PHENOMENOLOGICAL MODELLING OF STEAM EXPLOSIONS

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ABSTRACT

During a hypothetical core meltdown accident, an important safety issue to be addressed is the potential for steam explosions. This paper presents analysis and modelling of experimental results.

There are four observations that can be drawn from the analysis: (1) Vapor explosions are suppressed by noncondensible gases generated by fuel oxidation, by high ambient pressure, and by high water temperatures; (2) These effects appear to be trigger-related in that an explosion can again be induced in some cases by increasing the trigger magnitude; (3) Direct fuel liquid-coolant contact can explain small scale fuel fragmentation; (4) Heat transfer during the expansion phase of the explosion can reduce the work potential.

In this paper we also present a transient wave propagation formulation which incorporates models for all of these observed effects.

1. Introduction

The purpose of the steam explosion phenomena program at Sandia National Laboratories is twofold: (1) To experimentally identify the fuel-coolant mixing requirements, trigger energy, and other initial conditions which are necessary to trigger and propagate explosive interactions between water and molten light water reactor (LWR) materials; (2) To develop criteria to assess the consequences and the probability of steam explosions during a hypothetical core meltdown accident in an LWR.

In 1975 the Reactor Safety Study (WASH-1400)[1] identified the steam explosion as one of the many physical processes that could cause containment failure during a hypothetical core meltdown. The probability assigned to this event, .01, had large uncertainty bands of more than an order of magnitude. Subsequent research has attempted to reduce the uncertainty. Buxton concluded that during meltdown the probability of molten core contact with a significant water mass (10-35 Mg) is nearly one.[2] Also, experiments at small and intermediate scale[3-6] and subsequent analysis[7,8] have indicated that a steam explosion event with fuel fragmentation smaller than 4000 μm is quite likely under a variety of initial conditions. In this paper we present the results of analysis and phenomenological modelling that may explain these experimental observations.

A steam explosion can be viewed as consisting of four phases of energy transfer between the fuel and coolant:

- a) Coarse Intermixing. The molten fuel and liquid coolant are mixed and the heat transfer mode is quiescent; e.g., film boiling.
- b) Trigger. The fuel and coolant are somehow brought into liquid-liquid contact and rapid heat transfer begins.
- c) Propagation. The heat transfer process rapidly escalates as more of the fuel is fragmented and as more high-pressure coolant vapor is generated.
- d) Expansion. The high-pressure vapor expands against the surroundings causing destructive mechanical work.

In this paper we briefly outline the models used to investigate each of these four phases. More detailed descriptions of the analyses can be found in Refs. [7, 8]. In addition, we describe in some detail a newly developed transient propagation model. This model is unique because its general formulation allows the incorporation of a number of detailed fuel-coolant heat transfer and fragmentation mechanisms.

2. Overview of the Phenomenological Modelling

2.1 Fuel-Coolant Mixing

The initial configuration of the fuel and coolant prior to the explosive interaction is a significant factor in determining the mechanical work. The degree of coarse mixing, characterized by the fuel drop diameter and the local fuel-coolant mass ratio, is dependent upon experimental technique or the accident scenario. A past analysis[9] suggests that film boiling significantly enhances mixing. This condition is easily satisfied for LWR materials; however, no quantitative theory has been proposed.

Recently, experiments by Mitchell,[8] which use molten iron-aluminum oxide and water have significantly aided in quantifying this mixing process at intermediate scales. These experiments consisted of dropping fuel ($\approx$ 5 kg) into coolant ($\approx$ 200 kg). The fuel free fall velocity upon entering the water was about 5 m/s, and the associated Weber number was small in comparison to the critical value ($We_{crit} \approx 20$). The fuel fragmented in the water to about 10-20 mm diameter drops in $\approx$ 100 ms, before reaching the bottom of the water tank (depth - .5-.7 m). The fuel mixed with the water and dispersed through 50 percent of the tank volume.

