A DIFFERENT APPROACH TO FRAGMENTATION IN STEAM EXPLOSIONS

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ABSTRACT

Fragmentation of a high temperature liquid, which is embedded in a film boiling state within a low temperature liquid, has been the subject of numerous studies. For explosive interactions the fragmentation and subsequent energy transfer must be sufficiently rapid to support the formation of a shock wave. In previous studies, the principal interest was the rate at which these capillary size high temperature droplets could be fragmented and rapidly mixed with the surrounding liquid to cause heat transfer and vaporization on explosive timescales (generally less than milliseconds). Recent experiments have shown that such rapid fragmentation and mixing is difficult to achieve.

This paper proposes a different approach to fragmentation, namely that the principal fragmentation process is in the low temperature liquid and that the capillary size high temperature droplets do not substantially alter their dimensions during the propagation of the shock wave. Furthermore, if the hot material dimensions are altered, it is postulated that no substantive rapid mixing of the high temperature and low temperature liquids occurs. This approach to the detailed heat transfer mechanism during physical explosions results in a simple expression for the efficiency of such interactions that is consistent with large scale data. Furthermore, the mechanism for rapid fragmentation and the resulting rapid energy transfer rates are consistent with the small scale separate effects data from the spontaneous nucleation literature.

1.0 BACKGROUND

Rapid fragmentation has been a subject of major interest in steam explosion research since the beginning of analytical and experimental studies in this area. In particular, interest has focused on the fragmentation of the high temperature liquid droplets (fuel) as a result of the shock wave(s) that would develop during an explosive event. This is a natural consideration since the energy source for the explosion is in the hot material and the smaller droplets (or particles) the faster this energy can be released (assuming that rapid mixing also occurs) with thermal conduction in the fuel being the controlling energy transfer process. However, some studies with respect to this perceived process of rapid fragmentation and intermixing with the coolant have concluded that energy requirements strongly limit the capacity to rapidly mix materials as assessed by Henry and Fauske (1981) using mixing models published in the Recent calculations including the potential for a velocity literature (Cho et al., 1976). equilibrium of the two different liquids (Fauske, 1995) concludes that it is even more difficult to rapidly mix in a liquid-liquid configuration than was originally assessed. Furthermore, experiments directed at fragmentation of capillary size molten metal droplets in strong waves (100-400 bars) have shown that droplets may be difficult to fragment (Theofanous et al., 1994).

If such large pressures cannot cause rapid fragmentation how can explosive events escalate from very small (almost innocuous) events typical of systems with no external trigger (Henry and Fauske, 1979)?

Perhaps the most meaningful set of experiments related to hydrodynamic fragmentation are the shock tube experiments performed by Theofanous and his colleagues. In these tests, very large shock waves were imposed on high temperature molten aluminum droplets in a film boiling state within the surrounding water medium. Figure 1, which is taken from Theofanous et al. (1994), shows the major results from these experiments. In particular, those tests which were characterized as only "interactions" were characterized as "a few aluminum fragments in the millimeter size range and/or a largely unfragmented but high convulated aluminum mass". Furthermore, for temperatures less than 1400°C there was little oxidation of the aluminum droplet. These experiments indicate that the behavior of the aluminum has a much stronger function of the aluminum temperature than the imposed shock wave pressure, even though all of the experiments are within the range where substantial explosions have been observed in large scale tests (Long, 1957). For these large scale experiments, explosive interactions were observed for molten aluminum temperatures as slow as 670°C and with a strong external trigger. In fact, Long's experiments demonstrated that painting the inner surface of the water container prevented explosions and conversely an unpainted surface caused explosions.



Figure 1, Map of the various observed interaction regimes in "melt temperature"-"shock pressure" coordinates. The solid symbols are for the computer-controlled runs (see text).

