

# Thermal explosion under film boiling conditions

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(Received 27 September 1990)

**Abstract**—This study deals with thermal explosion in liquid metal–water systems. The heat transfer and the time scale for the fine fragmentation behind the front of the shock wave were assessed. It was shown that the direct liquid–liquid contact is impossible for most of the media of interest and the heat is transferred under film boiling conditions. The fine fragmentation seems to occur too slowly to support the propagation in the initial stage of the explosion. A modification of the propagation mechanism is suggested.

## 1. INTRODUCTION

THE PRESENT paper is concerned with vapor explosions in liquid metal–water systems. The large-scale vapor explosions have been described by use of a detonation model, which provides an overall conceptual picture of the process. According to this model, the sequence of events can be briefly described as follows [1–5]:

- (1) A coarse mixture is formed as a result of a pre-mixing process. The mixture—under film boiling conditions—consists of melt drops of the order of  $10^{-2}$  m, intermixed with a coolant.
- (2) A shock wave progresses through the mixture. Immediately behind the shock front all vapor condenses and direct liquid–liquid contact occurs.
- (3) A significant relative velocity between melt and coolant causes a hydrodynamically driven fine fragmentation. Rapid heat transfer to the coolant occurs.
- (4) The shock leaves behind a mixture at high pressure. As the pressure decreases, a vaporization and a subsequent expansion occur.

A certain modification of this model is suggested in this paper. The presented assessments show that the direct liquid–liquid contact is impossible for the systems of interest and that heat transfer takes place mainly under film boiling conditions. The fine fragmentation, in turn, seems to occur too slowly for the classical propagation mechanism to be operative, i.e. for the shock wave to be supported by rapid heat transfer due to fragmentation; this refers first of all to the initial stage of the explosion. An additional propagation mechanism is outlined.

## 2. TIME SCALE FOR FINE FRAGMENTATION

Let us consider a coarse mixture region of volume  $V$ , initially at rest. A shock wave is propagating

through the mixture, causing a steep rise in pressure and a subsequent condensation of coolant vapor of volume  $V_{\text{con}}$ . It should be stated that not all vapor condenses. As it will be shown later, a vapor film is expected to exist around melt drops behind the shock front. Assuming incompressibility of the melt as well as the liquid coolant one can assess a velocity  $w_0$  behind the front of the wave:

$$w_0 = w_{\text{det}} \alpha_v; \quad \alpha_v = \frac{V_{\text{con}}}{V}. \quad (1)$$

Here  $w_{\text{det}}$  denotes the wave velocity in the frame of the medium before the wave. Taking into account the significant difference between the density of the melt and that of the coolant one can suggest the following model of the velocity transient in the mixture:

- (1) The coolant reaches the velocity  $w_0$  virtually immediately.
- (2) The velocity of the melt drop  $w_D$  increases from zero to  $w_0$  according to the equation [6]

$$w_D = w_0 \left( 1 - \frac{\tau}{t + \tau} \right); \quad \tau = \frac{8}{3} D \frac{\rho_F}{\rho_C} \frac{1}{w_0}. \quad (2)$$

As  $w_D(t = \tau) = \frac{1}{2} w_0$ , the time  $\tau$  may be taken as the time scale for the velocity equalization. The difference between the velocity of the coolant and that of the drop is a prerequisite of a hydrodynamic fine fragmentation.

Fragmentation is the key to the enhanced heat transfer rate in the thermal explosion and there are many fragmentation concepts. From various research works it appears that in the reaction zone behind the shock front the hydrodynamic mechanism seems to be dominant [2, 3, 5]. The analysis of the drop fragmentation in a stream of other liquid concerns in general a direct liquid–liquid contact (see, e.g. ref. [7]). The question is whether the existence of the vapor film around the melt drop can affect the phenomenon. The answer seems to appear from the results presented by Nigmatulin [6]. According to these results the frag-