The main mechanism for this mixing is believed to be the boiling process. Hydrodynamic fragmentation alone cannot account for this rapid dispersal. The characteristic time for the fuel to fragment due to hydrodynamic forces is given by the relation[8]

$$\tau = \frac{5r_H}{U_{rel}} \sqrt{\frac{\rho_H}{\rho_c}} \qquad (1)$$

where ρ_H and ρ_c are the fuel and coolant liquid densities, r_H is the fuel radius, and U_{rel} is the relative velocity. For this case τ is approximately 400 msec. This time is too long compared to the observed time of 100 msec for total dispersal.

Application of these empirical observations to the full scale meltdown accident is quite difficult at this time. There are a number of factors that must be considered. First, the scale of the experiments is a factor of 1000 or more smaller than that of a reactor. Much larger fuel masses may inhibit mixing. Another factor which may inhibit mixing at full scale is solidification of the melt. Present experiments use melt superheats of $\sim$ 300 K which may not be prototypical. Finally, the meltdown progression in the reactor vessel and how it affects the fuel-coolant contact is not well known.

2.2 Steam Explosion Triggering

In the small scale experiments[3,5,8] which used reactor materials, the steam explosion was triggered by a pressure transient generated by either an exploding bridgewire or a mini-detonator in the water surrounding the fuel. Three initial conditions were altered during the experiments which caused the explosion to be suppressed: (1) the molten fuel composition was made more metallic; (2) the water subcooling was decreased to less than 24°C; (3) the ambient pressure was increased above .5 MPa. In all these tests the trigger energy was held constant (i.e.,

exploding bridgewire, $P_p = 1$. MPa). Past theories[10,11] have been used to explain these results. Also, other experimental investigators[12-17] have noted the same effect of ambient pressure on the explosion.

The physical mechanism causing this suppression appears to be identified with stabilizing the film. For example, the more metallic molten fuel quickly oxidizes in the steam film and generates a noncondensible gas (H_2)[5,8] which prevents film collapse. Increasing the ambient pressure increases the vapor film density, and thus the film behaves as a more effective 'spring' to resist film collapse.

This implies that an explosion can again be induced if the trigger energy is increased sufficiently to again cause film collapse. This hypothesis has been verified for the coolant temperature effect by recent experiments of Nelson[8] where a 10 MPa trigger pulse induced an explosion in water 14°C below saturation.

A model was developed to investigate film collapse behavior under varying initial conditions.[7,18] The model depicts a spherical molten fuel droplet immersed in a large volume of coolant (Figure 1). The model is similar in concept to that used by Kazimi[11] although the governing equations are different. In formulating this model, the following major assumptions were made:

    (1) The fuel-coolant system is spherically symmetric.
    (2) The fuel and coolant liquids are incompressible with constant properties and the vapor and other gases (if any) are ideal gases.
    (3) All vapor is either retained in the film around the drop or condenses at the coolant interface.

The governing equations are described in References 7 and 18. The model in Reference (7) assumes local equilibrium at the vapor-liquid interface (i.e., $P_v = P_{sat}(T_I)$), while the nonequilibrium model[18] considers the temperature of the vapor and the liquid near the interface to be different.

Application of a pressure pulse causes the vapor-liquid interface to be accelerated inward as the vapor condenses. As the film collapses, the film pressure rises. The predicted film collapse behavior is somewhat different for these models. For the equilibrium model the film does not collapse symmetrically but reaches a minimum thickness with a large film pressure rise. This can induce asymmetric collapse due to fluid instabilities. For the nonequilibrium model symmetric collapse can occur. In both models, film collapse is inhibited if the ambient pressure is increased, coolant temperature is increased or a noncondensible gas is introduced in the film.

