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VAPOR EXPLOSION PHENOMENA WITH RESPECT TO NUCLEAR REACTOR SAFETY ASSESSMENT

AUGUST W. CRONENBERG • R. BENZ

July 1978



IDAHO NATIONAL ENGINEERING LABORATORY

DEPARTMENT OF ENERGY

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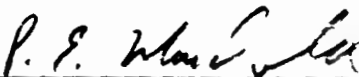
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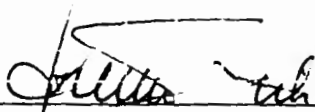
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**VAPOR EXPLOSION PHENOMENA WITH RESPECT TO
NUCLEAR REACTOR SAFETY ASSESSMENT**

by

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EG&G IDAHO, INC.

July 1978

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U.S. NUCLEAR REGULATORY COMMISSION
AND THE
DEPARTMENT OF ENERGY
IDAHO OPERATIONS OFFICE
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FOREWORD

The contents of this report are based on a chapter to appear in a forthcoming issue of "Advances in Nuclear Science and Technology". The work was begun under the sponsorship of the Division of Fast Reactor Safety Research, the U.S. Nuclear Regulatory Commission, and the Institute for Kernenergetik, the University of Stuttgart, in the summer of 1976, where the principal author was a guest researcher for two months. The work was completed during the principal author's last year at the University of New Mexico and at EG&G Idaho, Inc., as part of the Thermal Fuels Behavior Program being performed for the Light Water Reactor Safety Research Division of the U.S. Nuclear Regulatory Commission.

ABSTRACT

Stringent licensing procedures for commercial nuclear reactor operation require an in-depth analysis of the phenomena associated with postulated reactor core overheating accidents. One aspect of nuclear reactor safety assessment is a prediction of the consequences of interaction between molten fuel and coolant, in which rapid heat transfer from the fuel may lead to explosive vaporization of the coolant.

In this report some of the more recent theories relating to vapor explosion research for nuclear reactor safety assessment are critically reviewed and assessed. Specifically, the spontaneous nucleation and pressure detonation models are discussed at length. In addition, modeling of the fragmentation of hot molten fuel upon contact with liquid coolant, and energy considerations for rapid fine-scale intermixing of such fragmented fuel with coolant are discussed in detail. The purpose of such a review is to assess the current state of knowledge in this ongoing research field, and to gain insight into the basic phenomena that should be considered in assessing overall nuclear reactor safety under severe, hypothesized off-normal heat transfer conditions.

SUMMARY

One of the principal concerns in assessing the safety characteristics of large-scale nuclear power reactors is whether core overheating and subsequent fuel element meltdown in a liquid coolant environment can lead to explosive vaporization of the type observed in the BORAX-I and SPERT-ID destructive experiments and the SL-1 accident.

The purpose of this report is to critically review and assess some of the more recent theories and experiments relating to molten fuel-coolant interactions (MFCI) which might lead to explosive vaporization and to summarize and interpret the current state of understanding. Such knowledge is of importance in assessing the results of off-normal core behavior under various postulated conditions, where extensive fuel rod failure may occur with fuel in the molten state.

In addressing the vapor explosion problem, an area of primary importance is an understanding of the necessary and sufficient conditions for explosive vaporization. Two concepts that attempt to assess such conditions are the spontaneous nucleation and the pressure detonation model concepts. With respect to the former, a vapor explosion is considered possible only if the contact interface temperature established between the hot and cold materials is greater than the spontaneous nucleation temperature (that is, the temperature at which vapor nuclei form in a heterogeneous manner and include the wetting contact effects of nucleation at a liquid-liquid interface). A quite different approach considers that explosive vaporization is governed primarily by the fragmentation and intermixing process, such that fine-scale mixing between the cold and hot materials results in a nucleate-type boiling process which is sufficiently rapid to cause shock pressurization of the system. Several "triggers" have been postulated to initiate such fragmentation and intermixing, including pressure-induced detonation and film boiling destabilization. The pressure detonation concept, however, has been formulated into a rather detailed model, whereas the latter concept has not. Since the temperature conditions for film boiling destabilization and spontaneous nucleation appear to be similar, various simulant fluid experiments to test the spontaneous nucleation concept have been interpreted in light of both theories. With respect to pressure-induced triggering of fine-scale fragmentation and intermixing, preliminary experiments and associated modeling efforts indicate that such a mechanism may be valid, although for reactor materials and geometry, the necessary conditions appear to be difficult to obtain.

From the critical review presented, the conclusion reached is that although model details may differ, a consensus of opinion is emerging on the generalized necessary conditions for explosive vaporization. All model concepts are consistent in that an initial period of stable film boiling, separating molten fuel from coolant, is considered necessary (at least for large-scale interactions and efficient intermixing), with resulting breakdown of film boiling due to pressure and/or thermal effects, followed by intimate fuel-coolant contact, fine-scale fragmentation, and fuel-coolant intermixing which results in a rapid vaporization process sufficient to cause shock pressurization. One of the principal areas of difference is what constitutes the requisite condition(s) for rapid vapor production to cause

shock pressurization. Until such questions are settled, the important state variables (that is, temperature, pressure, and specific volume) for MFCI-induced vapor explosions cannot be accurately predicted.

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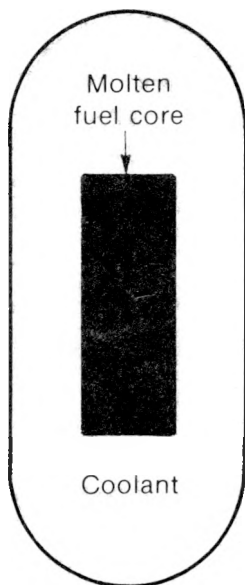
VAPOR EXPLOSION PHENOMENA WITH RESPECT TO NUCLEAR REACTOR SAFETY ASSESSMENT

I. INTRODUCTION

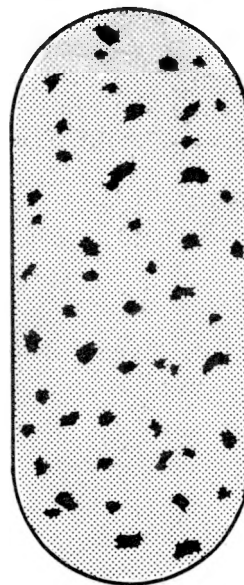
An important concern in the analysis of a hypothetical nuclear power reactor accident is an understanding of the consequences of reactor core overheating, leading to fuel melting and subsequent interaction of hot molten fuel with coolant. If such molten fuel-coolant interaction (MFCI) is of limited extent, the resultant work potential is relatively benign. However, as illustrated in Figure 1, it can be envisioned that under certain conditions core overheating may lead to a sequence of events resulting in the formation of an extensive amount of hot molten fuel in a liquid coolant environment, where such molten fuel may interact with the colder liquid coolant causing it to vaporize as a result of local heat transfer. If the local heat transfer process is rapid enough (for example, due to fine-scale fuel fragmentation and intermixing with the coolant), the vapor generation process may be extremely fast, such that shock pressurization of the system occurs. If the pressure pulse generated is of sufficient strength, then severe damage to or failure of the reactor vessel may occur. Such a process is often referred to as a "vapor explosion".

The implication of this type of occurrence, where the reactor vessel is breached and releases high temperature material which is radioactive, can be severe. Although such a vapor explosion accident has never been known to occur in an operating commercial power reactor, the small possibility of such an occurrence and the stringent safety requirements placed on the licensing of nuclear reactors for commercial use has stimulated research aimed at understanding the basic phenomena involved in such vapor explosions.

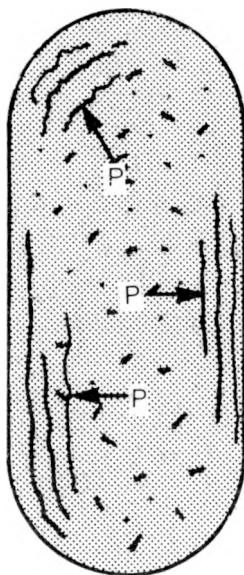
Although the general subject area of MFCIs is of interest in overall nuclear reactor safety assessment, where, for example, mild MFCI events can lead to off-normal coolant hydraulic effects, the present discussion concentrates on the specific case of severe MFCI-induced explosive vaporization, where a critical review of recent developments in the understanding of vapor explosion phenomena is presented. Emphasis is placed on reviewing and assessing the validity of assumed processes associated with several overall vapor explosion models, as well as an understanding of fine-scale fuel fragmentation and intermixing with liquid coolant, which is considered necessary for the occurrence of large scale explosions. In addition, considerations relevant to nuclear reactor systems are addressed. From such a critical review, it is hoped that the reader will obtain a better understanding of the major contributions in describing the necessary conditions for explosive vaporization, the detailed theoretical modeling of such conditions, the validity and limitations of the various proposed models, and the principal uncertainties that still exist at the time of this writing. First, however, a brief discussion of MFCI incidents (some of which can be classified as true vapor explosions) is presented. Following this discussion, various overall vapor explosion models are reviewed as well as modeling and experimental efforts on



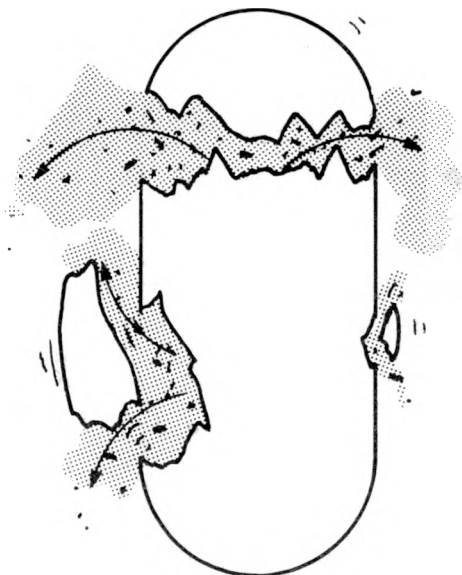
(a)
Core overheating-
fuel melting



(b)
Fine-scale fuel
fragmentation and
intermixing



(c)
Rapid vaporization
and shock pressurization



(d)
Potential reactor
vessel failure

INEL-A-7976

Fig. 1 Illustration of a hypothetical molten fuel-coolant interaction induced vapor explosion.

the fragmentation and intermixing processes. The relation of such models to reactor conditions is also presented, followed by summary and conclusion sections.

II. MOLTEN FUEL-COOLANT INTERACTION INCIDENTS

The general area of molten fuel-coolant interaction has been the subject of considerable research^[1-7]. This problem, however, is not only of interest with respect to nuclear reactor safety^[8] but also to the safety of the foundry^[2,9] and liquified natural gas^[10,11] industries. The problem is one of assessing the mechanisms involved in such interactions and the associated work potential resulting from the contact of a hot substance immersed in a colder fluid with attendant coolant vaporization and pressurization. As illustrated in Figure 2, such metal-coolant interactions can be considered vapor explosions