If strong shock waves do not create the fine scale fragmentation, what does initiate the explosive interaction and how does it escalate? Here we postulate that the fragmentation process that matters is the fragmentation of the low temperature liquid (coolant). Specifically, the fine spray resulting from the direct fuel-coolant contact when the interface temperature exceeds the spontaneous nucleation temperature (Fauske, 1974) is that fragmentation process. One test was performed with the host liquid (silicon oil in this case) at a temperature greater than the

spontaneous nucleation temperature of the entering droplet (pentane for these tests) but not at a sufficiently high temperature for the contact interface temperature to be greater than the spontaneous nucleation value for pentane. In this test the droplet contacted the surface, submerged and returned to the surface. After 77 msec a single explosive interaction was witnessed. This is not the type of interaction that would support the escalation of an explosive event. Conversely, Figure 2 shows the interactions, when the host liquid temperature is sufficiently high that the contact temperature exceeds spontaneous nucleation for pentane. As a result, vapor nucleation and inertially dominated bubble growth to sizes comparable to heated layer can occur on very short time scales. As estimated by Henry and Fauske (1979) this growth, and hence the fragmentation, can occur within intervals of the order 10 μ s (10⁻⁵ secs). Figure 2 shows a fine liquid spray at the bottom surface of the droplet forms "immediately" as it contacts the silicon oil. In these tests the framing rate for the high speed movies was 1000 frames per second so that the maximum resolution is 1 msec. However, this clearly shows that there is a substantial fragmentation (fine spray) of the coolant drop as it contacts the hot liquid surface. Furthermore, this fragmentation is of very small size (clearly much less than a millimeter) and this "spray" spreads in all directions. This initial fragmentation could begin to set up the system for an escalation of this initial event such that a shock wave could form. Should the very small droplets (<< 1 mm) created by this consequence of "violent boiling" subsequently collide with the high temperature fuel, experiments have shown that these vaporize completely on an explosive time scale (Henry and Fauske, 1979). Thus, fine scale fragmentation of the coolant, resulting from local contacts, can create an explosive situation. In the following discussion we consider how this relates to the development of an explosive configuration and the resulting energetics.



Figure 2, Illustration of explosive boiling immediately upon liquid-liquid contact. Temperature of the pentane droplet was 30°C; temperature of the oil was 238°C. The droplet impact velocity was 250 cm/sec.

2.0 THE PROPOSED MECHANISM

As discussed above rapid mixing of one liquid into another is difficult. This has been suggested by analysis and experiments appear to confirm this. Conversely, the rapid fragmentation of a liquid into a surrounding gaseous medium does not require substantial energy and has been experimentally observed to result from a single liquid-liquid contact. Therefore, the proposed mechanism focuses on the "coarse mixing" configuration (prior to the explosive interaction) and the fragmentation that could occur as a result of local contacts and the process that could limit the energy release.

Drainage of a high temperature melt into water, as occurred in the TMI-2 accident, is the configuration of interest for LWR safety assessments. During this event, the more dense high temperature melt will be entrained into the surrounding water with the melt having a characteristic dimension given by the capillary size (droplet radius) or larger (Russell and McCardell, 1989). Furthermore, this melt dimension characterizes the effective energy transfer, either due to the lack of further fragmentation on an explosive time scale or the lack of rapid liquid-liquid mixing.

The key assumptions for the proposed mechanism are:

1. The fuel does not substantially fragment and intermix with coolant during the pressure escalation interval (shock wave rise time) of approximately 1 ms. Hence, the fuel characteristic dimension during the pressure escalation is given by the capillary dimension

$$r = \sqrt{\frac{\sigma}{\left(\rho_{1} - \rho_{g}\right)g}} \approx \sqrt{\frac{\sigma}{\rho_{1}g}}$$
(1)

In this expression, σ is the melt surface tension, ρ_P is the melt density, ρ_g is the gas (vapor) density and g is the acceleration of gravity. This determines the characteristic size of the high temperature melt for the "coarse mixing" stage. Such sizes have been observed by Magallon and Hohmann for molten UO₂ into water. Furthermore, the assumption of no significant fragmentation and rapid mixing of the fuel material during the explosion, provides the basis for the process which limits the energy release.