The effect of introducing a noncondensible gas into the film is illustrated in Figure 2. By using the equilibrium model, we compare the film collapse behavior around an iron-oxide and an iron droplet for a fixed trigger energy. The initial conditions are characteristic of Nelson's single drop experiments.[5] The noncondensible gas acts to slow the interface collapse because the film thickness is large. When the trigger energy is increased (Figure 3), the minimum-approach thickness is much smaller although collapse does not occur. If the trigger energy is increased further collapse does occur.

The same trends in the film collapse behavior are seen if the ambient pressure or coolant temperature is increased. It appears that the suppression of the explosion under certain initial conditions is a function of the trigger magnitude. Therefore, given a large enough trigger, the film collapse and the subsequent vapor explosion can be induced.

2.3 Propagation Phase

Once the trigger induces film collapse the rapid heat transfer process begins. This induces a local pressure increase, and a collapse of nearby vapor films. The resulting effect propagates through the mixture. In the past there has been extensive research work involved in this phase of the explosion;[19-25] however,

at present relatively little is known about either how the explosion propagates or the mechanisms for fuel fragmentation and fuel-coolant heat transfer. Additional experiments and analysis are now being performed to study the propagation phase.

Nelson[5,8] has observed in single droplet experiments (fuel mass ≈ .1-1 gm) using FeO$_x$ and water that fine fuel fragmentation (D$_d$ ≤ 50 μm) triggered by a bridgewire occurs in less than 200 μsec. For the LWR accident environment, one important characteristic is that the molten fuel temperature is quite high (T$_H$ = 2000-3000K), while the coolant temperature is low (T$_c$ = 400-500K). Thus if the fuel and coolant are forced into liquid-liquid contact by the trigger pressure pulse, the local pressure could rise quite high as the coolant vaporizes and fragments the fuel. This concept of fragmentation was originally advanced by Bankoff.[26] Based upon it a simple mathematical model of fuel fragmentation was developed and applied to Nelson's small scale tests. This local pressurization model is based on the idea that establishing liquid-liquid contact at the termination of film collapse can generate a high pressure vapor which upon expanding fragments the fuel due to Taylor instabilities.[8] The volumetric rate of fragmentation, $\dot{V}_H$, is given by

$$\dot{V}_H \doteq A_p \sqrt{a_H \lambda_{crit}} \qquad (2)$$

where A$_p$ is the projected area λ_{crit} is the fuel critical Taylor wavelength, and the expected fuel fragment size,

$$\lambda_{crit} = 2\pi \sqrt{\frac{\sigma}{a_H(\rho_H - \rho_v)}} \qquad (3)$$

$$a_H = \frac{\Delta P_{con}}{2\rho_H r_H} \qquad (4)$$

where σ is the surface tension, a$_H$ is the acceleration and ΔP_{con} is the vapor pressure on contact. Once the fuel is fragmented it is assumed that it rapidly mixes with the local liquid coolant and thermally equilibrates. This assumption is approximately valid because the conduction heat transfer rate upon sudden fuel-coolant contact is quite high. This heat transfer generates high pressure coolant vapor which expands and forces the fuel droplet into subsequent fuel-coolant contacts, thereby causing more fuel fragmentation and vapor generation. This process continues until the fuel is fully fragmented and vapor begins to expand. Prediction of Nelson's test results is shown in Figure 4 for the coolant vapor expansion during and after the interaction. The model predicts a total fuel fragmentation time of about 100 μsec with the fragment diameters in the range of 10-25 μm. These results show good agreement with the data, and suggest that fragmentation induced by liquid-liquid contact is a possible mechanism in single droplet experiments with LWR materials.

Recent experiments by Mitchell[8] using Fe-Al$_2$O$_3$ and water have indicated that the rapid fuel fragmentation and heat transfer can also occur at a much larger scale (fuel mass ≈ 5 kg). Mitchell observed a rapidly propagating explosion through a coarsely mixed fuel-coolant system. Large peak pressures were generated (> 15 MPa) and a shock front propagating at 300-500 m/s was observed. Behind this front fuel appeared to be rapidly fragmented. To model this behavior we have developed a transient one-dimensional macroscopic propagation model. This model is presented in detail in Section 3.

