Thermal detonation wave in liquid lead – water mixture

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Abstract. It was developed the model of thermal detonation in a mixture of continuous liquid lead and dispersed steam/water particles. Stationary equations of mass, impulse and energy conservations laws for multiphase continuum are applied to describe internal structure of thermal detonation wave. They are supplemented by closing relations describing interfacial friction, heat transfer, and fragmentation. Conditions at leading shock wave and at Chapman-Jouguet plane are used as boundary conditions.

1. Introduction

The rupture of heat exchange tubes in the steam generator of the BREST-OD-300 lead-cooled reactor is classified as a design basis accident and is required detailed studies [1]. In the course of its development, various physical processes can occur which threat the safety of the nuclear power plant [2, 3]. One of the insufficient studied phenomena arising during the development of the accident of this type is the thermal interaction of the liquid lead coolant with the water discharged from the rupture. In studies [4-6], separate aspects of this phenomenon were studied: pressure waves in liquid lead generated by a drop of water boiling in the lead, the flow of lead caused by this interaction and its effect on neighbouring heat exchange tubes, the energy of the thermal interaction process and its potential for explosive interactions. Current research is a continuation of the mentioned studies. The subject of this research is the thermal detonation wave during the interaction of liquid lead with water.

The study [7] in 1975, was the first to formulate an analogy between the propagation of a detonation wave through a melt-coolant mixture and a detonation wave in a chemically reacting medium, the mechanism of which is well studied and the corresponding mathematical model is developed [8]. In the case of a melt-coolant mixture, the role of an exothermic chemical reaction that releases the energy is played by the fragmentation of the melt. Due to fragmentation, the area of the interphase surface increases significantly and the intensity of the transfer of thermal energy from the melt to the coolant sharply increases.

It is assumed that the melt fragmentation and the thermal energy transfer to the coolant occurs in a relatively narrow spatial region immediately behind the leading shock front until the achievement of hydrodynamic and thermodynamic equilibrium between the components (melt fragments and hot coolant) in Chapman – Jouguet plane, behind which the mixture expands as a homogeneous equilibrium flow without interaction of its components, which has a nonstationary character and depends on the explosion geometry. This detonation is called thermal detonation and it takes place both in systems with large melt droplets dispersed in a continuous coolant (traditionally considered...
case), and in systems with coolant droplets in a continuous melt phase ("inverted" configuration), Figure 1.

By analogy with the theory of chemical detonation, in thermal detonation, it is possible to calculate the parameters of the mixture in the Chapman – Jouguet plane only on the basis of conservation laws, without considering the complex kinetics of fragmentation and the heat transfer processes in the interaction zone, Figure 2.

It should be noted that, in contrast to the detonation of gaseous combustible mixtures, the construction of the shock adiabat for the case of thermal detonation is ambiguous and depends on the assumptions about the multiphase flow structure in this plane. The detonation adiabat itself (the Hugoniot adiabat) is determined by the parameters of the equilibrium mixture.

![Figure 1. Multiphase thermal detonation model: SW – shock wave, CJ – Chapman-Jouguet plane. Traditional system: 1 – coolant, 2 – melt droplets, 3 – vapor. Reverse configuration: 1 – melt, 2 – coolant droplets, 3 – vapor.](image1)

![Figure 2. Hugoniot adiabat and Chapman-Jouguet point for thermal detonation in multiphase mixture](image2)

It should be noted that the proposed model assumes the fulfillment of the condition of complete thermodynamic and mechanical equilibrium in the Chapman – Jouguet plane, which means the formation of a homogeneous mixture at the end of the fragmentation zone, all components of which have the same temperatures and velocities. Obviously, this condition can be assumed to be satisfied only when the melt is completely fragmented.

The study [7] has initiated further researches in this direction [9–11]. The authors of these papers focused their efforts on a more detailed description of the interphase interaction behind the shock wave, as well as on the softening of the requirement for complete melt fragmentation in Chapman – Jouguet plane [7]. An additional parameter was introduced into the mathematical model - the degree of melt fragmentation; to describe the processes behind the shock wave, one-dimensional stationary equations of a multiphase flow with the corresponding correlations for fragmentation, heat transfer, and friction were used. The Chapman – Jouguet plane was determined by the condition of equalization of the velocities of the melt and water, while the condition of equality of the flow velocity and the speed of sound was fulfilled.

In subsequent works [12-16], the theory of thermal detonation was improved. The study [12] analyzed the assumptions underlying the theory of Hugoniot adiabats. It was noted that intermediate states cannot be determined, despite the fact that the initial and final states on the Hugoniot adiabat are related by the Rayleigh line. It was also emphasized that the leading shock adiabat does not always
exist. The authors of [12] refused to introduce into the model a parameter characterizing the melt fragmentation degree, due to its uncertainty.

