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Shock waves in multiphase flow of fuel–coolant interaction

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Abstract — The interaction of fuel and coolant (FCI) is a complex multiphase process due to the fact that the fragmentation and heat transfer process are not easy to cast in simple mathematical formulas. This paper, a theoretical model has been developed by considering multiphase flow shock wave propagating of fuel–coolant interaction. Analysis of a steady-state vapour explosion in one dimension has been carried out by applying the conservation laws of mass, momentum, energy and the appropriate equation of state for an interaction of molten dioxide uranium and water. Using the model, we predicted the pressure magnitudes behind shock wave of vapour explosion varied with the initial volume fraction of vapour, melt mass concentrations, liquid entrained fraction and when they were considered as dangerous. © 2000 Éditions scientifiques et médicales Elsevier SAS

shock wave / fuel–coolant interaction (FCI) / Chapaman–Jouguet (CJ) pressure / void volume fraction / multiphase flow

Nomenclature

C	mass concentration	
f	mass fraction	
h	specific enthalpy	$\mathrm{kJ \cdot kg^{-1}}$
n	particle number density	
p	CJ pressure	bar
T	temperature	K
w	sound velocity	$\mathrm{m \cdot s^{-1}}$
x	mass concentration	

Greek symbols

α	volume fraction
ρ	density
K	isentropic exponent

Subscripts

l	phase (vapour, water, melt)
$l, 1$	phase before shock wave
$l, 2$	phase behind shock wave
h	homogeneous average
h, 1	mixture average before shock wave
h, 2	mixture average behind shock wave
1, 1	vapour before shock wave
1, 2	vapour behind shock wave
2, 1	water before shock wave
2, 2	water behind shock wave
3, 1	melt before shock wave
3, 2	melt behind shock wave
4, 2	entrained water behind shock wave
5, 2	entrained melt behind shock wave

1. INTRODUCTION

A vapour explosion is physical phenomenon in which rapid thermal energy transfer occurs during the mixing of a hot liquid (fuel) and a cold liquid (coolant). It results in a sharp rise of the system pressure followed by an explosion with destructive work done to the surroundings. Shamoun and Corradini et al. [1] conceptualised the vapour explosion process into four phases, mixing phase, triggering phase, propagation phase and expansion phase. These phases are a complex multiphase process due to the fact that the fragmentation and heat transfer process are not easy to cast in simple mathematical formulas. However, the theoretical models help one to understand the behaviour of this phenomenon [2–4]. For an accurate assessment of an energetic fuel–coolant interaction event based on the conceptual picture of the

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aforementioned four phases, mechanistic and thermodynamic models were proposed to simulate this phenomenon. Unfortunately, the current lack of understanding the detail mixing and fragmentation process has led the mechanistic model to invoke empirical coefficients for the rapid fuel fragmentation and heat transfer processes to fit the model predictions with actual data. Nelson and Duda's experimental observations [5] have shown that the assumption of complete fuel fragmentation in a vapour explosion by the shock adiabatic thermodynamic model results in overestimation for the shock pressure, propagation velocity, and work output. So, Board et al. [6] proposed the fine fragmentation behind a shock front and following steam production and expansion as the driving force for transferring shock waves in self sustaining detonation waves. Their remark that not all melt behind shock front may participate in the energy transfer process was generally accepted. Scot et al. [7] assumed the homogeneous mixture was relaxed and resulted in interesting estimations, one of them is the thickness of the "discontinuity" front depending on the initial particle size. However, in the absence of a complete mechanistic model and numerical computations with very fine discretization grid discriminating regions of near and far, a shock wave model may be considered an attractive alternative for an accurate assessment of the vapour explosion process if spatial difference in equilibrium can be accounted for.

In this paper, a model of shock waves of multiphase flow based on the shock adiabatic thermodynamic model proposed originally by Landau [8] has been developed. The model can relax the condition of complete fragmentation of the fuel in the vapour explosion process and predict the pressure's output under assuming the various parameters' values. From these analysis, we can judge the dangers of FCI.

2. THEORETICAL MODEL

The shock adiabatic model suggests that in an energetic fuel–coolant interaction (FCI), a pressure pulse is generated due to a rapid thermal energy transfer from the fuel to the coolant. The propagation of this pulse results in shock wave that spatially propagates in the medium, collapses the vapour film that blankets the fuel, and causes fine fragmentation of the fuel. The mixture behind the shock wave attains thermal and mechanical equilibrium at the high pressure, which is followed by an expansion process driving the shock forward. By using the analogy between the thermal and chemical detonation, for a given set of initial conditions, there is only one state for the material behind the shock front that can make the reaction stable. The state corresponds by analogy to the Chapaman–Jouguet detonation point (CJ point).