## NOMENCLATURE

$Bi$	Biot number; $Bi = hr_0/\lambda_F$	$w_0$	coolant velocity
$c_p$	specific heat	$We$	Weber number; $We = D\rho_C w_0^2/\sigma$ .
$D$	diameter	Greek symbols	
$Fo$	Fourier number; $Fo = \lambda t/c_p \rho r_0^2$	$\alpha_v$	cf. equation (1)
$h$	heat transfer coefficient	$\beta$	cf. equation (7)
$Nu$	Nusselt number; $Nu = hD/\lambda_C$	$\gamma_n$	cf. equation (10)
$Pr$	Prandtl number; $Pr = c_p \rho v/\lambda$	$\delta$	thickness
$q$	heat flux	$\mu_n$	cf. equation (11)
$Q'$	transferred heat	$\nu$	kinematic viscosity
$Q''$	available heat	$\lambda$	thermal conductivity
$\bar{Q}$	dimensionless heat	$\rho$	density
$r$	radial coordinate	$\sigma$	surface tension
$r_0$	radius of a sphere	$\tau$	cf. equation (2).
$Re$	Reynolds number; $Re = wD/\nu$	Subscripts	
$t$	time	C	coolant
$T$	temperature	D	drop
$T_1$	contact temperature	det	shock wave
$T_s$	saturation temperature	F	melt
$\bar{T}$	dimensionless temperature	FR	fragmentation, fragments.
$V$	volume		
$V_{con}$	cf. equation (1)		
$w$	velocity		

mentation of the drop is caused by the Rayleigh–Taylor instability due to action of the stream on the vicinity of the stagnation point. The vapor film does not change the stagnation pressure. By virtue of this fact the influence of the vapor film may be neglected and the interaction can be considered to be determined—at least as a first approximation—by the Weber number

$$We = \frac{D\rho_C w_0^2}{\sigma} \quad (3)$$

According to the range of the Weber number, various modes of the drop's fragmentation have been observed [2, 6, 7]. For thermal explosion to occur, only the catastrophic break up of the drop directly to small fragments seems to be adequate. It takes place for  $We > 1000$  [6] (Kim [7] suggests  $We > 1300$ ). As will be shown later, even with this mode the fragmentation takes a relatively long time. Inasmuch as the decrease in the velocity  $w_0$  results in a longer fragmentation time and the interfacial area for  $We < 1000$  spreads out less effectively, the assumption  $We > 1000$  seems to be acceptable.

According to Nigmatulin [6] the process occurs in two stages.

(1) A step increase in the coolant velocity from zero to  $w_0$  occurs for  $t = 0$ . In the interval  $0 < t < t_{FR}$  the drop remains as one unit. The characteristic fragmentation time  $t_{FR}$  is given as:

$$t_{FR} = \frac{D}{w_0} \left( \frac{\rho_F}{\rho_C} \right)^{1/2} \quad (4)$$

(2) The break up to small fragments takes place in the interval

$$t_{FR} < t < 5t_{FR}.$$

Let us assume the following typical sizes: the diameter of the melt drop in the coarse mixture  $D = 10^{-2}$  m, and the diameter of the fragment after break up  $D_{FR} = 10^{-4}$  m [2, 3, 7]. Taking  $\sigma = 1 \text{ N m}^{-1}$  one obtains from (3) for  $We > 1000$  the velocity  $w_0 > 10 \text{ m s}^{-1}$ .

This allows us to assess the upper bound of the characteristic fragmentation time  $t_{FR}$ . It yields  $1.5 \times 10^{-3}$  s for Al and  $3 \times 10^{-3}$  s for  $\text{UO}_2$ . The comparison of  $t_{FR}$  with the characteristic time of velocity equalization  $\tau$  gives the following.

(a) For the drop:

$$\frac{\tau}{t_{FR}} = \frac{8}{3} \left( \frac{\rho_F}{\rho_C} \right)^{1/2} > 1. \quad (5)$$

This shows that in the initial break up stage of duration  $t_{FR}$  the velocity difference is significant.

(b) For the fragments:

$$\frac{\tau}{t_{FR}} = \frac{8}{3} \left( \frac{\rho_F}{\rho_C} \right)^{1/2} \frac{D_{FR}}{D} \ll 1. \quad (6)$$

Apparently, rapid velocity equalization takes place and the relative velocity is believed to be very small. This velocity, however, is not equal to zero. The decrease both in velocity and in diameter diminishes the Reynolds number  $Re$  and the velocity equalization became less efficient than it appears from equation (2), which holds for  $Re > 50$ .