The studies [13, 14] were devoted to the analysis of KROTOS experiments using the thermal detonation model. The authors, using the experimental values of the wave pressure and the velocity of its propagation, determined the initial state of the mixture, the fragmented melt fraction, and the expansion work.

In the research [15] the model of thermal detonation was supplemented with a model of microinteractions of a melt with a coolant, according to which the melt debris formed as a result of fragmentation does not thermally interact with the entire coolant, but only with its part, thereby providing a more powerful interaction. As a result, the calculations performed in [15] confirmed that even in very "lean" mixtures (with a low melt content), supercritical detonation is possible.

In [16], the results of studies of the propagation of thermal detonation waves through mixtures: uranium dioxide – water, aluminum oxide – water, steel – water using the Hugoniot adiabat method are presented. The mathematical model uses the concept of microinteractions, and also takes into account the partial fragmentation of the melt, for which a parameter which consider the degree of fragmentation is introduced.

2. The model description

We will consider a system of three phases: 1- continuous liquid lead (subscript \(m\)), 2- large drops of water inside vapor bubbles (index \(d\)), 3- small drops or fragments of water inside vapor bubbles (index \(f\)). Each phase is characterized by its own volume fraction \(\alpha\). These phases completely occupy any local volume of the considered region; therefore, \(\alpha_m + \alpha_d + \alpha_f = 1\).

Each phase is described by own density, velocity and temperature, all the phases have the same local volume of the considered region; therefore, \(\alpha_m + \alpha_d + \alpha_f = 1\).

Due to the difference in velocities between the melt and the large water droplets surrounded by vapor bubbles, fragmentation of these droplets into small fragments occurs, leading to an increase in the heat exchange surface between the melt and the vapor -water medium, which causes an increase in heat transfer and expansion of vapor.

We will describe the studied system using stationary equations of conservation of mass, momentum and energy of a multiphase medium [16, 17]:

\[
\frac{d}{dx} (\alpha_m \rho_m V_m) = 0, \quad \frac{d}{dx} (\alpha_d \rho_d V_d) = -\Gamma_f, \quad \frac{d}{dx} (\alpha_f \rho_f V_f) = +\Gamma_f, \tag{1}
\]

\[
\frac{d}{dx} (\alpha_m \rho_m V_m^2) = -\alpha_m \frac{dP}{dx} + K_{dm}(V_d - V_m) + K_{fm}(V_f - V_m), \tag{2}
\]

\[
\frac{d}{dx} (\alpha_d \rho_d V_d^2) = -\alpha_d \frac{dP}{dx} + K_{dm}(V_m - V_d) - \Gamma_f V_d, \tag{3}
\]

\[
\frac{d}{dx} (\alpha_f \rho_f V_f^2) = -\alpha_f \frac{dP}{dx} + K_{fm}(V_m - V_f) + \Gamma_f V_d, \tag{4}
\]

\[
\frac{d}{dx} (\alpha_m \rho_m V_m h_{sm}) = R_{dm}(T_d - T_m) + R_{fm}(T_f - T_m) + V_m K_{dm}(V_d - V_m) + V_m K_{fm}(V_f - V_m), \tag{5}
\]

\[
\frac{d}{dx} (\alpha_d \rho_d V_d h_{sd}) = R_{dm}(T_m - T_d) + V_d K_{dm}(V_m - V_d) + K_{dm}(V_m - V_d)^2 - \Gamma_f h_{sd}, \tag{6}
\]

\[
\frac{d}{dx} (\alpha_f \rho_f V_f h_{sf}) = R_{fm}(T_m - T_f) + V_f K_{fm}(V_m - V_f) + K_{fm}(V_m - V_f)^2 + \Gamma_f h_{sd}, \tag{7}
\]
Equations (1)-(7) use standard notation: $\rho$ – density, $V$ – velocity, $T$ – temperature, $P$ – pressure, $h_c$ – stagnation enthalpy, which is defined as $h_c = e + P/\rho + V^2/2$, $e$ is internal energy; the values $K$ and $R$ describe the friction and heat transfer between the phases, $\Gamma_f$ – the fragmentation rate of large water droplets.

The melt density and internal energy are functions of its temperature $\rho_m = \rho_m(T_m)$ and $e_m = e_m(T_m)$. The densities of the $d$-phase and $f$-phase are determined by the volumetric vapor content in these phases, $\rho_d = (1 - \varphi_d)\rho'(P) + \varphi_d\rho''(P)$, $\rho_f = (1 - \varphi_f)\rho'(P) + \varphi_f\rho''(P)$, where $\varphi_d$ and $\varphi_f$ are the void fractions in the $d$-phase and $f$-phase.