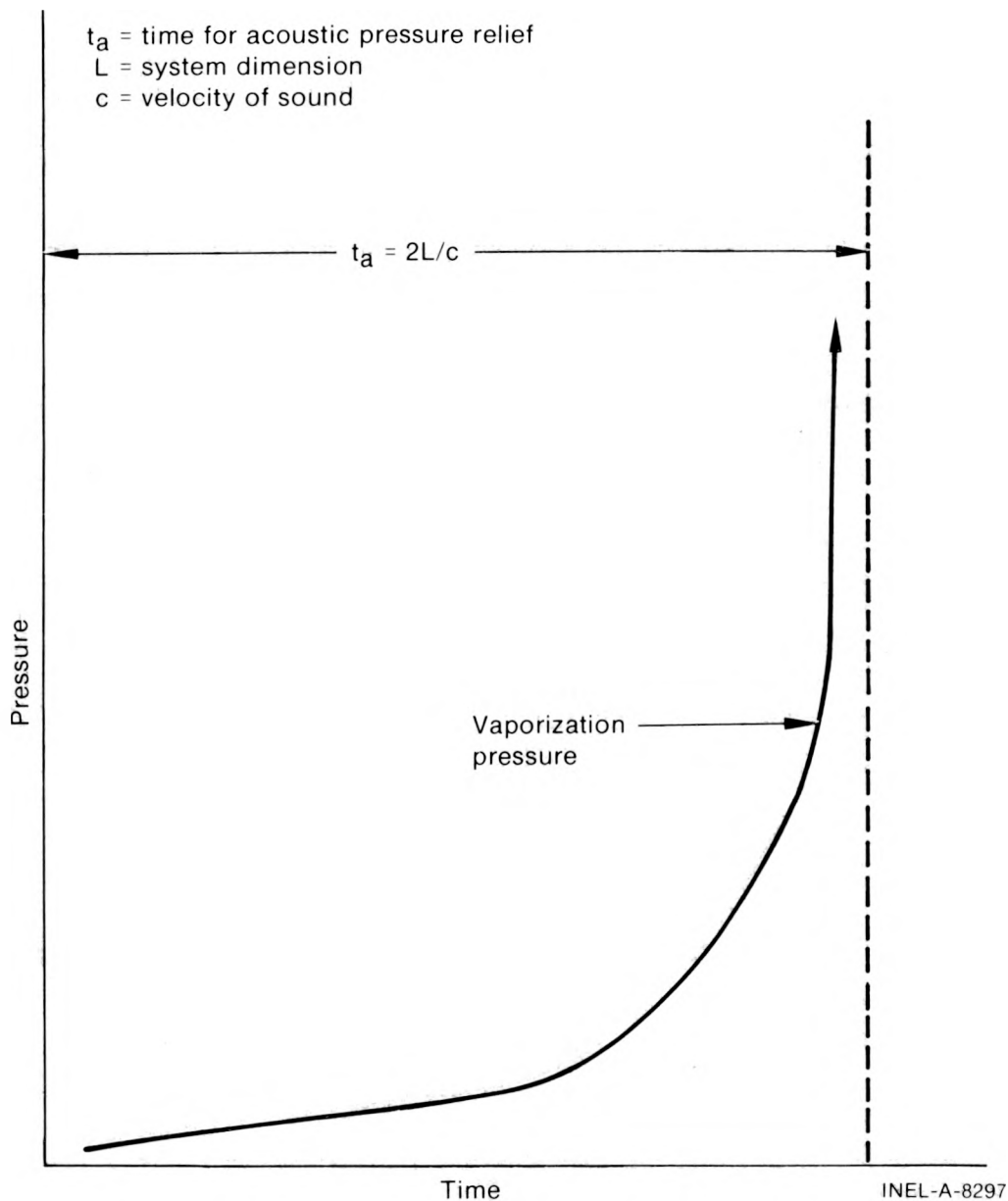


Fig. 2 Transient pressurization characteristics resulting from explosive vaporization.

when the rate of pressure buildup occurs faster than pressure relief in the surrounding liquid. Such a situation will lead to a shock-type pressure pulse and the possibility for severe damage to the confining system, depending on the rate and extent of volume expansion of the working fluid.

Early industrial experience has shown that vapor explosions often result during the accidental spillage of molten metals onto damp surfaces. One such incident, described by Long^[2], resulted when molten steel slag was accidentally spilled into an open trough containing water, causing extensive foundry damage. Epstein^[3] documented other examples of metal-water explosions. In one case, the loading of wet scrap aluminum into a furnace produced an explosion causing six deaths, four injuries, and approximately one million dollars in property damage.

As illustrated in Table I, several molten fuel-coolant interactions have occurred in test reactor systems, some of which can be classified as true vapor explosions. One of the first indications of a MFCI in a nuclear reactor was a result of the core-meltdown accident of the experimental Canadian NRX test reactor^[12] (Table I). During a low-power experiment, failure occurred in the shutdown-rod system due to a concurrence of mechanical defects and operating errors. Hurst^[13] concluded, in his analysis of this accident, that the damage to the calandria tubes was a direct cause of either a uranium-steam or uranium-water interaction, which was of a nonchemical nature. Evidence of a similar type fuel-coolant interaction (FCI) in a fast reactor dates back to the Experimental Breeder Reactor-I (EBR-I) (U-Zr alloy fuel) meltdown with NaK coolant^[14,15]. Although no evidence of severe pressurization was found, apparently coolant boiling resulting from a MFCI played a major role in damage to the core^[15].

Following the NRX incident, a destructive reactor experiment was performed with the Boiling Water Reactor (BORAX) facility^[16,17]. As described by Dietrich^[16], "A power excursion melted most of the fuel plates. The pressure resulting from the molten metal in contact with the reactor water burst the reactor tank and ejected most of the contents of the shield tank into the air. Analysis of mechanical damage indicated that the peak pressure was at least as high as 6000 psi." Dietrich concluded that no evidence existed of any significant chemical reaction, but rather that the explosion was of a thermal nature.

The first fatal reactor accident occurred on January 3, 1961 as a result of the explosion of the experimental military Stationary Low Power Reactor-I (SL-1), a boiling water reactor^[18]. Although other causes have been postulated, the most plausible explanation is that the accident resulted primarily from the withdrawal of a control rod, leading to a nuclear excursion, fuel-element failure, and violent interaction between molten fuel and water. The magnitude of the indicated pressures generated in this accident led to the development of a series of experiments which concentrated interest on the mechanisms for MFCI. Results of the controlled destructive experiments with the Special Power Excursion Reactor Test-Idaho (SPERT-ID) core also indicated that the explosion was primarily of a thermal nature, with an estimated 10% maximum energy release due to chemical reaction effects^[19-22].

TABLE I

SOME WATER REACTOR ACCIDENTS AND EXPERIMENTS INVOLVING METAL-WATER INTERACTION

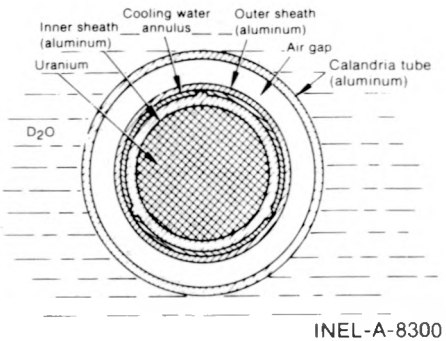
Date of Occurrence	Reactor	a) Fuel b) Coolant c) Moderator	Fuel-Coolant Geometry	Cause	Description of Events	Primary Factors Influencing Reactor System Damage
12/12/52	NRX	a) Natural-U clad with Al b) H ₂ O c) D ₂ O		Control rod malfunction during an experiment on the reactivity of the reactor at low power. The object of the experiment was to compare the reactivity of irradiated fuel with fresh fuel. The normal water coolant flow for some of the rods was reduced for this experiment.	<p>A postaccident investigation led to the conclusion that the reactor went supercritical by about \$0.6 and that the power rose to about 20 MW(t). Although the reactor was capable of operating at power levels up to 30 MW(t), the reduced cooling rate for the test resulted in coolant boiling and steam pressure buildup, causing eventual melting of several rods and subsequent interaction between U and Al with the water coolant.</p> <p>Analysis of the accident indicated that the exothermic chemical reaction was not significant in itself. However, the attendant hydrogen release from this reaction, which came in contact with air, resulted in an H-O explosive reaction, such that the core and calandria tubes were damaged beyond repair. There was no evidence of a shock-type steam explosion.</p>	<p>a) Coolant vaporization leading to fuel rod meltdown</p> <p>b) Steam pressure buildup (non-explosive)</p> <p>c) Hydrogen-oxygen explosion</p>

TABLE I (continued)

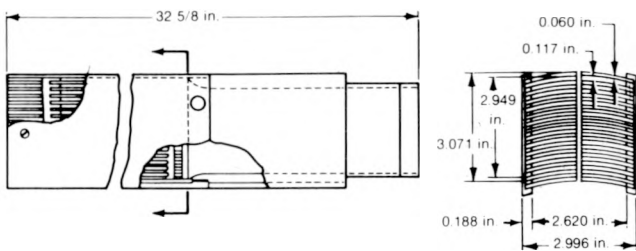
Date of Occurrence	Reactor	a) Fuel b) Coolant c) Moderator	Fuel-Coolant Geometry	Cause	Description of Events	Primary Factors Influencing Reactor System Damage
1954	BORAX-I	a) U-Al Alloy clad in Al b) H ₂ O c) H ₂ O	 INEL-A-8302	Destructive experiment initiated by 4%-k _{eff} control rod ejection.	Analysis of the accident indicated that most of the fuel plates melted or partially vaporized. However, postaccident debris indicated that although the U-Al fuel melted during the transient, the cladding remained solid. The total energy release was 135 MW-s, resulting in a pressure peak of about 650 atms. The reactor tank was burst by the blast and most of the shield tank contents were ejected into the air. The control rod mechanism (mounted on a heavy plate), weighing approximately one ton, was thrown 30 ft into the air. The shutdown mechanism was due to core mechanical expansion and coolant boiling.	a) Although high speed motion pictures indicated a light flash lasting 0.003 s as peak power was reached, the flash was gone before any material was ejected from the reactor tank; thus indicating that the mechanical damage was a result of a thermally induced steam explosion rather than a chemical explosion. b) Postaccident analysis indicated that the fuel was molten at the time of interaction, while the Al cladding remained in the solid state. c) Extensive fuel fragmentation occurred.

TABLE I (continued)

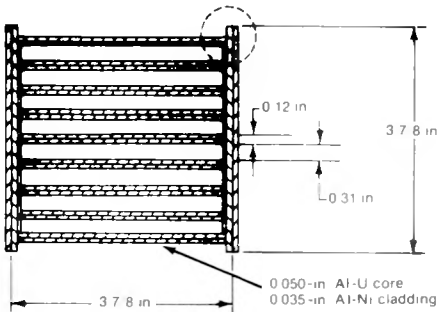
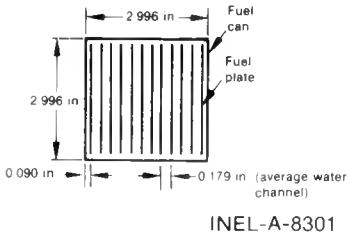
Date of Occurrence	Reactor	a) Fuel b) Coolant c) Moderator	Fuel-Coolant Geometry	Cause	Description of Events	Primary Factors Influencing Reactor System Damage
1/3/61	SL-1	a) 93% enriched U ²³⁵ , clad with Al b) H ₂ O c) H ₂ O	 <p>INEL-A-8299</p>	Excessive control rod withdrawal leading to a nuclear excursion, fuel element failure, and violent interaction between metal and water.	<p>Analysis of the accident indicated that the excess reactivity resulted in partial fuel element meltdown and vaporization. Inter-mixing of the vapor driven solid/molten metal with water led to violent steam formation and some metal-water chemical reaction. The formation of a steam void terminated the nuclear transient. However, the steam pressure (estimated to have reached 700 atm) caused the pressure vessel to rise approximately 9 ft above its normal position, shearing off all piping in the process, and ejecting the loose control rod plugs upward, resulting in their penetration in the ceiling above. Two of the fatalities were instantaneous, as a result of the mechanical blast damage. The third fatality was due to radiation exposure and flying debris.</p> <p>The mechanical damage was the result of a shock-type metal-water thermal explosion, being approximately 1% of the total nuclear energy released.</p>	a) Essentially all mechanical damage to the reactor system can be attributed to the thermally induced steam explosion. Calculations indicated that at the time of the steam vapor expansion, the Al cladding was solid, while the U metal was partially vaporized.

TABLE I (continued)

Date of Occurrence	Reactor	a) Fuel b) Coolant c) Moderator	Fuel-Coolant Geometry	Cause	Description of Events	Primary Factors Influencing Reactor System Damage
11/5/62	SPERT-ID	a) U-Al alloy clad in Al B) H ₂ O C) H ₂ O	 <p>INEL-A-8301</p>	Destructive experiment initiated by a power excursion.	<p>The destructive test was instrumented with a special capsule to measure transient power, energy, fuel-plate surface temperature, moderator flow, pressure, and strain. The data obtained indicate a period of 3.2 ms and a peak power of 2300 MW(t). Pressures of 270 atm were recorded. Approximately 35% of the core experienced melting with all 270 fuel plates in the core having undergone some degree of melting.</p> <p>Postaccident analysis indicated that approximately 20 kg of a sponge-like metallic material fragmented to sizes from 0.003 in., to a few inches in diameter. Chemical analysis of this material indicated a content, by weight, of 65% Al, and 6.7% U; the rest being insoluble residue (Fe, etc.). The extent of Al-H₂O chemical reaction was considered small with respect to the pressure pulse. The blast pressure was considered to be caused by a steam explosion resulting from thermal interaction between the molten fuel plates and the water.</p> <p>The maximum surface temperature at the time of the destructive pressure pulse was estimated to be about 600°C; the interior portion of the U-Al fuel was about 1200°C.</p>	<p>a) The metal-water chemical reaction did not appear to be the primary cause of the observed pressure pulse.</p> <p>b) Fuel-plate analysis indicated that approximately 35% of the core was molten at the time of the blast.</p> <p>c) Extensive fragmentation resulted.</p> <p>d) A steam explosion resulted, considered to be caused by a thermal interaction between metal and water.</p>

Uncertainty still exists as to the mechanism of and factors influencing such thermal explosions. However, it is generally recognized that extensive fuel fragmentation and intermixing with coolant occurs, with intimate contact between the hot and cold materials, resulting in a heat transfer and coolant vaporization process sufficiently rapid to cause shock pressurization of the working fluid (coolant). If such interaction is coherent and large scale in nature, severe damage to the reactor system can result. Milder fuel-coolant interactions can also occur, as demonstrated in numerous in-pile and out-of-pile experiments, which can result in a rather violent vaporization process; however, such interactions are not considered to be true vapor explosions unless severe shock-pressurization occurs. Evidence indicates that the SL-1, BORAX-I, and SPERT-ID incidents can be categorized as undergoing true vapor explosions, whereas the NRX and EBR-I incidents can be categorized as being due to milder MFCI. However, because of redundant safety systems, such energetic interactions have not occurred in modern commercial power reactors and their probability of occurrence is low^[8].