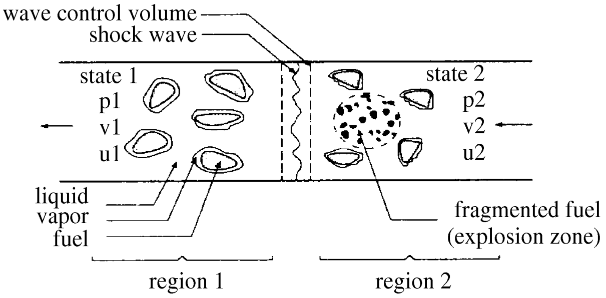

Figure 1. Schematic of the reaction regions 1 and 2 separated by a shock wave.

According to the experimental observations, it was found that not all the fuel in an energetic vapour explosion event fragments and transfers its internal energy to the coolant. In fact, only a small percentage of the total mass of the fuel was found broken into fine particles. So, we consider that the control volume of a FCI system behind the shock is divided into two zones, the explosion zone and the nonexplosion zone as shown in *figure 1* according the Shamoun and Corradini [1].

We assume that the thickness of the shock front is small and that no fragmentation, interfacial heat and mass transfer practically take place. According to the no mechanical phase coupling model [9, 10], for multiphase, the local volume averaged equations give as follows:

$$\Delta(\alpha_l \rho_l w_l) = 0 \tag{1}$$

$$\Delta\left(\alpha_l \rho_l w_l^2\right) + \alpha_l \Delta p = 0 \tag{2}$$

$$\Delta\left[\alpha_l \rho_l w_l \left(h_l + \frac{1}{2} w_l^2\right)\right] = 0 \tag{3}$$

$$\Delta(\alpha_l \rho_l w_l C_{il}) = 0 \quad \text{for } \alpha_l \geq 0 \tag{4}$$

$$\Delta(w_l n_l) = 0 \qquad \text{for } \alpha_l \geq 0 \tag{5}$$

2.1. Multiphase

The problem is considerably simplified with the assumption that all the velocities are equal, $w_l = w_{\mathrm{h}}$, where

$$w_{\mathrm{h}} = \frac{1}{\sqrt{\rho_{\mathrm{h}} \sum_{l=1}^{l_{\max}} [\alpha_l / (\rho_l a_l^2)]}}$$

is homogeneous mixture sound velocity for small pressure amplitude.

The mass conservation of a single velocity field is then

$$\begin{aligned} &\alpha_{l,2}\rho_{l,2}w_{\mathrm{h},2} - \alpha_{l,1}\rho_{l,1}w_{\mathrm{h},1} = 0 \quad \text{or} \\ &\frac{\alpha_{l,2}\rho_{l,2}}{\rho_{\mathrm{h},2}} - \frac{\alpha_{l,2}\rho_{l,2}}{\rho_{\mathrm{h},2}} = 0 \quad \text{or} \\ &x_{l,2} - x_{l,1} = 0 \end{aligned} \tag{6}$$

which says the field mass concentration remains constant across the shock front. This is a remarkable equation. It indicates that such calculation is conveniently performed if one uses the definition of the mass concentrations:

$$x_l = \frac{\alpha_l \rho_l}{\rho_{\mathrm{h}}} \tag{7}$$

Thus, the homogeneous density can be expressed by

$$\rho_{\mathrm{h}} = \frac{1}{\sum_{l=1}^{l_{\max}}(x_l/\rho_l)} \tag{8}$$

The mixture mass conservation results in

$$\rho_{\mathrm{h},1}w_{\mathrm{h},1} = \rho_{\mathrm{h},2}w_{\mathrm{h},2} = \rho_{\mathrm{h}}w_{\mathrm{h}} \tag{9}$$

Using the mixture mass conservation the mixture momentum equation can be transformed in

$$\begin{aligned} &\rho_{\mathrm{h},2}w_{\mathrm{h},2}^2 = \rho_{\mathrm{h},1}w_{\mathrm{h},1}^2 + p_2 - p_1 = 0 \quad \text{or} \\ &(\rho_{\mathrm{h}}w_{\mathrm{h}})^2 = \frac{p_2 - p_1}{1/p_{\mathrm{h},1} - 1/p_{\mathrm{h},2}} \end{aligned} \tag{10}$$