3. Description of interphase interaction

We will assume that the dispersed formation (a large drop of water inside a vapor bubble) has a spherical shape. The resistance force to the movement of this dispersed particles in a continuous medium of liquid lead is described as follows:

$$F_d = \frac{1}{2} C_{D,dm} \rho_{ef} \frac{L_d^2}{4} |V_m - V_d| (V_m - V_d) \tag{8}$$

Here $C_{D,dm}$ is the drag coefficient of a dispersed particle of the $d$-phase, $L_d$ is the diameter of this particle. The quantity $\rho_{ef}$ describes the effective density of the medium that surrounds the dispersed particle under consideration, $\rho_{ef} = (\alpha_m \rho_m + \alpha_f \rho_f) / (\alpha_m + \alpha_f)$. Taking into account (8) we can conclude, that

$$K_{dm} = \frac{3}{4} \frac{C_{D,dm}}{L_d} \rho_{ef} \alpha_d |V_m - V_d| \tag{9}$$

In present work, following [17], we use the constant value $C_{D,dm} = 2.5$ to take into account the increase in resistance during fragmentation of a dispersed particle.

The value of $K_{fm}$ is determined in a similar way:

$$K_{fm} = \frac{3}{4} \frac{C_{D,fm}}{L_f} \rho_m \alpha_f |V_m - V_f| \tag{10}$$

where $C_{D,fm}$ is the drag coefficient of a dispersed particle of the $f$-phase, which we will assume as $C_{D,fm} = 0.4$, $L_f$ is the diameter of this particle.

The quantities $R_{dm}$ and $R_{fm}$, which describe the interfacial heat transfer, are expressed in terms of the heat transfer coefficients as follows:

$$R_{dm} = 6\alpha_d \frac{h_{dm}}{L_d} \quad R_{fm} = 6\alpha_f \frac{h_{fm}}{L_f} \tag{11}$$

Here $h_{dm}$ and $h_{fm}$ are the coefficients of heat transfer from the melt to particles of the $d$-phase and $f$-phase, respectively. We will assume that they are constant, $h_{dm} = h_{fm} = 10^3 W/(m^2K)$, as was suggested in [17].

Fragmentation of large water droplets inside a vapor bubble, or $d$-phase, as far as the authors know, has not been previously studied. Let us assume that in the detonation wave, due to the difference in velocities between the carrier medium (liquid lead) and the $d$-phase particles, the fragmentation of which occurs according to the boundary layer stripping mechanism. The resulting fragments have a fixed initial size $L_0$, and consist of vapor and water in the same mass proportion as the initial parent particle. We will use the model proposed in [18]. In accordance with it, a fragmented dispersed particle loses its mass $m$ at a rate:

$$\frac{dm}{dt} = c_{frag} |V_d - V_m| \pi L_d^2 \sqrt{\rho_d \rho_{ef}} \tag{12}$$
The empirical constant $c_{\text{frag}}$ is approximately $1/6$. Multiplying the equation (12) by the number of dispersed particles of the $d$-phase per unit volume, we obtain $\Gamma = \alpha_d V_d - V_m \sqrt{\rho_d \rho_{\text{ef}} / L_d}$, it was taken into account that the product of all constants is equal to one.

4. Hugoniot adiabat

We obtain the first integrals of the system of differential equations (1)-(7). Adding equations (1) and integrating the total equation, we obtain the formulation of conservation of the mass flow of the multiphase mixture:

$$\alpha_m \rho_m V_m + \alpha_d \rho_d V_d + \alpha_l \rho_l V_l = \text{const}_1$$

(13)

Similarly, from the equations of the momentum of each phase (2)-(4) it follows that the flux of the impulse of the multiphase mixture is conserved:

$$\alpha_m \rho_m V_m^2 + \alpha_d \rho_d V_d^2 + \alpha_l \rho_l V_l^2 + P = \text{const}_2$$

(14)

In the same way, from equations (5)-(7), we obtain the formulation of conservation of the energy flux of the multiphase mixture:

$$\alpha_m \rho_m V_m h_{\text{sm}} + \alpha_d \rho_d V_d h_{\text{sd}} + \alpha_l \rho_l V_l h_{sf} = \text{const}_3$$

(15)

We will consider a thermal detonation wave in a multiphase mixture in a coordinate system moving with this wave. The parameters of the initial mixture will be denoted by the subscript 0. The subscript 2 will denote the parameters of the equilibrium multiphase mixture after the completion of the interphase interaction. Then, based on the first integrals (13)-(15), we can obtain the equations connecting the parameters of the multiphase flow in sections 0 and 2:

$$\rho_2 V_2 = \rho_0 V_0,$$

$$h_2 + \frac{1}{2} V_2^2 = h_0 + \frac{1}{2} V_0^2$$

(16)

$$\rho_0 = \frac{\alpha_m \rho_m h_{\text{m0}} + \alpha_d \rho_d h_{\text{d0}}}{\alpha_m \rho_m + \alpha_d \rho_d}.$$ 

(17)

$$h_0 = \frac{\alpha_m \rho_m h_{\text{m0}} + \alpha_d \rho_d h_{\text{d0}}}{\alpha_m \rho_m + \alpha_d \rho_d}.$$

(18)

After algebraic transformations of equations (16), (17), we obtain the Hugoniot adiabat equation:

$$(P_2 - P_0)(v_2 + v_0) - 2(h_2 - h_0) = 0$$

(20)

Here $v_0 = 1/\rho_0$ and $v_2 = 1/\rho_2$ – specific volumes of the multiphase mixture in planes 0 and 2.