2.4 Expansion Phase

The expansion phase is associated with serious mechanical damage, i.e., containment failure. Some preliminary analysis has been done   to address this area. We will only discuss the expansion of t' fuel-coolant mixture in this paper while the fluid-structure response is discussed in a separate work.[28] Past efforts in this area[29-30] have entirely focused upon the Liquid Metal Fast Breeder Reactor (LMFBR) and the structural response of the LMFBR to a fluid expansion caused by a vapor explosion or other processes.

In the reactor vessel the expansion of high pressure vapor can accelerate a liquid slug causing reactor vessel head impact and subsequent missile generation. The initial mass of coolant involved in the interaction, its thermodynamic state, and the subsequent heat transfer during the expansion will determine how much work is derived from the explosion. At present small scale experiments[5,8] indicate a conversion ratio of the fuel thermal energy to mechanical work of approximately 3-15 percent, while intermediate scale tests[6,8] have produced explosions with a conversion ratio in the range of 0-2 percent. In a hypothetical meltdown scenario, the manner in which fuel and coolant mix prior to an interaction again plays a significant role in determining the work output. If the fuel is dispersed in a large volume of coolant ($m_H/m_c \ll 1$), more cold liquid can become entrained in the vapor during expansion. Since cooling can occur with both initially mixed water and with entrained water, condensation and pressure reduction can occur. In contrast, if the fuel is dispersed in a small mass of coolant ($m_H/m_c \gg 1$), heat transfer can only occur with the entrained coolant. In either case the conversion ratio might be reduced due to heat transfer. In addition, the geometry within the reactor vessel after the meltdown can affect mixing and the expansion-work; although the quantitative effect is not well known.

A preliminary analysis examining this heat transfer effect is briefly presented. The coolant liquid entrainment rate is based upon a Taylor instability model. The governing equations and detailed results can be found in Reference 27. Parametric calculations were done for the expansion in full scale assuming no core structure or upper internal structure is present after the meltdown. In the analysis the hot coolant vapor in the fuel-coolant interaction zone accelerates a voidless coolant slug and entrains coolant liquid. This liquid reduces the vapor pressure and the slug kinetic energy. The calculations consider that 1-20 percent of the molten core comes to thermodynamic equilibrium with an equal mass of coolant ($m_H/m_c = 1$) after the explosion propagation. This mass ratio assumption is reasonable because it represents the midrange value of m_H/m_c, which is still a major unknown at this time. It thus accounts for heat transfer with both the coolant that is initially mixed with the fuel and that coolant entrained from the surroundings during the expansion. Some results are shown in Figure 5 and compared to an isentropic expansion. One can see that the percentage reduction in slug kinetic energy is strongly dependent on the mass of coolant, M_c, participating in the explosion; for $i.e. M_c = 1000$ kg the slug kinetic energy is reduced by a factor of five while for $i.e. M_c = 4000$ kg the reduction is a factor of two. This result corresponds to a fuel thermal energy to mechanical work conversion ratio of 1-2 percent.

3.0 A Transient-Propagation-Phase Model

Physically the propagation phase of the vapor explosion is composed of a series of vapor-film collapses. Each film collapse causes the enclosed drop to fragment and release thermal energy through accelerated vaporization of the surrounding coolant. This increase in vapor production results in elevated pressures which stimulate an even more rapid collapse of the neighboring vapor films.

The analogy of a string of dominoes is appropriate to this problem. The system is stable as long as one of the dominoes is not pushed into its neighbor; however,

if one of them is pushed, the chain reaction begins and propagates as if each succeeding domino was larger than the last.

A mixture theory must be used to accurately model this problem. The theory must include three materials; the fuel droplets, the vapor films surrounding each droplet, and the liquid coolant in which the droplets are immersed. Furthermore, from the physical description of the film-collapse process, we see that the local description of the vapor-film geometry is of major importance.