An overview of current international MFCI research activities is given in Reference 23 and illustrated in Table II for light water reactors (LWRs) and in Reference 24 and Table III for liquid metal fast breeder reactors (LMFBRs). However, the safety concerns for the two systems are somewhat different. With respect to LMFBRs, the questions of vapor explosion potential and milder MFCI leading to coolant voiding (with a potentially positive void coefficient) are both of primary importance. For LWRs, however, the effects of coolant expulsion are not as critical in comparison, due to an overall negative void coefficient. Thus, for LMFBRs two important concerns exist – vapor explosion potential and milder MFCI-induced voiding; whereas for LWRs, violent vapor explosions are of primary interest. As stated previously, this report is limited to a discussion of various modeling concepts associated with MFCI-induced vapor explosions, rather than a general discussion of all aspects of molten fuel-coolant interaction^[a]. In the following section, a critical review is presented of two overall vapor explosion model concepts in view of the basic physical phenomena assumed in each model.

[a] Present discussion is limited to the highly improbable core-meltdown accident with accompanying potential for a thermal vapor explosion, and should not be considered applicable to other hypothesized loss-of-coolant accidents^[25,26].

TABLE II

STEAM EXPLOSION RESEARCH PROGRAMS WITH RESPECT TO
CORE MELTDOWN ASSESSMENT PROGRAMS^[23]

	<u>Sandia Laboratories</u>	<u>Joint Research Center at Ispra, Italy</u>		<u>Argonne National Laboratory</u>	
Test configuration	Stationary vapor-blanketed droplet in closed chamber	Shock tube	Drop test in 300-closed tank	Drop tests in closed vessel	Various modes of forced contact
Hot phase	Steel, corium	UO ₂ , steel, zircaloy-4, corium	UO ₂ , steel zircaloy-4, corium	Mineral oil	Aluminum
— Cold phase	Water	Water	Water	Freon-22	Water
Temperature of hot phase (°C)	T _{mp} to (T _{mp} + 500)	1500 to 2900	1500 to 2900	100 to 220	300
Mass of hot phase (kg)	0.02	0.12 to 0.15	3	5	0.10
Mass of cold phase (kg)	2	0 to 22	0 to 200	10	1
Temperature of cold phase (°C)	25 to 90	20 to 220	20 to 220	-40	25
System pressure (atm)	1 to 5	1 to 25	1 to 25	1 to 50	1

TABLE III
EXPERIMENTAL LMFBR FUEL-COOLANT INTERACTION RESEARCH PROGRAM^[24]

Out-of-Pile Experiments				
Laboratory	UO ₂	Na	Contact Mode	Test Conditions
Grenoble, France	5 g	4 g	UO ₂ into Na	Rod failure, joule heater
	3 to 5 kg	225 g	Na into UO ₂	Pool geometry, induction heated
Japan	20 g	30 to 200 g	UO ₂ into Na	Dropping, radiant heated
CNEN, Italy	10 g	7 g	UO ₂ into Na	Rod failure, joule heater
Ispra, Italy	3000 g	70 g	UO ₂ into Na	Dropping, radiant heated
ANL, U.S.	7 to 10 g	300 g	UO ₂ into Na	Dropping, induction heated
	30 g	5 to 10 g	Na into UO ₂	Dropping, induction heated
	500 g	5 to 10 g	UO ₂ into Na	Dropping, thermite heated
In-Pile Experiments				
Laboratory	UO ₂	Test Conditions		
Petten, Netherlands	100 g	Single-rod, fresh fuel, loss-of-flow (LOF) simulation		
ANL (series)				
(S)	28 to 286 g	1 to 7 rods, fresh fuel, transient- overpower (TOP)		
(H)	68 to 472 g	1 to 7 rods, fresh and irradiated fuel, TOP (50¢/s)		
(E)	45 to 472 g	1 to 7 rods, fresh and irradiated fuel, TOP (\$3/s)		
(L)	456 to 470 g	7 rods, fresh and irradiated fuel, LOF		
(R)	200 to 1200 g	1 to 7 rods, fresh fuel, LOF		
Sandia	64 g	1 rod, fresh fuel, with and without Na, prompt burst		

III. VAPOR EXPLOSION MODELS

Basically, two different approaches have been adopted in assessing the vapor explosion problem: the equilibrium thermodynamic models which estimate the maximum work potential available, and the transient heat transfer and fluid dynamics models which attempt to describe the actual phenomena and rate processes involved.

The thermodynamic approach was first employed by Hicks and Menzies^[27] to estimate an upper limit on the expansion work of the coolant due to a MFCI. This work is calculated to be equal to the change in internal energy of the fuel during an isentropic expansion from a compressed state, defined by the amount of energy added to the core fuel, to an expanded state, defined by the boiling temperature of the fuel at atmospheric pressure. By use of a different equation-of-state for sodium coolant, Judd^[28] obtained a somewhat higher ($\sim 30\%$) estimate of the ultimate work potential. However, such thermodynamic approaches do not describe the necessary conditions for explosive vaporization, nor the details of the physical phenomena or rate processes involved. A more mechanistic approach to the problem has been the development of several transient models, the two most important being the spontaneous nucleation and pressure-induced detonation models. A critical review of these two transient model concepts is presented in the following sections.

1. SPONTANEOUS NUCLEATION

As illustrated in Figure 3, the spontaneous nucleation model proposed by Fauske^[29,30] considers that for a large-scale vapor explosion to occur, the conditions for liquid-liquid contact must exist such that the contact interface temperature established between the molten fuel and coolant must exceed that for spontaneous nucleation [Figure 3(a)]. The contact interface temperature (T_I) in the absence of solidification of the hot material can be described as

$$T_I = \frac{T_H (k/\sqrt{\alpha})_H + T_C (k/\sqrt{\alpha})_C}{(k/\sqrt{\alpha})_H + (k/\sqrt{\alpha})_C} \quad (1)$$

where

T = temperature

k = thermal conductivity

α = thermal diffusivity

H = hot material

C = coolant.

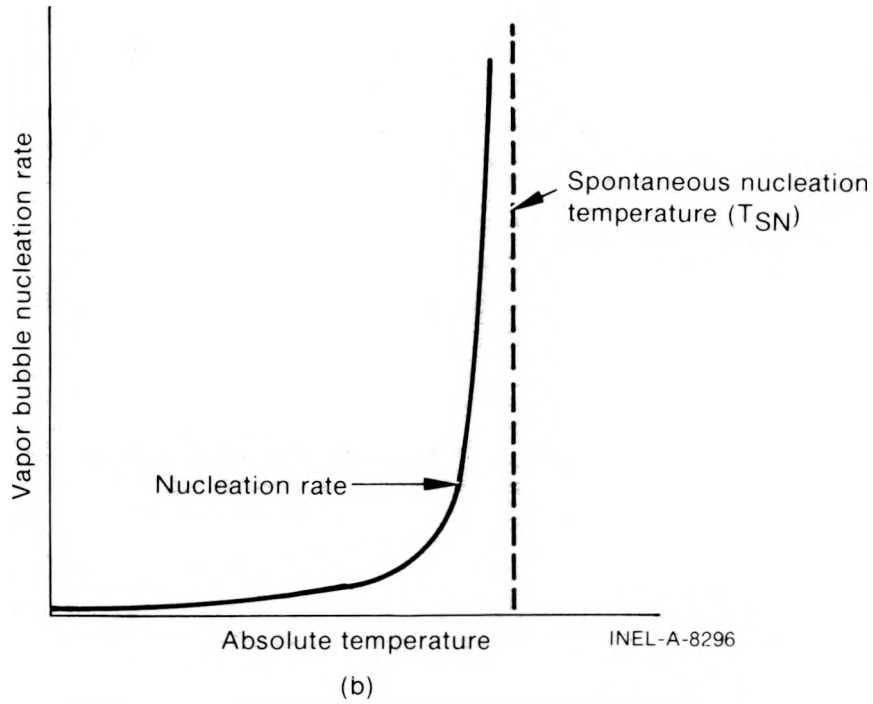
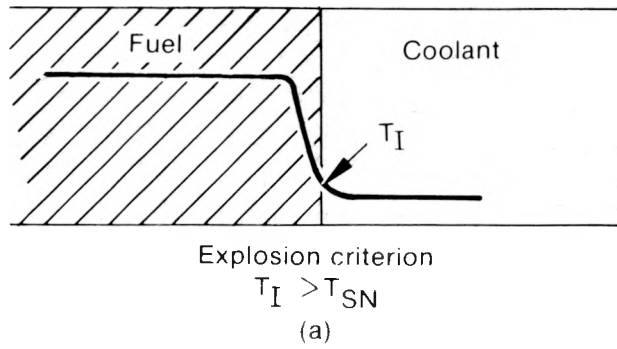


Fig. 3 Illustration of spontaneous nucleation model.

To assess the temperature at which spontaneous nucleation occurs (T_{SN}), Volmer's well-known rate equation is used, such that

$$J = \text{const} \exp (-W/kT) \quad (2)$$

where

- J = the rate of bubble nucleation per unit volume
- k = Boltzmann's constant
- W = reversible work of formation of a critical vapor embryo in the liquid and is given by

$$W = 16\pi\sigma^3 / 3(P_v - P_\ell)^2 \quad (3)$$

where

- σ = surface tension of the pure liquid
- P_v = vapor pressure
- P_ℓ = liquid pressure.

As shown in Figure 3(b), the nucleation rate remains small until the temperature of the liquid reaches a critical value, where J increases rapidly. For vapor nucleation in the bulk of a pure liquid, this temperature limit is referred to as the homogeneous nucleation temperature (T_{HN})^[a] and can be approximated as about 90% of the thermodynamic critical temperature, T_c ($\simeq 647$ K for water and $\simeq 2570$ K for sodium). However, for the case of partial liquid contact with another substance, the effect of the wetting characteristics at the contact interface must also be considered, such that Equation (3) is multiplied by a wetting factor, expressed as

$$f(\theta) = \frac{2 + 3 \cos \theta - \cos^3 \theta}{4} \quad (4)$$

where θ = the contact angle established between the two materials. For perfect wetting $\theta = 0^\circ$ and $f(\theta) = 1$, which gives the upper limit of the spontaneous nucleation temperature (T_{SN}); that is, the homogeneous nucleation temperature. Only for a high degree of nonwetting is T_{SN} significantly lower than T_{HN} , where for example as θ approaches 180° T_{SN} approaches the saturation temperature.

As can be seen by inspection of Equation (1), the interface temperature approaches that of the hot material when the thermal conductivity of the coolant is relatively low compared to that of the hot material. As a result, forced contact between such molten fuel and coolant may lead to the condition that $T_I > T_{SN}$, which is the situation for molten UO_2 quenched in water. If sufficient heat transfer surface area is available through the process of fuel fragmentation and intermixing, and if the system is constrained such that a rapid rate of pressure buildup cannot be relieved, then a shock-type vapor explosion is

[a] The homogeneous nucleation temperatures calculated from Equation (2) for various fluids are: Freon-22 (326 K), n-pentane (421 K), ethanol (468 K), sodium (2300 K), and water (575 K).

postulated to occur. However, it has been argued^[29] that fission gases, radiation, and other nucleation aids in a reactor environment tend to initiate boiling prior to the spontaneous nucleation threshold being reached, such that relatively mild pressurization events would normally occur. However, energetic vapor explosions of the type observed in the SPERT-ID, BORAX-I, and SL-1 events can occur if intimate contact for a constrained system is established. For LMFBR materials, such as UO_2 fuel and Na coolant, such explosions are ruled out *a priori* for the reactor conditions of large UO_2 -Na masses, since in this case the contact temperature is calculated to be well below that for spontaneous nucleation of sodium. Only for the laboratory case, where a small mass of Na might be entrapped by UO_2 and slowly heated to its spontaneous nucleation temperature, is a vapor explosion considered possible. Armstrong's experiments^[31,32] have been interpreted in Reference 29 in this manner. However, in a recent paper by Anderson and Armstrong^[33], both UO_2 into Na and Na into UO_2 are considered to behave in a similar manner; both producing laboratory-scale vapor explosions under favorable conditions (to be discussed later). Thus, the statement that vapor explosions have not been observed for the UO_2 into Na experiments appears to be subject to interpretation.