The energy conservation for each velocity field is then

$$\begin{aligned} &\alpha_{l,2}\rho_{l,2}w_{\mathrm{h},2}\left(h_{l,2} + \frac{1}{2}w_{\mathrm{h},2}^2\right) \\ &\quad - \alpha_{l,1}\rho_{l,1}w_{\mathrm{h},1}\left(h_{l,1} + \frac{1}{2}w_{\mathrm{h},1}^2\right) = 0 \end{aligned} \tag{11}$$

After applying the field and the mixture mass conservation equation and using the last form of the momentum equation the single field energy conservation results in

$$h_{l,2} - h_{l,1} - \frac{1}{2}(p_2 - p_1)\left(\frac{1}{\rho_{\mathrm{h},1}} + \frac{1}{\rho_{\mathrm{h},2}}\right) = 0 \tag{12}$$

The assumption that the multiphase flow consists of steam and water which are in thermodynamical equilibrium reduces equation (10) to one derived by Fischer [11] in 1967.

For frozen two-component flow we have

$$\begin{aligned} &(T_{1,2} - T_{1,1})C_{p,1} - \frac{1}{2}p_1\left(\frac{p_2}{p_1} - 1\right) \\ &\quad \cdot \left[\frac{x_1}{\rho_{1,1}}\left(1 + \frac{p_1}{p_2}\frac{T_{1,2}}{T_{1,1}}\right) + \frac{1 - x_1}{\rho_{2,1}}\left(1 + \frac{\rho_{2,1}}{\rho_{2,2}}\right)\right] \\ &= 0 \end{aligned} \tag{13}$$

2.2. Melt-coolant interaction detonations

In the fuel coolant interaction detonations molten material is premixed with liquid being in thermal non-equilibrium. The melt is in state of film boiling. The incoming shock wave causes instability and fragments the melt. The generated microscopic particles released their thermal energy by directly contacting with the surrounded coolant. This interaction is short distance interaction. It may happen so that the coolant can be specified as follows.

One very useful simplification for such analysis is proposed by Shamoun and Corradini [1]. The authors proposed that the entrained melt f_3x_3 intermixed with the entrained liquid $f_2x_2 = f_2(1 - x_1 - x_3)$ reach thermal equilibrium. They have common pressure p_2 and common mixture temperature T_{m}. This in fact specifies the thermal energy release behind the shock and makes the short distance entrained liquid fraction f_2 be function of the initial parameter, a consequence is not recognised by the authors. So, we are looking for the effect of these unknown variable values on CJ pressures, which satisfy the Chapman–Jouquet condition behind the detonation front.

The densities and enthalpies required for this computation are functions of the pressure and temperature before and behind the shock, respectively.

We assume that the pressure wave first causes the micro-fragmentation and acceleration of the fine particles into the short distance liquid. Then the shock discontinuity comes. In this case the mass conservation (6) holds. The homogeneous mixture densities are then

$$\rho_{\mathrm{h},1} = \frac{1}{\frac{x_1}{\rho_1(p_1,T_{1,1})} + \frac{x_2}{\rho_2(p_1,T_{2,1})} + \frac{x_3}{\rho_3(p_1,T_{3,1})}} \tag{14}$$

$$\begin{aligned} \rho_{\mathrm{h},2} = &\left[\frac{x_1}{\rho_1(p_2,T_{1,2})} + \frac{(1 - f_2)x_2}{\rho_2(p_2,T_{2,2})} + \frac{(1 - f_3)x_3}{\rho_3(p_2,T_{3,2})}\right. \\ &\quad \left. + \frac{f_2x_2}{\rho_1(p_2,T_{\mathrm{m}})} + \frac{f_3x_3}{\rho_3(p_2,T_{\mathrm{m}})}\right]^{-1} \end{aligned} \tag{15}$$

where f_2 indicates the fraction of x_2 being within the short distance liquid. f_3 is the fraction of the melt being fine fragmented.

Then the shock adiabatic for each phase is:

(1) primary steam:

$$h_{1,2} = h_1(p_1, T_{1,1}) + \Delta h \tag{16}$$

where

$$\begin{aligned} &\Delta h = \frac{1}{2}(p_2 - p_1)\left(\frac{1}{\rho_{\mathrm{h},1}} + \frac{1}{\rho_{\mathrm{h},2}}\right) \\ &h_1(p_2, T_{1,2}) = h_{1,2} \quad \text{or} \quad T_{1,2} = T_1[p_2, h_{1,2}] \\ &\rho_{1,2} = \rho_1(p_2, T_{1,2}) \end{aligned}$$

(2) not entrained liquid:

$$\begin{aligned} &h_{2,2} = h_2(p_1, T_{2,1}) + \Delta h \\ &h_2(p_2, T_{2,2}) = h_{2,2} \\ &\rho_{2,2} = \rho_2(p_2, T_{2,2}) \end{aligned} \tag{17}$$

(3) entrained liquid and melt:

$$\begin{aligned} &f_2 x_2 h_{4,2} + f_3 x_3 h_{5,2} = f_2 x_2 h_{2,1} + f_3 x_3 h_{3,1} \\ &h_1(p_2, T_\mathrm{m}) = h_{4,2} \\ &\rho_{4,2} = \rho_1(p_2, T_\mathrm{m}) \\ &h_3(p_2, T_\mathrm{m}) = h_{5,2} \\ &\rho_{5,2} = \rho_3(p_2, T_\mathrm{m}) \end{aligned} \tag{18}$$

(4) the temperature of not entrained melt is constant.