Mixture theories which include the effects of local geometry such as the vapor-film collapse are called structured mixture theories. The theory used to obtain the calculations in this work is derived in References (31-32). It has been previously applied to study the behavior of bubbly liquids.[34-35]

The bubbly-liquid and the vapor-explosion problem are similar in that each exhibits a cavitation behavior as the individual bubbles or vapor films expand or collapse. In each case, a mixture theory is required in which the gas or vapor constituent has a pressure which differs from the surrounding liquid. This pressure difference drives the collapse of the vapor film. It is a dynamic phenomenon which should not be confused with static pressure differences created by surface tension effects. Surface tension effects produce pressure differences which are negligible in this problem.

In the present work this pressure difference is coupled to the motion of the vapor film-coolant interface by means of a Rayleigh cavitation equation.[35] A precise derivation of the cavitation relation appropriate to this problem is included in Reference (18). The necessity of including this equation precludes the use of conventional two-phase flow theories since these formulations are derived with the assumption that the vapor and liquid constituents are at equal pressures.

For the purpose of achieving a tractable problem, the formulation was restricted to situations in which the drops, vapor-films, and coolant experienced identical translations. Also, at any given point in the mixture, a single droplet radius and vapor film radius were used to describe the mixture. These assumptions result in mass and momentum conservation laws which are similar to their conventional single-material counterparts. The material response descriptions and the mass and energy exchange relationships have been left general so as to allow to inclusion of all of the possible mechanisms for fragmentation described previously.

3.1 Numerical Technique

Provided we are willing to sacrifice some computational efficiency, existing wave propagation codes designed to solve conventional continuum relations can be modified to solve the equations described in the previous section. This is a feasible approach since the mass equation and the momentum equation retain the conventional forms for single-material mechanics problems.

We have chosen to modify the one-dimensional Lagrangian wave propagation code, WONDY IV.[36] The explicit, finite-difference scheme used in WONDY IV is structured so that as a particular mesh point is advanced in time, the new position is first computed from known values of the pressure and the mixture momentum balance, and then the new density is computed from the balance of mixture mass. To complete the cycle of computations, the equation-of-state subroutine is then called in which a new value of pressure and internal energy is computed by simultaneously solving the constitutive equation for pressure and the energy balance equation.

This format is useful for our problem since the mixture mass and momentum equations are already built into the code. The remaining field equations in the mixture formulation are local statements; that is, they do not contain spatial gradients, and can be solved in the equation-of-state subroutine.

The new equation-of-state subroutine is constructed in the following manner: first, the old and new values of density, ρ, are linearly interpolated to give a continuous value of ρ across the time step; then the energy equations along with

the vapor-film collapse relations are viewed as a set of ordinary differential equations in time; finally, these equations are integrated from the old value of time across the time step to the new value of time by means of a Runge-Kutta technique. This provides the new value of mixture internal energy and the new value of mixture pressure which is required to continue the computation.

This computational scheme has proven useful in a variety of similar problems wherein complex differential relations are integrated in the equation-of-state subroutine.[37-38] In particular, accurate modelling of experimental data for pressure waves propagating in bubbly liquids has been achieved. In general we have found that the Runge-Kutta integration scheme can be replaced by more accurate methods without altering the results. Also, because of the rate-dependent nature of the film collapse relations, the usual artificial viscosity terms found in this type of wave code can be eliminated.

3.2 Sample Results

Figure 6 contains two wave profiles at 0.14 ms and 0.26 ms after initiation of the trigger pulse. The trigger pulse which occurs on the right boundary is a square wave input 10 MPa in amplitude and 10 μs in duration; however, trigger pulses as low as 1 MPa result in an explosion in this example. The mixture is modelled after Michells experiments[8] and contains 20 percent by volume of 10-mm diameter molten fuel drops with 0.2-mm thick vapor films. Both the pressure within the vapor film and within the surrounding coolant are plotted. At the head of the left-traveling wave is a pressure spike which is a result of film collapse and coolant impact on the fuel drops. In this calculation fragmentation by cavitation converts 10 percent of the impact energy into new fuel-coolant surface area by using a surface tension coefficient of 0.4 N/m. The resulting vaporization of the coolant after impact is evidenced by a buildup of pressure behind the pressure spike. This broad region of elevated pressure in turn initiates the final expansion phase of the vapor explosion.