Other experimental findings which tend to discount the spontaneous nucleation-contact interface criterion are the R-22^[a]/water experiments of both Anderson and Armstrong^[33] and those of Enger and Hartmann^[10]. With respect to the latter experiments, the contact temperature was pointed out to be below that for homogeneous nucleation [$T_{\text{HN}}(\text{R-22}) = 53^\circ\text{C}$], yet vapor explosions occurred. Fauske^[29] attributed this discrepancy to transient variations in the interfacial surface energy (that is, dynamic surface tension effects) during the initial stage of contact. However, since R-22 has been shown to spread easily on cold water^[34], the spontaneous nucleation temperature would be expected to be near the homogeneous nucleation temperature.

While the question still remains as to whether or not achievement of the spontaneous nucleation temperature is a necessary condition for the occurrence of vapor explosions, several interpretations have been postulated to account for an experimentally observed delay period from time of contact to onset of rapid vapor production and pressurization. Henry and Fauske^[35-37] have attempted to account for such a delay period in the context of the time required to attain spontaneous nucleation from the onset of liquid-liquid contact. Although the time scale for establishment of the interface temperature is 10^{-12} s, assessed from the relaxation time for thermal vibration propagation (α/c^2 , where c is the velocity of sound in the conducting material), Henry et al^[35-37] hypothesized that vapor bubble nucleation cannot proceed until a thermal layer has developed in the coolant phase which is sufficiently thick to support a vapor embryo of the critical size (that is, $R_c = 2\sigma/\Delta P$). The time scale for commencement of bubble nucleation after contact is assessed considering the pressurization effects of liquid-phase expansion during development of such a thermal layer. The problem in such an assessment is one of determining the relief time and associated thermal layer thickness for the formation of critical size embryos (here called the critical thermal layer). For the case where the critical thermal layer is developed before pressure relief (for example, a fluid with a high diffusivity and a low velocity of

[a] Called Refrigerant-22 or Freon-22, the chemical formula being CHClF_2 .

sound, and a system with a relatively long distance to the free surface), a vapor explosion is considered to be temporarily suppressed if the pressurization exceeds the critical thermodynamic pressure, P_c .

For the opposite situation where rapid pressure relief occurs, the time period (t_n) elapsed between contact and the inception of a critical size bubble embryo is considered^[35-37] to be governed by the sum of three waiting times

$$t_n = t_a + \frac{1}{JV} + \frac{2\ell}{c} \quad (5)$$

where t_a is the acoustic relief time for liquid phase thermal expansion (which occurs during the initial period of contact between the hot and cold fluids), $\frac{1}{JV}$ is the waiting time until bubble nucleation, and $2\ell/c$ is the time period necessary for a pressure gradient to develop in the vicinity of the nucleated bubbles so that inertial bubble growth is possible. In Equation (5), J is the nucleation frequency per unit volume, V is the bubble volume, ℓ is a characteristic distance to a free interface, and c is the velocity of sound.

The time for the vapor bubble to grow (t_g) from nucleation to the limit of its stable region can be calculated from the inertial bubble growth equation such that

$$t_g = \frac{R_b(t) - R_c}{\sqrt{2/3} (\Delta P / \rho_\ell)} \quad (6)$$

where

$R_b(t)$ = time-dependent bubble radius

R_c = critical bubble radius

ρ_ℓ = liquid density

ΔP = average driving pressure from bubble inception to the maximum stable bubble limit.

However, during this growth period additional bubbles can form such that if the contact temperature is considerably higher than the spontaneous nucleation value, the nucleation rate is rapid enough to cause bubble interference. Such a condition will lead to vapor blanketing between the two previously contacting liquids, which in turn reduces the energy transfer process.

To assess whether such vapor nucleation will lead to either explosive boiling or simple vapor blanketing of the hot surface, a maximum site density (based on pressurization sufficient to suppress further nucleation) is compared with an interference site density ($N = 1/D_B^3$). By evaluation of the maximum stable bubble diameter (D_B^2) from the ideas

outlined above, Henry et al^[35-37] found that larger-diameter cold droplets submerged in a hot liquid result in site density interference leading to protective vapor blanketing rather than explosive boiling. An analytic prediction of this behavior is shown in Figure 4 for single droplets of Freon-12 (cold phase) submerged in oil (hot phase) and compared with experimental data. With respect to large cold droplet systems, it is hypothesized that film boiling will occur at high interface temperatures because of a well-developed thermal boundary layer and the large frequency of nucleation. As a result, such large cold droplets should remain in a film boiling condition until either they break up into smaller droplets or film collapse of the surrounding hot fluid occurs. If, at that time, the interface temperature still exceeds that for spontaneous nucleation, a potentially explosive interaction is considered possible.

Several authors have critiqued the work of Henry et al^[35-37] and proposed alternate arguments for a period of stable film boiling for the condition of $T_I > T_{SN}$. Board and Hall^[38] have proposed that at temperatures above T_{SN} , rapid bubble growth and coalescence quickly leads to the formation of a stable vapor film which limits the vapor generation process (which agrees with Henry's arguments). However, they propose that at temperatures just below T_{SN} , bubble growth and coalescence conditions are such that the total volume of vapor generated is greater than that above T_{SN} ; thus, the condition where $T_I < T_{SN}$ should lead to a more energetic situation than when $T_I > T_{SN}$. Board and Hall^[38] consider the Leidenfrost point (T_{Leid})^[a], or minimum temperature for stable film boiling (assumed to be below T_{SN}), as a better indicator of a threshold temperature for an energetic interaction. Besides questions relating to the validity of the interface-spontaneous nucleation criterion, arguments have also been presented which are at variance with other aspects of the model and with the interpretation of associated simulant fluid experiments.

W. B. Hall^[44] has presented calculations for bubble growth with acoustic loading, indicating that it is not necessary to await relief in order for bubble growth to proceed, the time period being dependent on the site density (N). Such results are in basic disagreement with the arguments of Henry et al^[35-37] for suppression of nucleation due to acoustic loading. However, Hall's formulation appears to be correct since an acoustic loading term is coupled directly with the Rayleigh bubble growth equation. The acoustic loading term is given as

$$\Delta P = 4\pi N R^2 \dot{R} \rho c \quad (7)$$

[a] From a thermodynamic viewpoint, one estimate of the minimum wall temperature to sustain film boiling (that is the Leidenfrost temperature) is $27/32 T_c$ ^[39]. However, for a pool boiling situation the minimum temperature for film boiling may be somewhat higher for small spheres^[40] and large subcooling^[41], based on hydrodynamic theory. At this time, an *a priori* assessment of T_{Leid} cannot be made with confidence, although for well wetted systems, the thermodynamic approach appears to correlate data quite well^[42]. For poorly wetted systems, T_{Leid} may approach the saturation temperature T_{sat} ^[42,43].

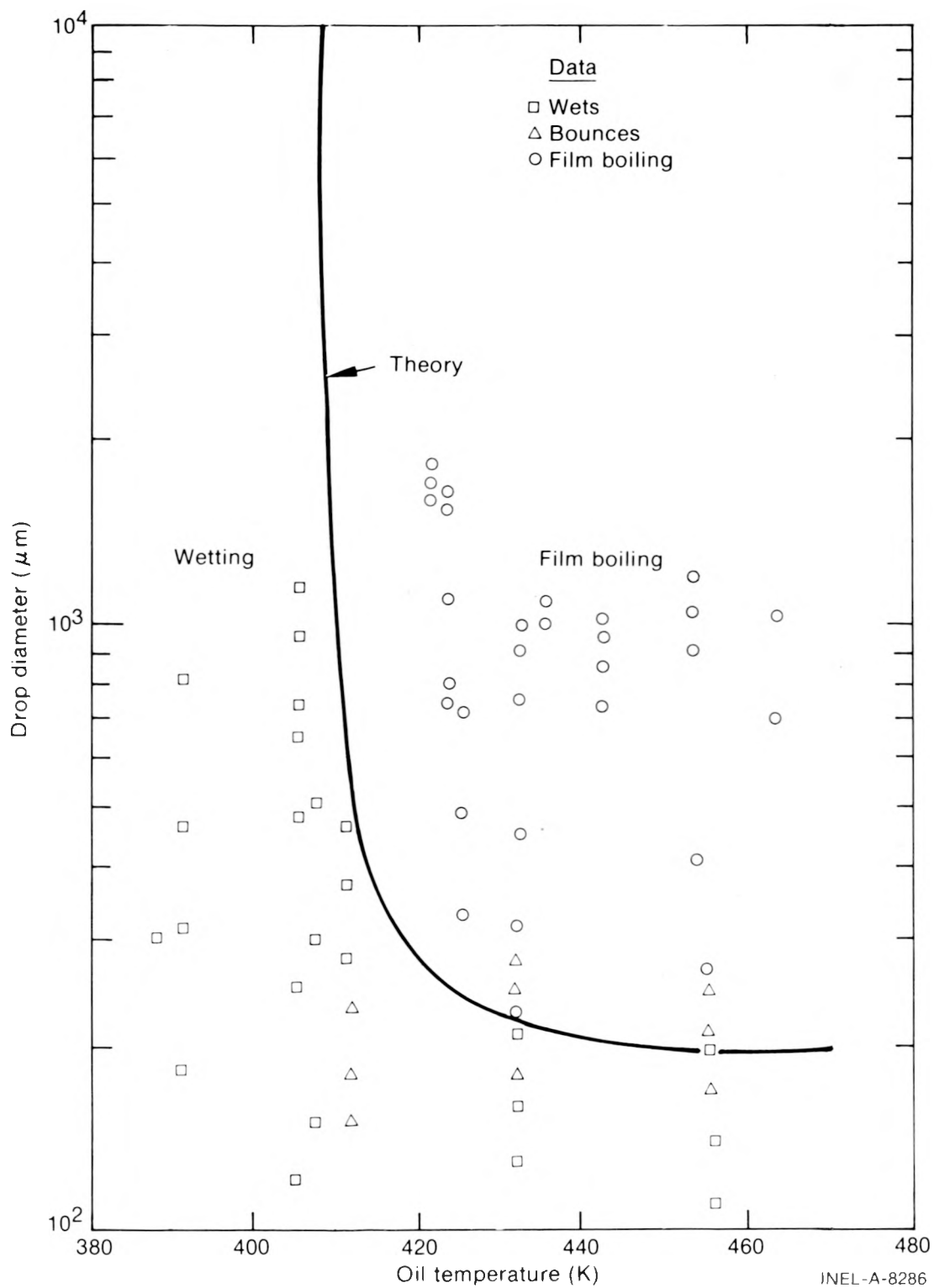


Fig. 4 Small drop interaction behavior for film boiling and capture of Freon-12 on a mineral oil surface^[37].