The definition of the homogeneous velocity of sound written in terms of the mass concentrations gives

$$\frac{1}{(\rho w_\mathrm{h})^2} = \sum_{l=1}^{l_{\max}} \frac{x_l}{(\rho_l a_l)^2} \tag{19}$$

Thus, the Chapman–Jouquet condition is defined as

$$\frac{1}{(\rho_\mathrm{h} w_\mathrm{h})_2^2} = \frac{1}{(\rho_\mathrm{h} w_\mathrm{h})^2} = \frac{1/\rho_{\mathrm{h},1} - 1/\rho_{\mathrm{h},2}}{p_2 - p_1} \tag{20a}$$

or

$$\begin{aligned} &\frac{x_1}{[\rho_1(p_2, T_{1,2}) a_1(p_2, T_{1,2})]^2} \\ &\quad + \frac{(1 - f_2)x_2}{[\rho_2(p_2, T_{2,2}) a_2(p_2, T_{2,2})]^2} \\ &\quad + \frac{(1 - f_3)x_3}{[\rho_3(p_2, T_{3,2}) a_3(p_2, T_{3,2})]^2} \\ &\quad + \frac{f_2 x_2}{[\rho_1(p_2, T_\mathrm{m}) a_1(p_2, T_\mathrm{m})]^2} \\ &\quad + \frac{f_3 x_3}{[\rho_3(p_2, T_\mathrm{m}) a_3(p_2, T_\mathrm{m})]^2} = \frac{1/\rho_{\mathrm{h},1} - 1/\rho_{\mathrm{h},2}}{p_2 - p_1} \end{aligned} \tag{20b}$$

3. METHOD OF SOLUTION

(1) Assume as initial values at the beginning of the interactions as follows:

$$\begin{aligned} &P_2 = p_1 + \Delta p, \quad \text{where } \Delta p > 0 \\ &T_{1,2} = T_{1,1}\left(\frac{p_2}{p_1}\right)^{(k_1 - 1)/k_1} \\ &T_{2,2} = T_{2,1} \\ &T_\mathrm{m} = T_{1,1} \\ &\rho_{\mathrm{h},2} = \rho_{\mathrm{h},1} \end{aligned}$$

(2) Iterated and calculated the enthalpy of vapour, the temperatures of water $T_{2,2}$, entrained water and melt mixtures T_m using equations (16), (17) and (18), respectively.

(3) According to equation (15), to calculate the mixture density $\rho_{\mathrm{h},2}$ behind shock wave front.

(4) From equation (20), the new pressure behind shock wave front p_2 is computed.

(5) Repeating steps (2)–(4) until the CJ pressure difference between two iterations is smaller than the control precision.

4. RESULTS

For the mixture consisting of uranium dioxide and water, *figure 2* shows the CJ pressure behind the shock wave as a function of void fraction for different mass concentration of melt. From this diagram, one can realise that the CJ pressures sharply increase with the volume fraction decreasing of vapour. Increasing of the melt the mass concentration x_3 up to about 30 %, the CJ pressure is largest.

The behaviours of mixtures having small amount of melt (lean) have been shown in *figure 3*.

Under the small values x_3, the value of mass concentration of melt hardly effect on the pressures, and for void fraction larger than 10 %, the CJ pressure has low risk. However, even very small amount of entrained water may cause at low void fractions potential considerable

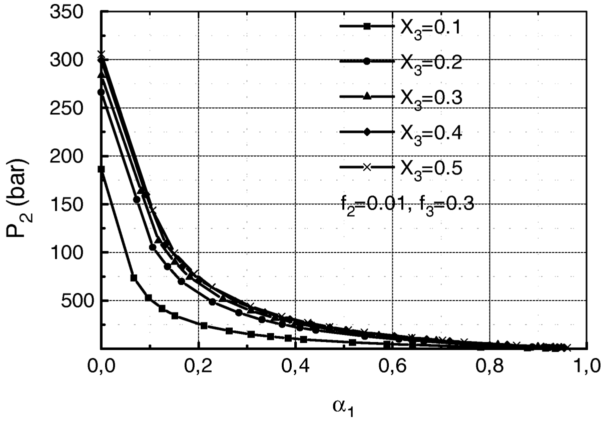

Figure 2. The CJ pressure behind shock wave as a function of the initial volume fraction of vapour: large melt mass concentrations.