- 2. Fragmentation of the coolant is due to violent boiling (spontaneous nucleation) mechanisms and is principally due to inertially dominated bubble growth inside of the coolant immediately following contact. Since the potential for inertial bubble growth is reduced by an increasing ambient pressure, the coolant fragmentation process eventually shuts down when the local pressure approaches half of the critical pressure (Henry and Fauske, 1979).
- 3. Energy transfer from the fuel to the coolant is determined by the thermal penetration distance (x_{con}) into the capillary size fuel droplets

$$x_{con} = \sqrt{\alpha \tau}$$

where α is the melt thermal diffusivity. In essence only a thin layer on the outer surface of each fuel droplet supplies energy to the coolant during the explosive interaction. This energy transfer occurs as the very small coolant droplets (<< 1 mm) contact the surface, vaporize some, or all, of the droplet mass and possibly fragment further during this internal (τ is taken to be the rise time for the shock wave ~ 1 ms). If it is assumed that all fuel droplets are initially at the capillary size and that the droplet surfaces are uniformly cooled to the spontaneous nucleation temperature (T_{sn}) (300°C for water) by the extensive droplet interactions with the surface, the conversion efficiency for heat removal from the droplets (η_{hr}), in terms of the total energy contained in the fuel above local saturation can be expressed by

$$\eta_{\rm hr} = \left[\frac{T_{\rm fuel} - T_{\rm sn}}{T_{\rm fuel} - T_{\rm sat, atm}}\right] \frac{1.5 \, x_{\rm con}}{r} \tag{3}$$

In this calculation it is assumed that there is a linear profile through the conduction layer from 300°C at the surface to the initial fuel temperature (T_{fuel}) with $T_{sat,atm}$ being the coolant saturation temperature at the atmospheric condition. It is noted that this characterizes the heat transfer process and by straightforward thermodynamic analyses only about one-third of this energy can be realized as work. Thus the mechanical conversion efficiency (η_m) is taken to be ($\eta_{hr}/3$).

The process which is involved with this mechanism is one in which one or more local contacts begin a small pressurization and fine scale fragmentation of the coolant in the immediate locale of the contact. These local contacts may cause the fuel droplet to move within the surrounding vapor layer and the local pressurization may cause additional local contacts of droplets in the immediate vicinity. It should be noted that this does not mean that contacts are not occurring all the time; quite the opposite. However, if the vapor layer is too extensive (low subcooling for the coolant medium) the implication of a local contact may not be significant compared to the current quantity of vapor. Hence, the liquid-liquid system may find it difficult to create an escalating condition. Certainly Longs experiments (1957) found that explosive interactions were not initiated for water temperatures above 71°C (160°F).

Figure 3 illustrates an escalating situation that can lead to the formation of a shock wave and cause more fine scale fragmentation, i.e. an unstable situation. Notice from the figure that the oscillations of fuel droplets within the existing vapor cavity could be convenient whereby additional fragmentation and vaporization occur during the timeframe of the energy transfer. Such droplet oscillations within vapor cavity are discussed by Fry and Robinson (1979) but are suggested to be too slow to participate in the explosive interaction. However, given the substantial pressure differences that could be imposed on the vapor cavity, fuel droplet oscillations should not be ruled out as one means of causing substantial energy transfer.



Figure 3, Schematic of how a physical explosion can be initiated and escalate d.

A few other observations should be made with respect to the mechanism. Firstly, there are a number of experiments that have used external triggers to initiate explosive interactions. In this regard, the role of the external trigger has been identified as the mechanism to "collapse the stable vapor film", i.e. one which prevents liquid-liquid contact. For this unstable situation, there is no such behavior as a "stable vapor film". With the influence of gravity initially and secondly the imposition of an external trigger, local contacts should occur continuously. The only question is whether there are sufficient local contacts occurring that the rate of vapor formation could begin to escalate into a shock wave. Thus, the role of an external trigger may be to (1) initiate local contacts and (2) cause fine scale fragmentation of the <u>coolant phase</u> as the surrounding coolant medium is accelerated through the vapor layer. Moreover, there could be some fragmentation of coolant into the vapor layer resulting from the expansion side of the trigger pulse due to cavitation within the coolant. Any of these could provide the necessary local coolant fragmentation to begin an escalating situation.