where

N = site density

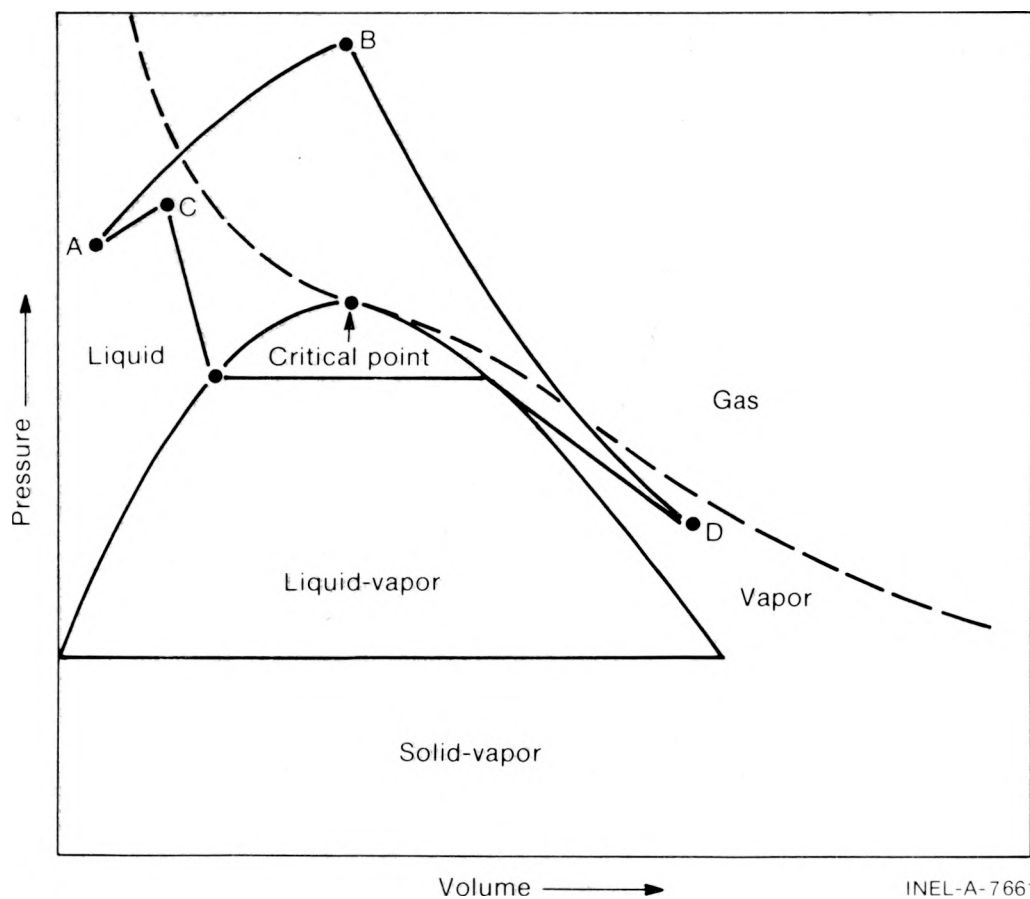
R = radius

\dot{R} = velocity

ρ = density

c = speed of sound.

Another consequence of the spontaneous nucleation model is that if the system pressure (P_{sy}) is above the thermodynamic critical value (P_c), discrete phase change will not occur; thus, an explosion is considered to be prevented if $P_{sy} > P_c$. However, as illustrated in Figure 5, work is a path function, such that rapid heating of a supercritical fluid, prior to inertial relief of the constraining system, can lead to an expansion process into the vapor regime which can be explosive, the rate processes being the determining factor.



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Fig. 5 Illustration of various expansion processes for a rapidly heated supercritical fluid (Paths A-B and A-C are prior to inertial relief), indicating work is a path function.

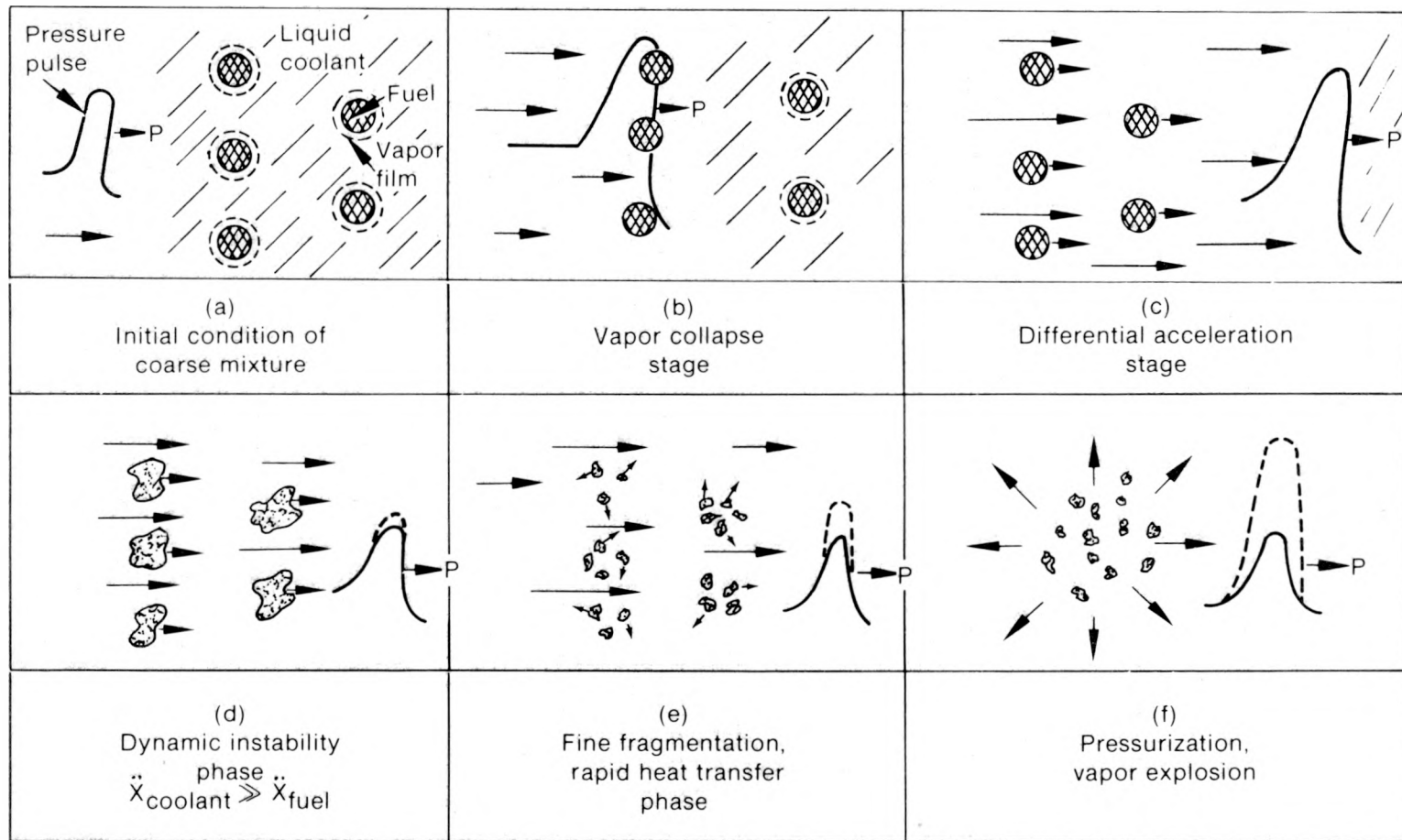
Other than Henry's Freon into oil (or water) studies (where the minimum Freon droplet size is assessed for explosive vaporization), no detailed coupled fragmentation-spontaneous nucleation model has been developed to date that answers questions concerning the mechanism and kinetics of the fragmentation-intermixing-heat transfer processes (for a large-scale system) versus the kinetics and energy associated with such nucleation. A complete description of the processes involved from nucleation through fragmentation, intermixing, and eventual explosion appears to be necessary at this time. Cho et al^[45,46] have begun to investigate such questions, particularly mixing requirements which are discussed in a later section.

Several other important factors have yet to be incorporated into this model concept with respect to assessing spontaneous nucleation for actual reactor materials and system conditions. For example, the work potential associated with a vapor explosion is mass-dependent, yet the amount of interacting material has not been discussed in the context of this model. With respect to the kinetics of phase change, it has been assumed that for perfect contact between two interacting fluids, Volmer's well-known rate equation applies, thus assessing homogeneous vapor nucleation for the liquid coolant but ignoring the effects of homogeneous solid nucleation in liquid fuel. In References 47 and 48 it has been demonstrated that Volmer's equation also describes the kinetics of solid phase nucleation in the melt and that under perfect contact quenching conditions, liquid UO_2 will undergo similar homogeneous solid crystal nucleation^[49-51]. This important effect has not been accounted for in the model or the simulant fluid experiments of Henry et al^[35]. It is felt that the effects of simultaneous solid- and vapor-phase nucleation for two dissimilar fluids have yet to be dealt with in a rigorous manner and that the present understanding of vapor nucleation from solid surfaces indicates that nucleation kinetics for such a simultaneous process may be quite different than for liquid-liquid systems.

Besides the concept that spontaneous vapor bubble nucleation is a necessary condition to cause explosive vaporization, Board et al^[38,52,53] have suggested an entirely different approach for explosive vaporization. Their model concept and variations of it are discussed in the following section.

2. PRESSURE-INDUCED DETONATION MODEL

Board et al^[38,52,53] have proposed the theory of explosive fuel-coolant interaction by pressure-induced detonation, similar to that of detonating chemical explosions. As illustrated in Figure 6, the model assumes that a strong shock front propagates steadily through a region of coarsely mixed molten fuel and coolant, the initial pressure trigger being considered sufficient to cause collapse of any preexisting vapor. As the pressure wave passes the interaction region, the flow velocity differential between the dense fuel and lighter coolant are considered sufficient to cause fine-scale fragmentation. As a result, the front leaves behind finely fragmented fuel in intimate contact with the coolant, eventually resulting in vaporization sufficiently rapid to cause shock pressurization and



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Fig. 6 Descriptive illustration of pressure detonation model.

explosion. Some uncertainties with respect to the model are: the source of the initial pressure pulse, the requisite condition of a predispersed coarse mixture, and the mechanism for rapid, fine fragmentation by dynamic instability.

At present, the requirement of rapid, fine fragmentation and intermixing is receiving considerable attention, since without such rapid fragmentation and intermixing, increased pressurization and eventual detonation ceases. The time for breakup is important to the analysis, since slow fragmentation (after the pressure pulse has traveled downstream of the interaction zone) would not result in superposition of pressurization, but rather a series of pressure waves which would eventually damp out.

To calculate the fragmentation time, the semiempirical relation of Simpkins and Bales^[54] was used for the breakup of a single droplet accelerated in a gas velocity field. The resulting breakup time is calculated to be

$$t_b = 44 \text{ Bo}_{L-V}^{-1/4} \sqrt{\frac{\rho_d}{\rho_f}} \left(\frac{R_d}{V_r} \right) \quad (8)$$

where

ρ_d = drop density

ρ_f = fluid density

R_d = drop radius

V_r = velocity of the drop relative to the surrounding medium

Bo_{L-V} = bond number for a liquid-vapor system which is calculated as

$$\text{Bo}_{L-V} = \frac{\rho_d g R_d^2}{\sigma} \quad (9)$$

where

σ = interfacial tension

g = acceleration of the drop due to drag.

To estimate the relative velocity after the shock front passes the drop, the mixture velocity at the Chapman-Jouguet point is used. For gas shocks, this is satisfied only if the drop is accelerated by the drag of the surrounding fluid and the fluid velocity remains constant through the fragmentation zone. However, these assumptions may not apply to the liquid-liquid system. To account for the situation of a liquid-liquid mixture, Bankoff et al^[55,56] suggested that a modified Bond number (Bo') be used, such that

$$Bo'_{L-L} = Bo_{L-V} \left[\frac{(\rho_d - \rho_f)\sigma_d}{(\sigma_d - \sigma_f)\rho_d} \right] \quad (10)$$

where σ is the surface tension of the droplet (d) and fluid (f). Such a correction is relatively minor in importance. However, Bankoff et al^[55,56] also investigated the effects of mass ratio on the relative velocity obtained between the droplet and coolant fluids and the time of breakup. Basically, a momentum balance is written for the coolant and droplet fluids to determine the time-dependence of the relative velocity, V_r . The resultant expression for this velocity is

$$\frac{1}{V_r} \frac{dV_r}{dt} = - \frac{C_D A \rho_f}{2} \left[\frac{1}{m_d} + \frac{1}{m_f} \right] \quad (11)$$

where

C_D = drag coefficient (assumed to be 2)

A = projected area of the drop

m = mass.

Considering both the mass effect for a multiple droplet configuration and the Bond number for liquid-liquid systems, the time for breakup is calculated as

$$t_b = 33 Bo'_{L-L}{}^{-1/4} \sqrt{\frac{\rho_d}{\rho_f}} \left(\frac{R_d}{V_r} \right) \left(1 + \frac{m_d}{m_f} \right). \quad (12)$$

As can be seen, the mass ratio effect predominates over that introduced by the modified Bond number for liquid-liquid systems.

A comparison of the time for breakup using the Board-Hall versus the Bankoff assumptions indicated that the breakup time estimated by Board and Hall (single droplet) can lead to fast fragmentation which is necessary for sustaining a detonation wave, whereas if the mass ratio (multiple droplets) effects are considered, the time for breakup is much slower and does not meet the criteria for sustaining the pressure wave. However, it is

important to note that the semiempirical relation of Sempkins and Bales^[54] used in both calculations was developed based on data for liquid drop breakup in a gas environment; thus, Bankoff's arguments may not apply to the liquid-liquid system.