### 3. HEAT TRANSFER

The temperature of the interface between melt and coolant  $T_1$  is often estimated by means of the well-known relation of Carslaw and Jaeger:

$$T_1 = \frac{T_F \beta_F + T_C \beta_C}{\beta_F + \beta_C}; \quad \beta = \sqrt{\lambda c_p \rho}. \quad (7)$$

For molten  $\text{UO}_2$  at 3000 K and water at 300 K one obtains  $T_1 = 1500$  K [2]. It is both higher than the critical temperature of water and lower than the melting point of  $\text{UO}_2$ . It has to be stated that the relation (7) is inadequate for the geometry of a coarse mixture. This remark—apparently correct—does not change the following significant conclusion: for corium as well as most liquid metals the melting temperature is higher than the critical temperature of water and, consequently, direct liquid–liquid contact is impossible for these media. For fine fragmentation to occur, a hot medium should be in the liquid state. By virtue of these facts the existence of a stable vapor film around melt drops behind the shock front is to be expected.

Let us consider the heat transfer from the melt to the coolant within the reaction zone. According to the results given previously, two stages of the process have to be taken into account.

- (1) For the period of time of duration  $t_{FR}$  a melt drop of diameter  $D = 10^{-2}$  m is immersed in a coolant stream of significant velocity.
- (2) For the period of time of duration  $4t_{FR}$  melt fragments of diameter  $D_{FR} = 10^{-4}$  m are immersed in a coolant stream of insignificant velocity.

Film boiling is assumed to take place. Our goal is to assess the melt temperature and the heat transferred as functions of initial parameters of the melt and of the coolant. Finding an exact solution to such a problem seems to be a rather complex task. Appropriate relations for film boiling forced convection are not known. In order to estimate the heat transfer, the following conclusions, relative to the film boiling on a sphere in forced convection, seem to be instrumental.

(1) According to Wilson [8], the rate of heat transfer is determined solely by material constants and the Peclet number of the coolant, and in the case of large subcooling (which takes place in the reaction zone as a result of the steep rise in pressure), does not depend on the sphere temperature; the thickness of the vapor film adjusts itself continually to maintain the heat transfer rate as the sphere cools.

(2) According to Witte and Orozco [9], as subcooling increases, the energy used to form vapor becomes a smaller fraction of the total energy transferred from the sphere; the size of the wake is decreased and the vapor hydrodynamics take on lesser importance.

A simple model based on the foregoing is suggested. Let us assume that the heat flux to the coolant is

expressed in the same way as the forced convection heat flux from a bubble or from a drop, i.e. it is determined by the interface temperature (in our case the saturation temperature) together with the coolant bulk temperature  $T_C$ , and the heat transfer coefficient is given by the relation [6]

$$Nu = 2 + 0.46 Re^{0.55} Pr^{0.33}. \quad (8)$$

$$q = h(T_s - T_C). \quad (9)$$

The temperature of the melt drop can be obtained from the well-known solution for the sphere with prescribed, constant heat flux at its surface. The flux is given by (9) and the temperature is obtained from [10]

$$[T_F - T(r, t)] \frac{\lambda_F}{qr_0} = 3Fo - \frac{1}{10} \left[ 3 - 5 \left( \frac{r}{r_0} \right)^2 \right] - \frac{r_0}{r} 2 \sum_{n=1}^{\infty} \left[ \frac{\sin \left( \gamma_n \frac{r}{r_0} \right)}{\gamma_n^2 \sin \gamma_n} \exp(-\gamma_n^2 Fo) \right]; \quad \gamma_n = \text{tg } \gamma_n \quad (10)$$

where  $T_F$  is the initial melt temperature. The heat flux is evidently underestimated, as the vapor formation is neglected. With its utmost simplicity, the presented model is expected to give the correct assessment. To check its usefulness, a similar analysis of the forced convection film boiling around a cylinder was made; it resulted in a heat transfer rate about 20% lower than that given by the classical correlation of Bromley. The upper bound of the heat transfer is determined as a result of a forced convection without vapor blanketing. The saturation temperature  $T_s$  in relation (9) is then replaced by the interface temperature  $T(r_0, t)$  and the temperature of the drop is given by [10]

$$\frac{T_F - T(r, t)}{T_F - T_C} = 1 - \frac{2r_0}{r} \sum_{n=1}^{\infty} \frac{\sin \mu_n - \mu_n \cos \mu_n}{\mu_n (\mu_n - \sin \mu_n \cos \mu_n)} \times \sin \left( \mu_n \frac{r}{r_0} \right) \exp(-\mu_n^2 Fo); \quad \text{tg } \mu_n = \frac{\mu_n}{1 - Bi}. \quad (11)$$

The heat transfer coefficient is obtained from relation (8).