3.0 COMPARISON WITH EXPERIMENTAL OBSERVATIONS

Table 1 lists the pertinent properties of many materials used as fuels in large scale vapor explosion experiments. For this simple evaluation the potential for oxidation of the fuel (if it is metallic) has not been considered. Also, the considerations for aluminum and tin have assumed

Table 1						
Calculations of the Explosion Efficiencies for Various Materials						
Used as "Fuel" With Water as the Coolant						
	Aluminum	Tin	UO ₂	AR_2O_3	Fe	Water
Density (kg/m ³)	2700	7000	9000	3800	7000	1000
Surface Tension (N/m)	0.84	0.51	0.5	0.5	2	0.05
k (W/m/K)	251	72	3.3	7.5	20	0.6
c (J/kg/K)	1050	300	600	1300	680	4200
α (m ² sec)	8.9E-5	3.4E-5	6.1E-7	1.5E-6	4.2E-6	1.4E-7
$x_{con}(m)$	3.0E-4	1.8E-4	2.5E-5	3.9E-5	6.4E-5	1.2E-5
r (m)	5.6E-3	2.7E-3	2.4E-3	3.6E-3	5.3E-3	2.2E-3
η_{hr}	0.057	0.071	0.015	0.015	0.016	0.008
η_{m}	0.019	0.024	0.005	0.005	0.0054	0.002

an initial fuel temperature of 800°C which is consistent with the experiments reported by Fry and Robinson (1979).

The first interesting aspect is that aluminum and tin can be considered to be more energetic than uranium dioxide. The second interesting feature is that the mechanical conversion efficiencies (ratios) are close to those that have been reported in the literature for those experiments where such efficiencies could be estimated. Figures 4 and 5, taken from the large scale thermite (Ab, O₃ and Fe) reported by Buxton et al. (1979), show a comparison with the proposed approach. It should be noted that the assessment of work done during the explosion has an accuracy of, at best, a factor of two. In this regard, the comparison of the model and the data is as accurate as the data.



Figure 4, Plot of estimated explosion efficiency versus water quantity present before the explosion for iron-thermite into water (Fe and $A\mathbb{P}_2O_3$). (Taken from Buxton et al., 1979.)



Figure 5, Plot of estimated explosion efficiency versus melt quantity present before the explosion for iron-thermite into water (Fe and $A\mathbf{R}_2O_3$). (Taken from Buxton et al., 1979.)

Frost, Bruckert and Ciccareli (1993) have reported mechanical energy conversion ratios of 0.0011 and 0.0026 for a stratified tin-water system. These values are bounded by the calculated values for tin in Table 1. In addition, Fuketa, Yamano and Inoue (1993) reported such ratios for fuel-coolant interactions representative of a reactivity initiated accident state. Figure 6 shows the results for in-reactor tests for uranium dioxide fuel and water and Fig. 7 shows a similar representation for an out-of-reactor test using a pulsed stainless steel rod in water. The information in Fig. 6 slightly exceeds the values in Table 1 but considering the inherent uncertainties of the data, the calculation is in good agreement with the approach. The information given in Fig. 7 shows energy conversion ratios are less than or equal to those calculated values for iron-water system. (For this assessment iron and steel are taken to be the same.)

It is also interesting in this regard to investigate the implications of this proposed mechanism on the SL-1 accident. As described by Thompson (1964), the SL-1 fuel were plates with a 1.27 mm aluminum nickel uranium alloy fuel clad by 0.89 mm of aluminum nickel on each side. For the sake of these analyses it is sufficient to assume that these alloys behave like pure aluminum. Since there was water on both sides of the fuel element, the characteristic dimension for heat removal is half the thickness of the element or 1.53 mm. As listed in Table 1, the thermal penetration for aluminum in 1 msec is 0.3 mm hence the heat transfer efficiency is calculated to be 20% with the resulting mechanical work conversion being 7%. Anderson and Armstrong (1973) tabulated the results of the assessments for total energy available and the destructive energy output from the SL-1 accident. The references for this tabulation were the SL-1 project final report (1962) and the evaluations performed by Procter (1967). This tabulation results in an assessment of 65 MW-sec of thermal energy available with a measured destructive output of 6 MW-sec, i.e., a 9% conversion ratio. Hence, the proposed mechanism is



Figure 6, Mechanical energy conversion ratio versus initial internal fuel rod pressure. (Taken from Fuketa et al., 1993.)