Contrary to such arguments that hydrodynamic fragmentation in a liquid-liquid system is more difficult to achieve than for the gas-liquid case, Patel and Theofanous^[57] have shown experimentally that hydrodynamic breakup of mercury in water, under shock tube conditions, leads to rather efficient fragmentation, which appears more likely to occur than the expected results based on the theory for gas-liquid systems. For liquid-liquid systems Taylor-type^[a] instabilities are considered to be the controlling factor.

Further investigations with respect to liquid-liquid systems appear to be warranted since without a quantitative knowledge of such fragmentation, the detonation concept cannot be accurately assessed. It is important to note that thermal effects should be accounted for in any final assessment of the fragmentation process since, in reality, a highly nonisothermal situation exists.

Williams^[58] also investigated the assumptions of the Board-Hall model and concluded that the probability of fine-scale fragmentation is greatly overestimated. His critique was made based on an assessment of the magnitude of the initiating pressure shock necessary to accelerate the fuel to a velocity corresponding to the Chapman-Jouguet point. For the $\text{UO}_2\text{-Na}$ fluid system, an initial pressure pulse of 80 to 700 bars was assessed, corresponding to a vapor void fraction of 0.5 to 0.1, respectively. The magnitude of such a pulse implies that the initiating or trigger event would be difficult to obtain and hardly less destructive than the vapor explosion itself. For heavy metal-water systems similar results can be expected, since such material properties as the speed of sound and isentropic bulk modulus are not that dissimilar from the $\text{UO}_2\text{-Na}$ system. Williams also discussed the dispersive characteristics of shock waves in the context of the Board-Hall model. He points out that sharply defined pressure waves undergo multiple partial reflections at the interface between mixture constituents, resulting in an attenuated wave. Multidimensional effects must also be considered with respect to reactor systems. Investigations^[58,59] of the Board-Hall assumptions also indicate that the reaction zone must be rather large, on the order of reactor systems dimensions; thus, the fact that most small, out-of-pile experiments do not result in shock-type vapor explosions may not be relevant to the question of whether such explosions can occur in a nuclear reactor. Recent calculational results of Sharon and Bankoff^[59] indicate that for high pressure shocks (~ 3000 to 8000 atm), a rather long relaxation length (several meters)^[b] is required for good intermixing of fuel and coolant (the relaxation length being defined as the distance from the leading edge of the shock front to the point of velocity equilibrium between fuel and coolant). With respect to geometry

[a] A Taylor instability is that which is due to an acceleration perpendicular to the interface of two fluids of different densities, where relative velocity effects between the fluids are unimportant.

[b] Dependent on the drag coefficient, particle (drop) size, densities, and breakup time.

considerations, it thus appears that a preliminary critique of the detonation concept indicates rather large system dimensions would be required (for reactor fuel-coolant materials) to meet detonation conditions (that is, dimensions greater than those common to reactor design concepts). Prototypic experiments may ultimately be necessary, although the cost would be phenomenal. Therefore, continued analytical investigation at this time appears to be appropriate.

Gunnerson and Cronenberg^[40] have investigated the initial blanket-coarse mixture geometry assumed by Board-Hall, where a vapor blanket is considered to initially surround the fuel particles. The results of their work are shown in Figure 7 and indicate that particle diameter has a large effect on the minimum temperature necessary to sustain film boiling. This minimum temperature is predicted to increase with decreasing particle size and is estimated to be quite large for particle sizes of interest in MFCI analysis. As a result, the initial vapor blanketing condition assumed by Board and Hall may be unrealistic, depending on the particle size characterization assumed for the initial coarse mixture. Also, it should be noted that many dropping experiments of molten metals into water^[2,7,60-62] have resulted in extensive fragmentation in the absence of any significant velocity differential. As discussed in the following section, other heat-transfer-governed mechanisms (for example, boiling and solidification) may account for a rapid fine fragmentation-intermixing process, with attendant rapid heat transfer sufficient in nature to induce acoustic pressurization of the coolant and eventual downstream explosion. If it is demonstrated that this is true, the rather severe initial pressure trigger assumed by Board may not be necessary. It is suggested here that the kinetics of such alternate fragmentation mechanisms be investigated in the context of this model.

Recently, Anderson and Armstrong^[33] have proposed a model similar to that of Board and Hall^[52]. They consider that a vapor explosion occurs as a result of three independent steps: (a) an initial mixing phase, (b) a trigger and growth phase, and (c) a mature phase in which a shock wave accelerates the two liquids into a collapsing vapor layer, causing high velocity impact which finely fragments and intermixes the two liquids.

Of particular interest are the experimental results of Anderson and Armstrong^[33] which led to this concept. In one series of experiments, unrestrained drops of a hydrocarbon refrigerant (R-22) were poured into a water-filled container. The results of these tests showed that:

- (1) Pressurization rise times are relatively slow (0.5 to 4 ms)
- (2) The measured pressure history is strongly influenced by the geometry of both the water-filled tank and the Freon-22 mass
- (3) Interaction behavior changes at a water bath temperature of about 75°C
- (4) Peak generated pressures at a given delay time were doubled when a small quantity of a dye was added to the Freon-22

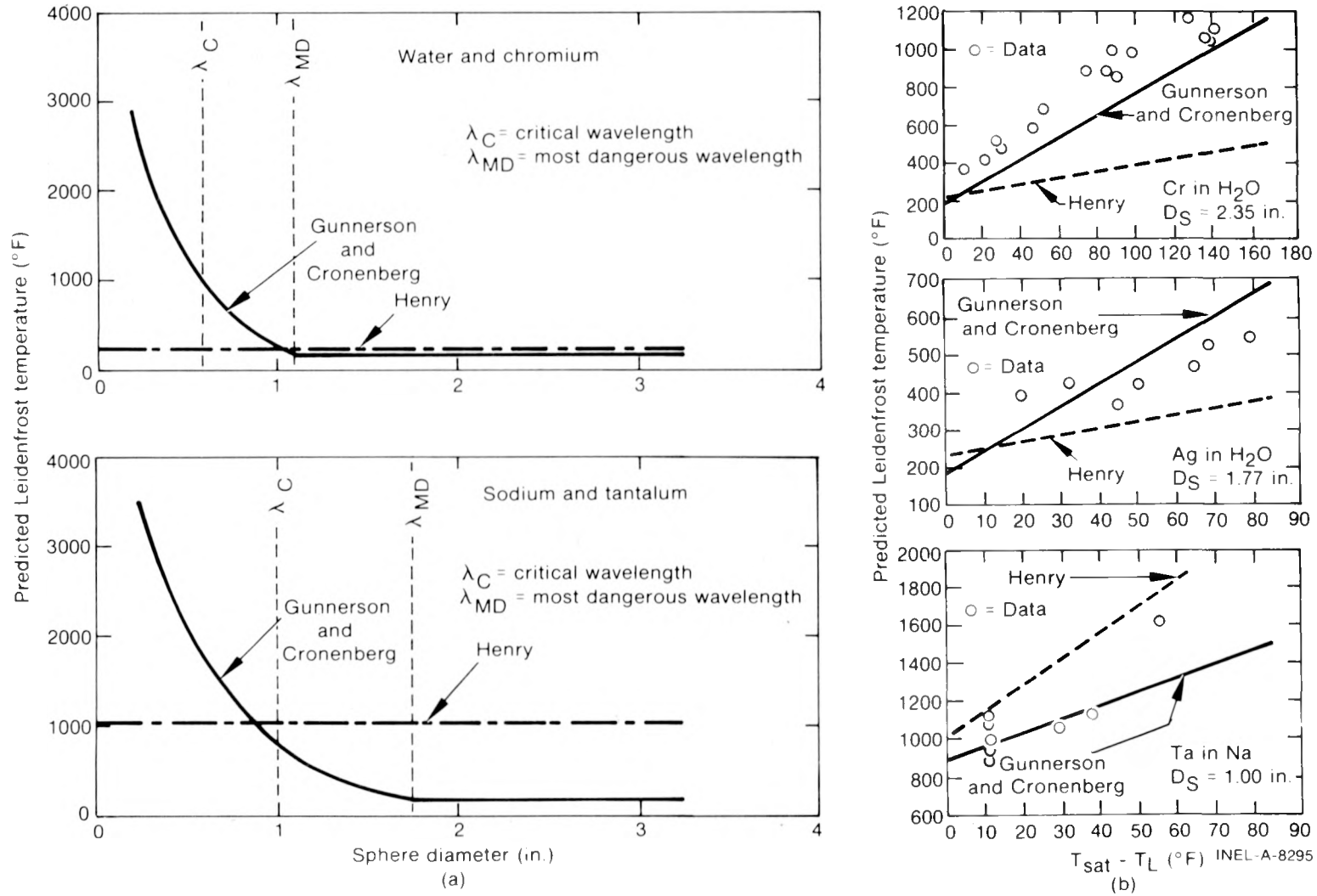


Fig. 7 Predicted Leidenfrost temperature versus (a) sphere diameter, and (b) degree of subcooling for three metal-coolant systems[40].

- (5) Delayed, high pressure events occurred in all water tests with water temperatures between 75°C and the maximum attainable system temperature of 99°C.

Such results indicated two types of interactions due to surface boiling characteristics. For the high temperature experiments, a period of film boiling enabled the R-22 mass to deeply penetrate into the water before a reaction was initiated, such that the inertial constraint of the water depth contributed to the generation of high pressure (rather than attributing this to the criterion of $T_I > T_{SN}$). Thus, Anderson and Armstrong^[33] postulated that high pressure explosions might also be produced with somewhat lower temperatures if R-22 was suddenly released well below the water surface. To test this hypothesis, R-22 was fully submerged in water by first enclosing it in a rubber prophylactic. The results of such constrained tests can be summarized as follows:

- (1) Subsurface release of Freon-22 into water below 60°C produced a qualitatively different kind of reaction than release into water above 70°C
- (2) Low temperature reactions were characterized by the immediate interaction at the Freon-water interface
- (3) High temperature reactions proceeded in two steps: first, the Freon-22 surface went into a film boiling condition; second, film destabilization by a surface mixing wave resulted in explosive reaction
- (4) The peak pressures in each test were directly proportional to the delay time between the vapor film formation and the appearance of the mixing wave
- (5) The relative efficiency ranged from 5% in low temperature experiments to 60% in high temperature experiments.

Although the conditions proposed for explosive interaction are consistent with such experimental findings, so too is the spontaneous nucleation concept, in that the high temperature tests were the most violent and satisfy the condition that $T_I > T_{SN}$. However, a thermodynamic prediction of the destabilization temperature for film boiling can be of similar magnitude as the threshold temperature for spontaneous nucleation^[42]; thus, such experiments can be interpreted in light of both factors. The fact that a wave-type disturbance appeared to trigger events lends added support to the shock-induced film boiling destabilization concept. Although Anderson and Armstrong^[33] present calculations supporting fine-scale intermixing of the two fluids, questions arise as to the assessed mixing energy requirements and the kinetic energy available upon vapor film collapse. This uncertainty arises as a consequence of assessing impact velocities and extent of fluid intermixing at the time of interaction.

Besides pressure or shock-wave-induced film boiling destabilization as a trigger for violent fuel-coolant interactions, Gunnerson and Cronenberg^[40,42] have indicated that such destabilization can also be induced by thermal conditions where an assessment of the minimum temperature for film boiling is assessed from thermodynamic considerations. The results of their work indicate that a strong shock wave may not be a necessary condition to cause initial vapor collapse, although such a shock wave may be necessary for fine-scale fragmentation and intermixing requirements.

From the preceding discussion it is apparent that a number of questions remain relating to the previously discussed model concepts for vapor explosion. Such questions are summarized as follows.

3. SUMMARY OF UNRESOLVED QUESTIONS

Some important questions which have not been resolved to date with respect to interpretation of experimental and modeling results are:

- (1) Did the experiments of Armstrong et al^[31,34] with UO_2 into Na produce explosions similar to the Na into UO_2 tests?
- (2) Are dynamic surface tension effects for the R-22/water experiments significant; that is, can the low temperature explosions be attributed to a low spontaneous nucleation temperature due to interfacial surface tension effects?
- (3) Is the interpretation of an interaction temperature valid; that is, at the end of a delay time, is the interaction initiated at the spontaneous nucleation temperature or at some threshold temperature at which film boiling becomes unstable?
- (4) Does a one-step, bulk-type interaction occur, as opposed to the propagating concept?
- (5) Is a preexisting vapor phase a necessary condition for efficient intermixing?
- (6) What effect does surface solidification of the hot phase, for reactor-type materials, have on the explosion process?
- (7) Is hydrodynamic fragmentation greater or less for liquid-liquid systems compared with gas-liquid systems?
- (8) Which factors primarily influence fragmentation and intermixing?