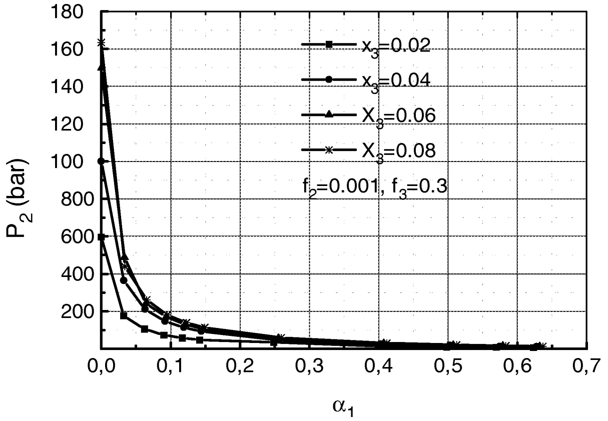

Figure 3. The CJ pressure behind shock wave as a function of the initial volume fraction of vapour: small melt mass concentrations.

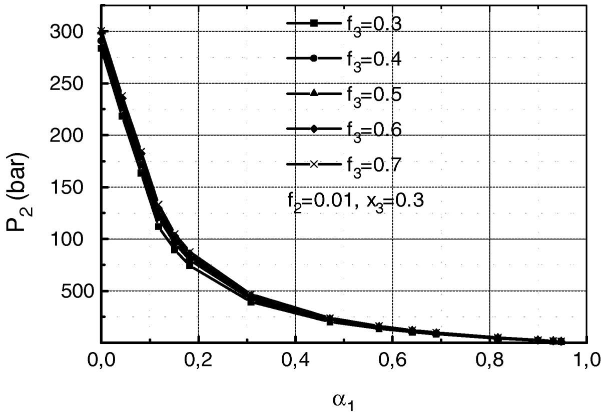

Figure 4. The CJ pressure behind the shock wave as a function of the initial volume fraction of vapour. Parameter: melt entrained fraction f_3.

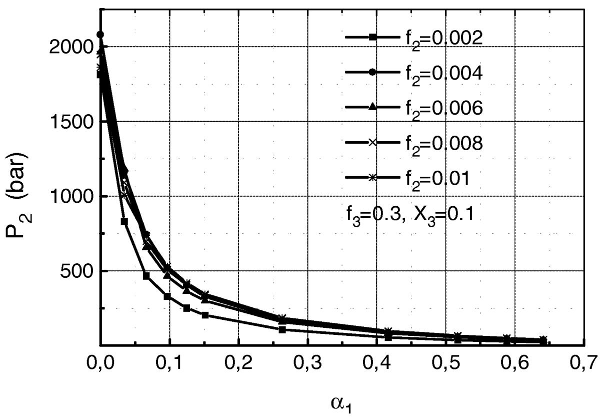

Figure 5. The CJ pressure behind the shock wave as a function of the initial volume fraction of vapour. Parameter: liquid entrained fraction f_2.

CJ pressures. This result confirms the warning expressed by Yuen and Theofanous [12] to consider lean mixture as potential explosion. So, one can see that the lean systems are very sensitive to void fraction.

Comparing the *figures 2* and *3*, we find that the pressures behind shock wave increase with the mass concentration of melt till the concentration of melt reached about 30 %.

Figures 4 and *5* show the pressures vary with various of the entrained melt and liquid fraction, respectively. The conclusion is entrained melt and liquid fractions hardly influence the pressure.

5. CONCLUSION

In this paper, we applied the shock wave theory in order to predict features of melt–water interaction. This model explains that the mixtures consisting of dispersed melt and dispersed water have detonation solution but there is no mechanism to explain the degree of melt fragmentation and water entrained brought in contact with the melt debris.

(1) The simulation results of shock wave show that the CJ pressures behind the shock wave are mainly influenced by the mass concentrations of melt and void fraction before the shock wave.

(2) The smaller the mass concentrations of vapour are, the higher the CJ pressure is. When melt mass concentration is about 30 %, the CJ pressure is highest.

(3) Even very small amount of entrained water may cause at low void fractions considerable detonation pres-

sures. This result confirms the warning expressed by Yuen and Theofanous in the situation.

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