#### 3.1. Heat transfer from the drop

The amount of heat transferred to the coolant may be expressed as

$$Q' = \pi D^2 q t_{FR} \quad (12)$$

where  $q$  is given by (9). Let us introduce an available heat  $Q''$

$$Q'' = \frac{\pi D^3}{6} \rho_F c_{pF} (T_F - T_C) \quad (13)$$

and the dimensionless, transferred heat  $\bar{Q}$

$$\bar{Q} = \frac{Q'}{Q''} = 3Fo Bi \frac{T_S - T_C}{T_F - T_C} \quad (14)$$

where the Fourier number  $Fo$  refers to the fragmentation time  $t_{FR}$ . It is worth noting that  $\bar{Q}$  depends on the velocity by a factor virtually equal to  $w^{-1/2}$  only. Taking  $w = 20 \text{ m s}^{-1}$  and  $D = 10^{-2} \text{ m}$  one obtains the factor  $3Fo Bi$  for  $\text{UO}_2$ , Al, and Cu equal to  $10^{-2}$ ,  $9.7 \times 10^{-3}$ , and  $1.4 \times 10^{-2}$ , respectively. Owing to the fact that  $T_F > T_S$  the heat  $\bar{Q}$  is in any case less than  $10^{-2}$ . To find the upper bound, one can evaluate the transferred heat  $Q'$  from relation (11). Considering (13) one obtains

$$\bar{Q} = \frac{Q'}{Q''} = 1 - 6 \sum_{n=1}^{\infty} \frac{(\sin \mu_n - \mu_n \cos \mu_n)^2}{\mu_n^3 (\mu_n - \sin \mu_n \cos \mu_n)} \times \exp(-\mu_n^2 Fo) \quad (15)$$

which also gives  $\bar{Q} < 10^{-2}$  for the media of interest. As will be shown later, the heat transfer from fragments is more significant. One can assume, consequently, that the heat transfer from the drop before break up can be neglected in the energetic considerations, irrespective of the existence or nonexistence of a vapor film. This heat transfer, however, should be taken into account when the melt temperature is determined. Let us introduce a dimensionless decrease of the drop's surface temperature  $\bar{T}$  as

$$\bar{T} = \frac{T_F - T(r_0, t_{FR})}{T_S - T_C} \quad (16)$$

The temperature  $T(r_0, t_{FR})$  is given by (10). This dimensionless drop  $\bar{T}$  for Cu and Al is less than 10%, but for  $\text{UO}_2$  it is  $\bar{T} = 0.62$ . This results from the relatively low thermal conductivity of this melt and from the significant temperature gradient involved. The heat is transferred first of all from the thin layer close to the surface. The difference between  $\text{UO}_2$  and the other melts considered becomes more visible when the upper bound of heat transfer is estimated. Introducing the decrease of temperature  $\bar{T}$  as

$$\bar{T} = \frac{T_F - T(r_0, t_{FR})}{T_F - T_C} \quad (17)$$

and evaluating  $T(r_0, t_{FR})$  from (11) one obtains for Al and Cu  $\bar{T}$  less than 7% but for  $\text{UO}_2$  it is  $\bar{T} = 0.44$ . As a possible result of this skin effect the following process should be taken into account: for the melts of low thermal conductivity the temperature of the drop's surface behind the shock front can fall to the melting point; the beginning of solidification can influence the fine fragmentation.