Although an answer to each of the above questions is important to a basic understanding of the factors influencing vapor explosions, the question of what factors primarily govern fine-scale fuel fragmentation and intermixing with coolant is considered to be of primary importance since such phenomena form an integral part of the vapor explosion process. Indeed, it is generally accepted that fragmentation and intermixing are necessary conditions for explosive vaporization. As a result, the fragmentation process and, more recently, intermixing considerations have received considerable attention in vapor explosion research. The following section discusses these two interrelated phenomena.

IV. FRAGMENTATION AND INTERMIXING CONSIDERATIONS

Although fragmentation and intermixing may not be sufficient in themselves to cause explosive vaporization, it is clear that a large effective heat transfer area between fuel and coolant must be generated in a rapid coherent manner if explosive vaporization is to occur. A discussion of these two important considerations is presented.

1. FRAGMENTATION

A rather extensive theoretical and experimental effort has been devoted to understanding the fragmentation process. Some of the more important modeling and experimental developments are reviewed considering four general categories, namely those categories that consider either hydrodynamic, boiling, internal pressurization, or solidification as governing effects. In addition, vapor blanketing effects are also discussed in this section in the context of both fragmentation and intermixing. Models which have been discussed in a previous paper^[4] are only briefly covered here, whereas the more recent developments and experiments are discussed in greater detail.

1.1 Hydrodynamic Effects

If a molten droplet is subjected to velocity induced surface forces sufficient to overcome the cohesive effects of surface tension, breakup of the droplet may occur. The potential to cause hydrodynamic breakup can be expressed in terms of the ratio of inertial to surface tension forces, which is commonly called the Weber number^[a].

$$We = \frac{\rho_c DV^2}{\sigma} \quad (13)$$

where

ρ_c = coolant density

D = diameter of droplet

V = velocity of droplet

σ = surface tension of droplet.

[a] The Bond number, Bo (that is, the ratio of buoyancy to surface tension forces), can also be used to assess hydrodynamic breakup and is related to the Weber number as $3/4 C_D We = Bo$, where C_D is a drag coefficient.

In some of the earliest experiments on impact fragmentation, performed by Ivins^[60], low-melting-point metals (tin, lead, bismuth, and mercury) were dropped from different heights into water at room temperature. Some of the results, shown in Figure 8, indicate that a fragmentation threshold occurs at a critical value between 10 and 20, which corresponds to that suggested by Hinze^[61]. Cho^[62] conducted similar experiments for the same materials while varying the quenching conditions and minimizing impact effects (that is, the Weber numbers were below the critical range). His work is summarized in Figure 9, which shows that thermal effects also influence the extent of fragmentation and may override those due to dynamic impact. This conclusion is also consistent with the recent experimental evidence of Lazarrus et al^[63], which showed that extensive fine

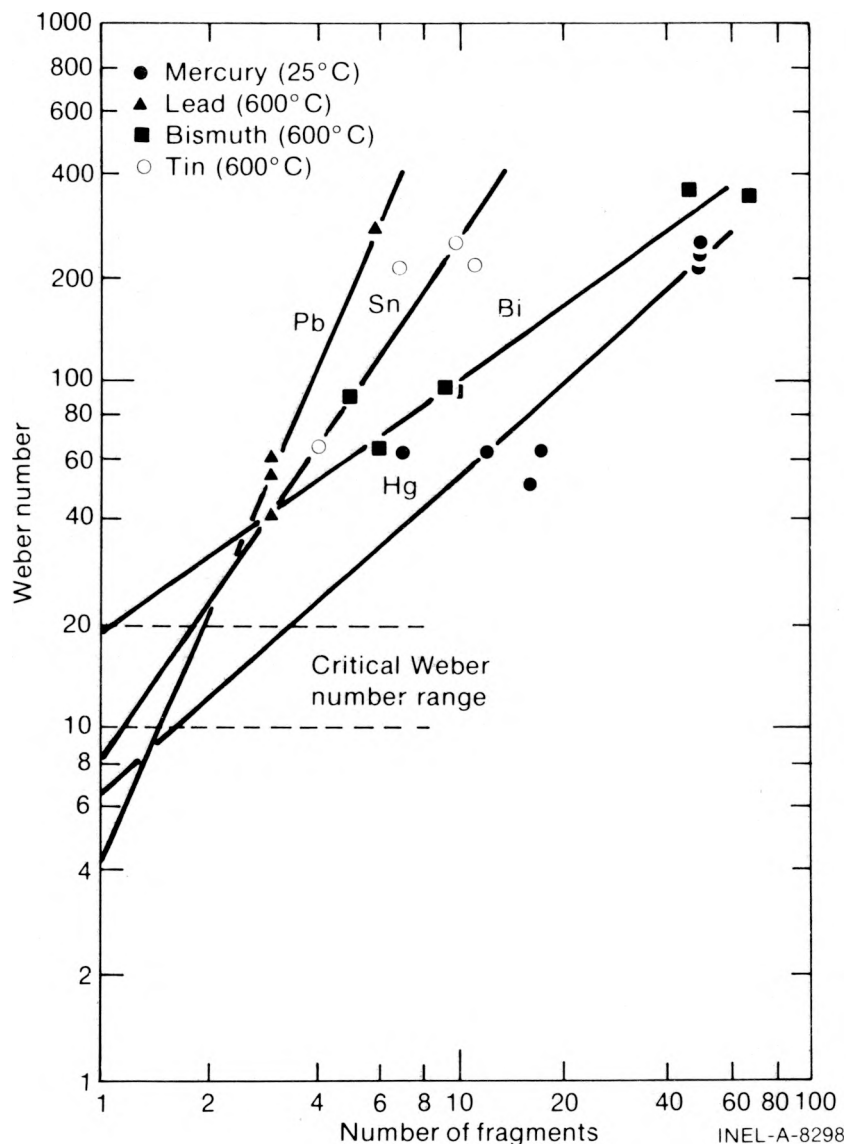


Fig. 8 Plot of Weber number versus number of fragments for molten metals dropped into room-temperature water^[60].

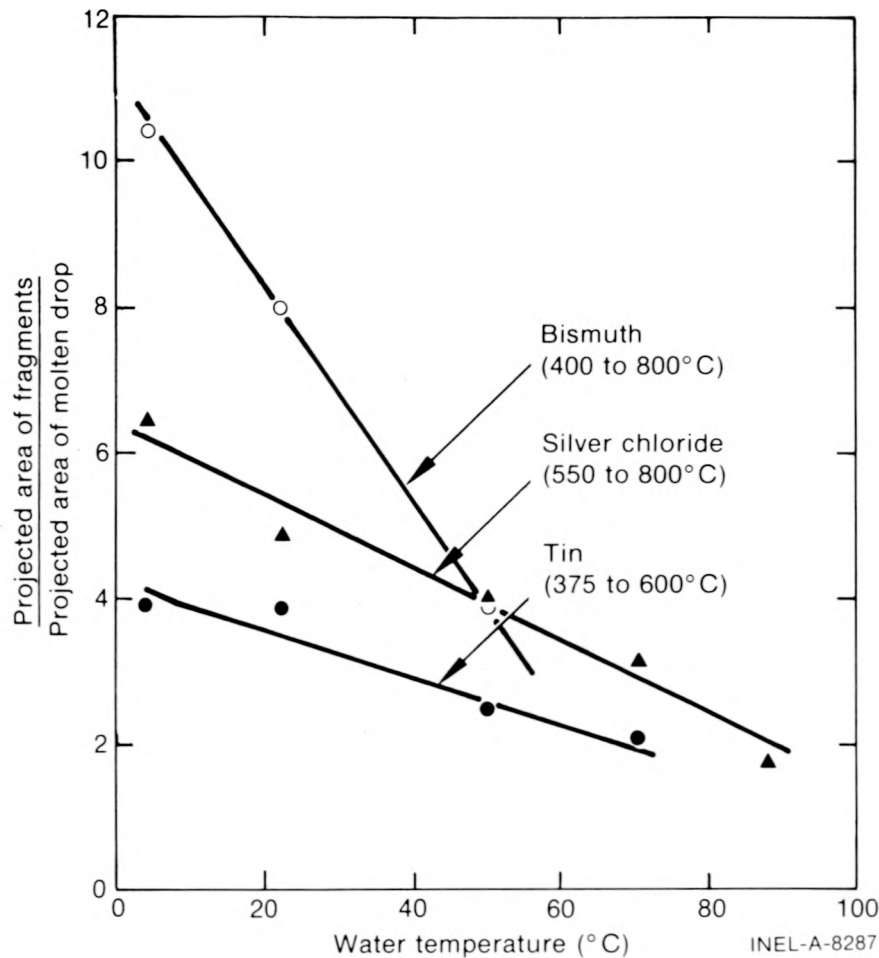


Fig. 9 Fragmentation of molten metals dropped into water, illustrating effect of coolant subcooling^[62].

fragmentation of molten Al_2O_3 occurred when in an inert-gas atmosphere of argon at 2.5 torrs. Such fragmentation was attributed to thermal stresses, and will be discussed later.

Helmholtz (parallel to the contact plane) and Taylor (normal to the plane) instabilities have also been suggested as breakup mechanisms^[64-67]. However, since the breakup of hot molten materials often occurs in the absence of a significant velocity differential for dropping experiments^[2,61,62,68], in-pile fuel rod failure tests^[69-71], and for true vapor explosions^[1,2,7,16-19], this indicates that the fragmentation process is not likely to be controlled by hydrodynamic considerations alone^[a], although such effects may enhance breakup. The occurrence of fine-scale fragmentation by thermal means appears likely^[1,2,4,7,60,62,64,67-69].

For jet-type fuel release from a failed rod, Weber numbers on the order of 10^3 are expected, based on ejection studies given in Reference 72 for a breach diameter of 0.25 cm

[a] Hydrodynamic fragmentation may, however, be of primary importance to some situations, but foundry accidents and the SL-1, SPERT-ID, and BORAX-I explosions do not indicate this conclusively.

and a velocity of 600 cm/s. However, Bradley and Witte^[73], in experiments with mercury jets into water, have shown that although some breakup occurs, it is much less than that for heated jets. Therefore, although the disruptive forces of impact and viscous drag may contribute to breakup, it appears that thermal effects play a more important role for high temperature materials.

Several other authors^[74-76] have considered various hydrodynamic-type fragmentation-intermixing models; the most detailed with respect to MFCI phenomena is presented by Roberts^[75]. He considers that the interface between two liquids will increase exponentially with time when one fluid is entrained in the other, due to the presence of spiral vortices (Figure 10) which result from an 'assumed' jetting process. Considering that surface and friction forces can be neglected and the relative velocity spatial distribution is the same at all times, the turbulent velocity is considered to be proportional to the square root of the energy content of the vortex. Based on this model concept, Roberts developed a set of equations for the theoretical description of the increase in surface area (A) and found that

$$A = \frac{A_0}{(1 - Bt\sqrt{A_0})^2} \quad (14)$$

where A_0 is the initial interface area, and B is a constant (s/cm) dependent on a number of scaling factors concerning the kinematics of turbulence and associated energy dissipation processes. Equation (15) predicts an "explosion" of the surface area and completion of energy release in a finite time given as

$$t = \frac{1}{B\sqrt{A_0}} \quad (15)$$

Two obvious questions with respect to this model are how the arbitrary constant, B, is to be assessed and how the energy needed to initiate the vortices is generated. In addition, the assumption of a vortex-type geometry for the intermixing of two dissimilar liquids may not be valid for the case where rapid heat transfer and phase change occur, with vaporization of the cold fluid and solidification of the hot material. It is therefore felt that the fragmentation-intermixing process of two liquids with highly dissimilar thermal conditions is not primarily governed by the formation of such vortices, although such a process may apply to the case of mixing two liquids at or near thermal equilibrium^[a].

A somewhat similar turbulent mixing model has been developed by Bruckner and Unger^[76]. They coupled the kinetic energy of the turbulent field with the heat flux between melt and coolant, assuming a certain degree of efficiency for the conversion of heat into mechanical energy. However, similar problems, as with Roberts^[75] model, exist with

[a] It is noted that if bubble growth and collapse are assumed, such collapse might initiate the formation of such a vortex^[77].