Figure 7, Mechanical energy conversion ratio versus input energy density. (Taken from Fuketa et al., 1993.)

in agreement with the observations from this destructive event particularly when considering the inherent uncertainties associated with evaluating the destructive energy and the use of a single value for the time response (1 msec).

This assessment for the SL-1 accident has an interesting insight. Namely, no fuel fragmentation is required to explain the destructive behavior in the accident. With the high thermal response fuel and small dimensions, the efficiency from the reactor system is higher, on a per unit mass basis, than for a system in which molten aluminum is poured into water and the droplets are determined by capillary effects.

Nelson (1993) has performed single drop experiments with aluminum and small triggers. These have been observed to produce significant thermal interactions with little oxidation in most cases. As a result of the triggered events, Nelson observed the bubble volume resulting from the thermal interaction with this volume generally growing to values of up to 1 liter in an interval from 3 to 5 msec. While the growth time is long compared to the explosive interaction, the final dimension of the bubble gives some indication of the work that was accomplished. In Nelson's experiments the mass of aluminum used varied from 1 to 10 grams. For the sake of this evaluation we will consider the sample to be 5 grams which corresponds to a droplet radius of 7.7 mm. Considering the initial temperature to be 1243 K, which was the case in experiment 38-3-1 as listed in the reference, the thermal energy available is about 4 KJ with the mechanical work associated with the bubble growth to 1 liter at an atmospheric pressure of 1 bar being approximately 100 J. This results in a mechanical conversion efficiency of 2.5% as compared with 1.3% from this proposed mechanism. Here again, the agreement is within the ability to resolve the actual work done as the result of an explosive interaction.

Numerous experiments have demonstrated the effect that ambient pressure has on suppressing vapor explosions (Henry and Fauske, 1979; Hohmann, 1979 and Hohmann et al., 1982). Since the fragmentation mechanism that started this escalation process is due to inertially dominated bubble growth, the implications on the extent of such growth as the ambient pressure increases is dramatic as discussed by Henry and Fauske (1979). Hence, the reason that such sensitivities could be observed in large scale interactions is the fact that the fundamental fragmentation process responsible for initiating, and subsequently escalating, the local events is strongly limited at elevated pressures. Such strong limitations have been observed in other spontaneous nucleation experiments (Avedisien, 1982).

Finally, a word of caution. Clearly the fuel is broken-up as a result of an explosive interaction as evidenced by post experiment debris sizes. However, it is not clear whether this breakup (and mixing) occurs on a time scale to support explosive interactions. Such post-experiment information may include evidence of whether the coolant or the fuel fragmentation is the dominant process but sorting out this puzzle is not easy.

4.0 SUMMARY

A model is proposed to characterize the fragmentation processes that occur during a physical explosion. This is a different approach from those proposed in the literature since the focus of the fragmentation is on the coolant, not the high temperature fuel droplets. This

fragmentation process is considered to be highly localized and thus requires a huge number of local interactions, each one of which can result in net vapor generation and a fine scale fragmentation for part of the surrounding coolant participating in this local contact. The resulting fine scale mist created by the fragmentation process has been shown experimentally to vaporize completely during a single contact with the high temperature melt. These interactions cause a sufficient pressurization to induce neighboring melt-coolant film boiling configurations to experience a substantial increase in the number of interactions. This then leads to an escalating event and the formation of a shock wave that does mechanical work.

With the postulate mechanism, the efficiency of physical explosions becomes a simple calculation. Comparisons of this calculation are in good agreement with the reported efficiencies with a variety of experimental systems reported in the vapor explosion literature. This proposed mechanism also identifies why physical explosions are relatively inefficient.

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