### 3.2. Heat transfer from fragments

Treating a single fragment after the break up as a drop of diameter  $D_{FR} = 10^{-4} \text{ m}$ , one can write relations analogous to (12), (13), and (14). As rapid velocity equalization takes place, forced convection can be neglected. In this limiting case the correlation (8) reduces to  $Nu = 2$ . Then, for  $t = 4t_{FR}$ , the factor

$3Fo Bi$  (cf. equation (14)) is virtually equal to unity for Al, Cu, and  $\text{UO}_2$ , which is 100 times greater than in the previous case of the drop. The decrease of the Nusselt number is tantamount to the decrease of the Biot number; e.g. for  $w = 0.1 \text{ m s}^{-1}$  it is  $3Fo Bi = 3$ . The weakness of these results seems to lie in treating the fragment as a single drop, immersed in a coolant of constant bulk temperature. In fact the products of the break up will occupy a limited region of size determined by the diameter of the drop, the velocity of the coolant, and the duration of the process. It is likely that the thermal layers around fragments will interfere or the vapor layers will coalesce; such a situation could evidently change the heat transfer conditions. Nevertheless, the following general consideration seems to be reasonable: the heat transfer within the reaction zone, essential to the thermal explosion, takes place after the break up of the coarse mixture. One should note that a significant part of the heat is transferred under film boiling conditions; this concerns first of all the medium of high melting temperature, e.g. corium.

## 4. MECHANISM OF PROPAGATION

Based on the classical paper by Hall and Board [1] as well as on the excellent review by Corradini *et al.* [3], one can condense the detonation model of thermal explosion as follows. A strong shock front progresses through the coarse mixture; behind the front the complete collapse of the vapor blanketing the melt occurs and the relative velocities between the liquid are sufficient to cause fine fragmentation of the melt which results in rapid heat transfer. This reaction zone is coupled to the triggering shock and propagates with it. The shock leaves behind a mixture at high pressure, and subsequent expansion drives the front forward.

On the grounds of the preceding considerations some criticisms need to be raised in this model.

(1) As was pointed out, for a number of melts direct contact with water seems to be impossible. Evidently, at elevated pressure the vapor layer is expected to be thinner, but the complete film boiling collapse cannot be assumed as a necessary condition for the explosion to occur.

(2) For the fine fragmentation to be completed within the reaction zone, the thickness of this zone has to be of the order of

$$\begin{aligned} \delta_{FR} &= (w_{det} - w_0) 5t_{FR} \\ \delta_{FR} &= 5 \frac{1 - \alpha_v}{\alpha_v} D \left( \frac{\rho_F}{\rho_C} \right)^{1/2}. \end{aligned} \quad (18)$$

For the media of interest  $\delta_{FR} \sim 10D(1 - \alpha_v)/\alpha_v$ . Evidently, this size should correspond to that of the high pressure region. The question is whether the thickness of the shock wave  $\delta$  fulfils this condition. According to experimental data, for the weak waves in the water-vapor mixtures the thickness  $\delta$  is of the order of a few

centimeters [6]. Then, for a weak triggering shock one can expect  $\delta < \delta_{FR}$ . In this case only a small part of the available energy can be released within the reaction zone. One can hardly expect the detonation wave to be amplified in these conditions.

On the other hand, many experiments indicate that the thermal explosion produces a shock wave which is similar to a detonation explosion wave. This contradiction is likely to be eliminated by a modification of the propagation mechanism. According to the detonation model, the rapid heat transfer from melt to coolant within the reaction zone causes simultaneously two distinct effects:

- (1) The shock wave, supported by part of the released energy, propagates through the coarse mixture.
- (2) The coolant temperature rises. The mixture, undergoing a vaporization and a subsequent expansion, can do work against its surroundings.

While the second effect is unquestionable, a supplementary energy source to support the propagation seems to be necessary. To find this additional propagation mechanism one can make use of the results presented by Nigmatulin [6]. From these results it appears that a strong amplification of the shock wave is observed in a two-phase mixture of water and vapor bubbles. The amplification is caused by a collapse of the bubbles and it depends considerably on the structure of the mixture. On the basis of this effect the following scenario is suggested.

(1) The coarse mixture is formed as a result of the premixing process. It is a mixture of the melt drops (around which the film boiling takes place), the vapor bubbles (the result of boiling), and the liquid coolant.