Conclusions

The quantitative nature of fuel-coolant mixing is unknown; however, observations indicate boiling processes can cause fuel breakup to 10-20 mm droplet diameters in about 0.1 s. In systems where this mixing occurs the effects of ambient pressure increase, coolant temperature increase, and fuel composition tend to suppress the initiation of an explosion; the phrase "tend to suppress" is important since elevated trigger pressures can override these effects and again induce an explosion.

While the final stages of film collapse and coolant-fuel impact are not totally understood, several promising mechanisms have been described. The net effect of these mechanisms is to mechanically fragment the fuel drop by allowing the vapor film to collapse. Upon collapse, the surrounding coolant converges and impacts the fuel drop. The increased evaporation after impact then re-establishes new vapor films and elevates the system pressure. This in turn accelerates the film collapse around the neighboring unfragmented fuel drops.

With the one-dimensional transient wave propagation model presented in Section 3, we have shown how this fragmentation process can easily build in efficiency with propagation distance.

Finally, we have shown that the release of mechanical work during the expansion phase of the explosion can be reduced by the effects of coolant liquid heat transfer during the expansion.
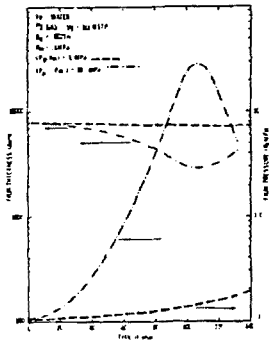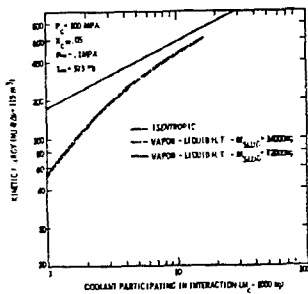
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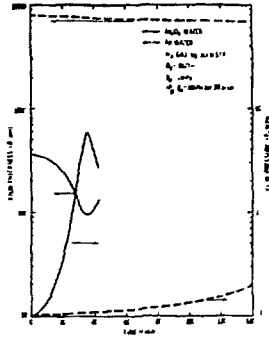(38) D. S. Drumheller, Inter. Jour. Solid & Struct., 14, 441, (1978).
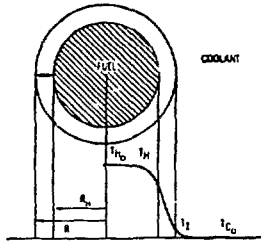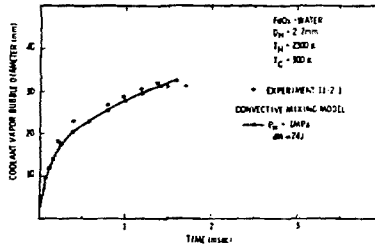
1. Schematic of the Dynamic Film Model

2. Vapor Film Collapse Behavior With and Without a Noncondensible Gas

3. Vapor Film Collapse Behavior With a Noncondensible Gas; for Different Trigger Magnitudes

4. Prediction of the Coolant Vapor Expansion During a Small Scale Explosion

5. Variation of the Slug Kinetic Energy at Impact with the Mass of Coolant Involved in the Explosion
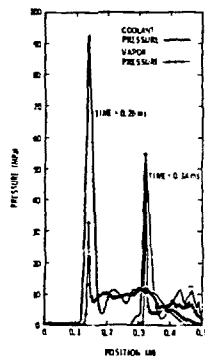
6. Prediction of the Pressure Generated by the Transient Propagation of the Explosion