) is the specific heat capacity of water, \(T_b\) is the boiling temperature at the current pressure, \(\Lambda\) is the latent heat of evaporation (it is assumed that vapor-liquid interface is at thermodynamic equilibrium, so that its temperature is equal to the boiling temperature at the current pressure \(T_b(P)\) corresponding to the saturation curve). The particle temperature \(T_s\) is much higher than \(T_b\) in the system considered, and we neglect its decrease due to short interaction time. The heat transfer coefficient \(h\) in (11) is evaluated for the film boiling regime as \([5]\)

\[
h = 2.98 \left( \frac{\rho_w \Lambda_w [\Lambda_w + 0.68 c_p (T_s - T_b)]}{d (T_s - T_b)} |\mathbf{V}_r| \right)^{1/2}
\]

The volume fraction of liquid water, \(\varphi_w\), appearing in the expressions for \(\mathbf{F}\) and \(\Gamma\), is related to the volume fraction of water-vapor mixture \(\varphi_m\) and mass fraction of vapor \(x_v\) (i.e., to the quantities entering the governing equations (1)–(3)) by

\[
\varphi_w = \varphi_m \frac{\rho_m (x_v) - \rho_v}{\rho_w - \rho_v}
\]

Droplet fragmentation in steam explosions is a complex physical process which can include both fluid dynamics (surface instability) and thermal (explosive boil-up of water) aspects. We adopt here a simple droplet breakup model based on the concept of critical Weber number: the condition for droplet breakup is

\[
We = \frac{\rho_w |\mathbf{V}_r|^2 d}{\sigma} > We_{cr}
\]

in which case the droplet diameter is reduced to \(d = We_{cr} \sigma/\rho_w |\mathbf{V}_r|^2\). In order to avoid possible unphysical values, the resulting diameter was limited from below by a prescribed value \(d_{\text{min}}\) which has to be chosen from experimental data on melt debris following steam explosions. Droplet breakup is taken into account as long as the vapor volume fraction in the water-vapor mixture is below the boundary of droplet flow regime: \(\varphi_v/(\varphi_v + \varphi_w) \leq 0.7\). In the Eulerian framework, melt drop diameter variation in fixed-mesh cells due to movement of melt particles is accounted for by solving the transport equation \(\partial d/\partial t + (\mathbf{V}_s \nabla) d = 0\).
3. Numerical method

Equations are solved numerically using the AUSM-family explicit numerical scheme AUSMPW+ [6] for the water-vapor mixture equations (1), (2), and WENO5 scheme for equations (3), (5). Since the melt particles are more inertial than water-vapor mixture due to high density of the material, algorithm is split into solution of transport equations for particles, then solution of ordinary differential equations describing the source terms (drag and evaporation), followed by the solution of transport equations for the mixture. Pressure $P$ is found from mixture density $\rho_m$ and mass fraction of vapor $x_v$ by inverting the equation of state (6). Solution of the stiff ordinary differential equations representing the exchange terms is performed by the VODE solver.

4. Results

4.1. Initial conditions

Consider propagation of pressure wave in a premixed water-steam-melt zone. As a model problem, 1D planar pressure wave was calculated with the following initial conditions: the initial mass fraction of vapor $x_v = 10^{-3}$, water temperature $T_w = 300$ K, pressure $P_0 = 1$ bar. The reference vapor density $\rho_0^v$ in (8) was calculated assuming the vapor temperature $500$ K, which reflects that in the subcooled (with respect to its saturation point $373$ K at the system pressure $P_0$) vapor phase can only exist initially if it is superheated due to interaction with hot melt. The melt particles were assumed to have temperature $T_s = 3000$ K, the initial diameter of melt droplet was taken $d = 3$ mm, the minimum particle diameter after fragmentation $d_{\text{min}}$, the critical Weber number $W_{\text{cr}} = 12$. The initial volume fraction of melt in the mixture was the main variable parameter in this study, it was varied in the range $\varphi_s = (1 - 5) \cdot 10^{-3}$.

Initially, all phases were non-moving ($V_m = V_s = 0$). The process was initiated by setting high pressure $P_{\text{ini}} = 20$ bar in a small domain $0 \leq x \leq x_0 = 0.1$ m near the left boundary (solid wall). The computational domain was extending to $x = X_{\text{max}} = 2$ m; the boundary conditions on the right boundary correspond to free outflow with the constant ambient pressure equal to $P_0$. The computational mesh was uniform, with the cell size of 1 cm (200 cell).

4.2. Pressure wave propagation

In Fig. 1, the pressure profiles at several instants are shown for three initial volume fractions of melt, $\varphi_s = 10^{-3}$, $2 \cdot 10^{-3}$, and $5 \cdot 10^{-3}$. It can be seen that in each case, the initial pressure disturbance generates the wave in which relative motion of water and melt intensifies evaporation, releasing a part of thermal energy of melt and converting it to mechanical energy supporting wave propagation. Evidently, the peak pressure in the propagating wave depends on the concentration of melt droplets in the mixture, with the maximum pressure by the time $t = 10$ ms reaching levels of $7.3$, $16$, and $72$ bar, respectively. Note that the pressure in the mixture behind the shock wave keeps growing with time due to continuing water evaporation by the hot fragmented melt particles. This evaporation, though, proceeds at lower rate than in the explosion wave because the relative velocity of melt particles and water is smaller due to melt particle entrainment by the expanding mixture. The structure of explosion wave is discussed in more details in the following section.

4.3. Structure of explosion wave

In order to elucidate the processes involved in the propagation of explosion wave, in Fig. 2, the pressure profile at $t = 10$ ms obtained for $\varphi_s = 2 \cdot 10^{-3}$ is plotted together with the evaporation rate $\Gamma$ (see (11)), as well as with the velocity profiles $u_m$ for water-vapor mixture, and $u_s$ for the dispersed particles. Since the melt particles possess approximately an order of magnitude larger density than the mixture, they are more inertial and react to the motion of mixture with some delay. Behind the shock, the mixture velocity is higher than that of particles; the mixture is accelerating particles, the relative velocity is high enough to cause immediate particle
Figure 1. Pressure profiles for initial volume fraction of melt $\varphi_s = 10^{-3}$ (a), $2 \cdot 10^{-3}$ (b), and $5 \cdot 10^{-3}$ (c).

fragmentation. Since the mixture velocity drops behind the shock, the phase velocities are equalized some 20 cm behind it, after which the mixture is decelerating the particles that gained momentum in the course of pressure wave propagation. Thus, the relative velocity (by magnitude) behaves non-monotonously, which is reflected by the local minimum of $\Gamma$.

It must be kept in mind that heat transfer from melt particles to water is affected by melt particle diameter $d$ in two ways. On one hand, fragmentation increases the specific surface area of melt droplets; at the same time, the velocity difference between water-vapor mixture and smaller droplet fragments is established faster, which decreases the heat transfer coefficient (12). Therefore, predictions of explosion features may be sensitive to the ultimate diameter of fragmented droplets $d_{\text{min}}$, as well as to details of fragmentation process.
5. Conclusions
The model for pressure waves due to interaction of high-temperature melt with water coolant is based on several simplifications in comparison with the multifluid models available in the literature. Nevertheless, possibility of describing the shock propagation has been demonstrated. Validation of the model against the experimental data, as well as comparison with the predictions obtained by multifluid code VAPEX-D is planned. The model will also be applied to the analysis of multidimensional configurations, in particular, of stratified steam explosions.

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