In equation (20), the specific volume $v_2$ and the enthalpy of the equilibrium mixture in plane 2 are determined by the pressure $P_2$ and the temperature $T_2$ of the mixture in this plane. By setting the temperature $T_2$ and determining the pressure $P_2$ from (20), we can calculate $v_2$, and on the plane $(v_2, P_2)$ draw a curve (Hugoniot adiabat) which will describe all possible states of the equilibrium mixture for given initial parameters of the multiphase mixture.

Figure 3 shows a typical Hugoniot adiabat for a mixture of liquid lead - vapor - water with initial parameters $(v_0 = 0.2906438 \cdot 10^{-3} \text{m}^3 / \text{kg}, \ P_0 = 0.8 \text{ MPa}, \ h_0 = 0.1733916 \cdot 10^5 \text{ J/kg}, \ T_{\text{m0}} = 800 \text{ K}, \ \varphi_0 = 0.5)$. It is also shown a point representing the initial state of the multiphase mixture and a tangent line drawn from the initial point to the adiabat. The slope of this straight line determines the speed of the detonation wave.

5. Leading shock wave

Let us consider the parameters of the mixture on the leading shock wave, the velocity of which $V_0$ is determined by the slope of the Rayleigh line to the Chapman-Jouguet point on the Hugoniot adiabat. In the plane of the shock wave, which will be denoted by the subscript 1, a pressure jump occurs, which causes discontinuities of some parameters relative to their initial values. We will assume that
the temperature of the melt in plane 1 does not change ($T_{m1} = T_{m0}$), and fragmentation of dispersed formations does not occur.

The mass flow rates of the melt and of the $d$-phase on the shock wave are conserved:

\begin{align}
\alpha_{m1} \rho_{m1} V_{m1} &= \alpha_{m0} \rho_{m0} V_{0}, \\
\alpha_{d1} \rho_{d1} V_{d1} &= \alpha_{d0} \rho_{d0} V_{0}
\end{align}

(21)

Since the temperature of the melt does not change, then $\rho_{m1} = \rho_{m0}$. Note that the velocities of the melt and $d$-phase are not equal in the shock wave.

The impulse flux of the mixture on the shock wave is also conserved:

\begin{align}
P_{1} + \alpha_{m1} \rho_{m1} V_{m1}^2 + \alpha_{d1} \rho_{d1} V_{d1}^2 &= P_{0} + (\alpha_{m0} \rho_{m0} + \alpha_{d0} \rho_{d0}) V_{0}^2
\end{align}

(22)

In addition, on the shock wave, the energy conservation law is fulfilled for each phase:

\begin{align}
h_{m1} + \frac{1}{2} V_{m1}^2 &= h_{m0} + \frac{1}{2} V_{0}^2, \\
h_{d1} + \frac{1}{2} V_{d1}^2 &= h_{d0} + \frac{1}{2} V_{0}^2
\end{align}

(23)

A multiphase mixture on a shock wave consists of a melt and a dispersed $d$-phase, so $\alpha_{m1} + \alpha_{d1} = 1$. The density and specific enthalpy of the $d$-phase are determined by the pressure and volumetric vapor quality on the shock wave: $\rho_{d1} = \rho_{d1}(P_{1}, \varphi_{1})$ and $h_{d1} = h_{d1}(P_{1}, \varphi_{1})$, and the specific enthalpy of the melt is expressed through the pressure on the shock wave: $h_{m1} = h_{m1}(P_{1})$. Equations (21) - (23) make it possible to determine the unknown values of the parameters on the shock wave (in plane 1): $\alpha_{m1}, \alpha_{d1}, V_{m1}, V_{d1}, P_{1}, \varphi_{1}$.

6. Conclusions

It was developed the model of thermal interaction of continuous liquid lead and dispersed steam/water particles. The model is based on a concept of multiphase thermal detonation wave. Stationary equations of mass, impulse and energy conservations laws for multiphase continuum are applied to describe internal structure of thermal detonation wave. Conditions at leading shock wave and at Chapman-Jouguet plane are used as boundary conditions. The model is aimed to study consequences of the water discharge into molten lead from the rupture of the heat exchange tube of the steam generator of the BREST reactor.
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