(2) A shock wave progresses through the mixture. Immediately behind the front of the wave the vapor bubbles collapse; this collapse supplies the energy to the wave. According to these conditions the wave is expected to be either maintained or amplified. Part of the vapor blanketing the melt condenses as well, which can contribute to this support.

(3) Within the reaction zone behind the front of the wave fine fragmentation and rapid heat transfer to the subcooled coolant occur. The coolant temperature rises. This energy transfer is irrelevant to the propagation mechanism. The pressure drops, which is conditioned by the structure of the wave.

(4) The mixture reaches its saturation point. Rapid evaporation and subsequent expansion occur.

The presented scenario is in the first part similar to the SWACER mechanism (Shock Wave Amplification by Coherent Energy Release), proposed by Lee *et al.* [11, 12] for chemical explosions. In both cases a preconditioned mixture has to be formed. The physical processes in this mixture can be thought of as the agents responsible for preparing the necessary conditions for the propagation mechanism to be operative. For chemical explosions, however, the mechanism is based on the principle that the time sequence of

chemical energy release is such that it is coherent with the shock wave it generates, thus adding strength to the shock wave as it propagates. For thermal explosion we suggest the disconnection of the propagation mechanism from the energy transfer to the coolant within the reaction zone.

The suggested model and classical thermal detonation are not mutually exclusive. For a strong shock the fine fragmentation and the energy release behind the front can run fast enough for both propagation mechanisms to be operative. This is probably the case in a fully developed thermal explosion.

## 5. CONCLUSIONS

The present study deals with thermal explosion in liquid metal–water systems. According to the presented assessments, the crucial heat transfer, leading to the explosion, takes place under film boiling conditions. The main conclusion of this paper is that the fine fragmentation of the hot phase seems to occur too slowly to support the propagation of the shock wave, at least as far as the shock is not strong enough. A modification of the propagation mechanism has been suggested. It consists of the disconnection of the propagation from the heat transfer from melt to coolant within the reaction zone. The shock wave is expected to be supported by the collapse of the vapor bubbles, which are inherent in the coarse mixture. The outstanding problems to be studied are the influence of the coarse mixture's structure on the propagation and the conditions of shock wave amplification.

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#### EXPLOSION THERMIQUE DANS DES CONDITIONS D'EBULLITION EN FILM

**Résumé**—L'étude concerne l'explosion thermique dans les systèmes métal liquide-eau. On évalue le transfert thermique et l'échelle de temps pour la fragmentation fine derrière l'onde de choc. On montre que le contact direct liquide-liquide est impossible pour la plupart des constituants usuels et que la chaleur est transférée dans les conditions de l'ébullition en film. La fine fragmentation semble apparaître trop lentement pour supporter la propagation dans le stade initial de l'explosion. Une modification du mécanisme de propagation est suggérée.

#### THERMISCHE EXPLOSION UNTER DEN BEDINGUNGEN DES FILMSIEDENS

**Zusammenfassung**—Die vorliegende Untersuchung beschäftigt sich mit thermischen Explosionen in Systemen aus flüssigem Metall und Wasser. Die Wärmeübertragung und der Zeitmaßstab für die Fragmentation hinter der Stoßfront wird abgeschätzt. Der direkte Kontakt der beiden Fluide erweist sich für die meisten interessierenden Medien als unmöglich, wobei die Wärmeübertragung unter den Bedingungen des Filmsiedens stattfindet. Die Fragmentation scheint zu langsam abzulaufen, als daß sie die Ausbreitung zu Beginn der Explosion unterstützen könnte. Abschließend wird eine Modifikation des Ausbreitungsmechanismus vorgeschlagen.

#### ТЕПЛОВОЙ ВЗРЫВ В УСЛОВИЯХ ПЛЕНОЧНОГО КИПЕНИЯ

**Аннотация**—Исследуется тепловой взрыв в системах жидкий металл-вода. Оцениваются теплоперенос и временной масштаб для процесса разделения на мелкие фракции за фронтом ударной волны. Показано, что прямой контакт жидкость-жидкость невозможен для большинства исследуемых сред и теплоперенос происходит в условиях пленочного кипения. Процесс разделения на мелкие фракции осуществляется слишком медленно и не может содействовать распространению начальной фазы взрыва. Предлагается механизм модификации процесса распространения.