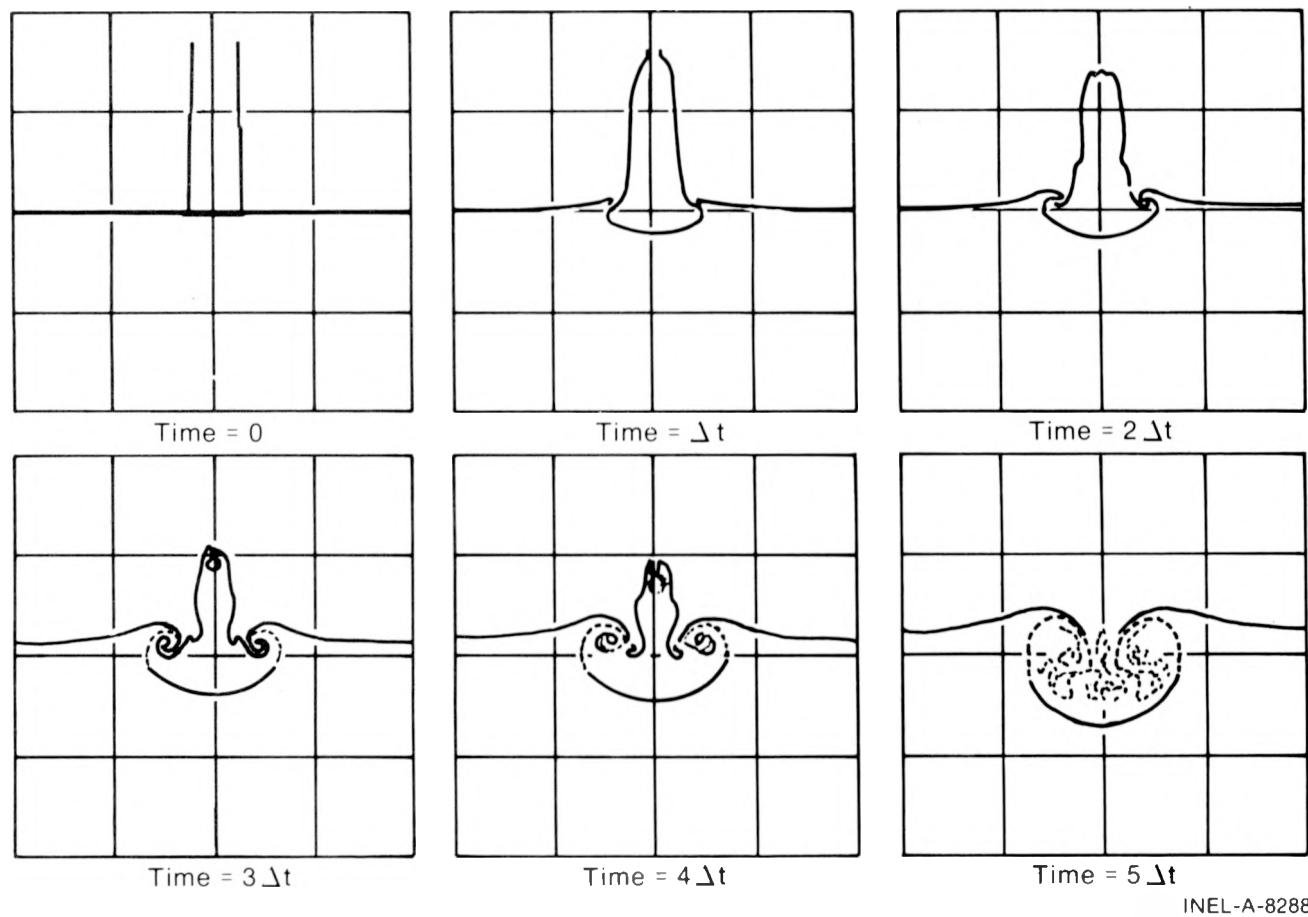


Fig. 10 Computer simulation of liquid jet penetration into another fluid^[75,86].

respect to assessing undetermined scaling constants. Until either experimental or theoretical values can be determined with respect to such constants, such a fragmentation model is of little engineering utility.

Besides such hydrodynamic considerations, the effects of bubble growth and collapse have received considerable attention as mechanisms for fine-scale breakup of molten fuel in coolant. These effects are discussed in the following section.

1.2 Boiling Effects

Vapor bubble growth and collapse have received considerable attention as a mechanism for fragmentation of molten materials quenched in coolant. Swift and Baker^[68] were the first to hypothesize that fragmentation might occur in the hydrodynamically violent transition and nucleate boiling regimes, based on their dropping experiments of various molten materials into water and sodium coolant.

In general, it can be said that the work potential for fragmentation can be related to some fraction of the bubble energy

$$E_b = \frac{4}{3}\pi R_b^3 |\Delta P| \quad (16)$$

where R_b is the maximum bubble radius and ΔP is the difference between the bubble and ambient coolant pressures. Various studies have been made to evaluate this energy by assessing both R_b and ΔP from either theoretical considerations or experimental data. As mentioned, Reference 4 contains a description of some of the boiling-fragmentation models in connection with MFCI analysis for LMFBRs. In the present discussion primary emphasis is placed mainly on modeling and experimental work associated with water coolant.

As discussed in References 77-84, several variations of the bubble growth and collapse mechanism have been developed to describe fuel fragmentation. Usually, such modeling work has been performed in conjunction with small-scale, out-of-pile experiments with molten metal samples being dropped into water. Basically, such models consider that quiescent film boiling, if it occurs initially, is destabilized (owing to various hypothesized 'triggers'), resulting in bubble formation at the hot surface. During expansion, spherical geometry is assumed, such that bubble growth is described by the well-known Rayleigh equation (usually neglecting viscous and surface tension effects)

$$R \frac{d^2 R}{dt^2} + \frac{3}{2} \left(\frac{dR}{dt} \right)^2 = (P_b - P_\infty) / \rho_c \quad (17)$$

where

R = bubble radius

P_b = bubble pressure

P_{∞} = ambient pressure

ρ_c = coolant density.

Buchanan^[77,78] assumes adiabatic expansion so that the mass of vapor in the bubble is constant, while Caldarola and Kastenberg^[79] consider vapor addition. Following the growth stage, initiation of collapse is assumed when the bubble has penetrated into the cold surrounding coolant. This general description of the initial sequence of events is common to the models described in References 77-81; however, the assumed collapse and fragmentation mechanisms are somewhat different. Buchanan^[77] considers that due to the presence of a molten heating surface, asymmetry of the collapsing bubble occurs, forming a high velocity coolant jet^[85] which penetrates the hot surface. Such coolant penetration into molten fuel results in turbulent mixing (similar to that described by Roberts^[75] and Christiansen^[86]), increased heat transfer area, and the formation of a new bubble leading to eventual fragmentation by a cyclic process of bubble growth, collapse, and jet penetration. Parametric calculations were carried out for the case of a fuel type considered to be seven times more dense than water coolant. Results indicate that the ratio of pressures in successive cycles depends on how the coolant is vaporized; that is, whether by heterogeneous or homogeneous nucleation. For a system external pressure of one bar, the cyclic pressure ratio is calculated to be

$$\frac{P_i - P_0}{P_{i-1} - P_0} = \begin{cases} 6.67 & \text{(heterogeneous nucleation)} \\ 2.90 & \text{(homogeneous nucleation)} \end{cases} \quad (18)$$

and the kinetic energy of the jet produced upon collapse is approximately 0.44 times the energy of the ultimate bubble. As illustrated in Table IV, the model predicts a buildup of energy from a small perturbation to a rather energetic process, indicating that the model might be applicable to MFCI analysis. As discussed in Reference 80, film studies^[87,88] with simulant materials show an interaction process which is increasing with the time. Likewise, asymmetric vapor collapse in the form of jets has been noted experimentally^[89]. Results of the model indicate that the jet energy, and thus, the fragmentation process, decreases with increasing system pressure. Evidence of such an effect has been observed for volcanic hydro-explosions where violent eruptions occur at small sea depths^[90]. The consequence of this result is that if the pressure of the initial cycle is not relieved, a 'self-limited' MFCI will occur^[a]. However, it is noted here that since the entire vapor produced during each cycle is assumed to collect in a single bubble, the model should only apply to small masses. It is also felt that the rather turbulent jet collapse and mixing process may lead to multiple-bubble formation with resultant energy density dissipation rather than an increasing energy density process, which is a direct consequence of the single bubble concept. It is suggested that visual experiments be conducted with this critique in mind.

[a] This would imply that increasing reactor system pressure diminishes the probability of severe MFCI, which is a similar consequence of the spontaneous nucleation model, although based on different reasoning.

TABLE IV

ILLUSTRATIVE CALCULATIONS FOR BUCHANAN'S MODEL, ASSUMING A SYSTEM PRESSURE
OF ONE BAR AND A HEAT TRANSFER COEFFICIENT OF $10^6 \text{ J/m}^2 \cdot \text{s} \cdot \text{K}$

Cycle (i)	Energy of Bubble $E(i)$ (joules)	Final Radius of Bubble $R_m(i)$ (cm)	Elapsed Time $t(i)$ (s)	Mass of Coolant (kg)	Peak Pressure Difference at R_m $P_i - P_o$ (bars)	Impulse at R_m ($\text{N/m}^2 \cdot \text{s}$)
1	1.261×10^{-4}	6.673×10^{-2}	2.687×10^{-3}	2.176×10^{-11}	3.339	5.354×10^{-3}
2	3.747×10^{-2}	4.453×10^{-1}	5.813×10^{-3}	6.487×10^{-9}	22.28	2.382×10^{-1}
3	$1.113 \times 10^{+1}$	1.971	1.197×10^{-2}	1.927×10^{-6}	148.7	1.060×10^1

Caldarola and associates^[79,91,92] have also considered the bubble growth and collapse mechanism of fine fragmentation. The simplified Rayleigh equation is again solved; however, the process is considered to be nonadiabatic such that an assessment of heating effects are determined from Schleutendahl's analysis^[93]. The extent of bubble growth is calculated until inertia forces are overcome, at which point the bubble collapse begins. Knowing $R_{b,max}$ and P_b at this time, the maximum bubble energy is determined. Results for the case of UO_2 and sodium at various temperatures are presented in Table V. Although the bubble pressure is maximum near the initial stage, the radius is minimum; thus, during some expanded stage, bubble energy is maximized. For sodium the maximum bubble energy is calculated to correspond to 52 atm pressure and a bubble radius of 3.14 cm. Since the temperature at this condition coincides with the minimum film boiling temperatures measured by Farahat^[94,95] in his tantalum-sphere sodium-coolant experiments, it was felt that the model might well explain fragmentation of UO_2 in Na (a similar analysis could be carried out for metal-water situations). However, it is noted that Farahat's experiments were carried out for solid tantalum spheres (1- to 1/2-in. diameter) with surface temperature conditions much lower than temperatures corresponding to molten UO_2 ; thus, his measurements of the minimum film boiling temperature may not accurately describe the actual situation for molten or solidified UO_2 at the small size of interest in MFCI analysis. It should also be noted that a rather large bubble size (3.14 cm) was predicted, which is greater

TABLE V
CALCULATION OF MAXIMUM BUBBLE RADIUS (R_b), PRESSURE
DIFFERENCE BETWEEN BUBBLE AND COOLANT (ΔP), MAXIMUM
BUBBLE WORK POTENTIAL ($\frac{4}{3} \pi R_b^3 |\Delta P|$), AND THE
APPROXIMATE ENERGY TRANSMITTED UPON BUBBLE COLLAPSE
(E_{tr}) VERSUS SODIUM TEMPERATURE^[79]

Temperature of Na (K)	R_b , maximum (cm)	$\Delta P \times 10^6$ (dy/cm ²)	$w_{max} \times 10^7$ (dy-cm)	E_{tr} (dy-cm)
550	1.73	0.92	1.995	$E_{tr} \approx 0.15 \times w_{max}$
650	1.85	0.924	2.43	$E_{tr} \approx 0.15 \times w_{max}$
750	2.025	0.934	3.25	$E_{tr} \approx 0.15 \times w_{max}$
850	2.26	0.92	4.45	$E_{tr} \approx 0.15 \times w_{max}$
950	2.58	0.85	6.12	$E_{tr} \approx 0.15 \times w_{max}$
1050	3.14	0.618	8.02	$E_{tr} \approx 0.15 \times w_{max}$
1150	4.29	0.026	0.858	$E_{tr} \approx 0.15 \times w_{max}$

than most experimental droplet sizes^[31,60,62,64,69,96-99]; thus, the vapor dome geometry assumed may not be realistic.

Caldarola and Kastenbergl^[79] also investigated the dynamics of bubble collapse in the form of microjets, illustrated in Figure 11. As a result of local impingement, an elastic wave

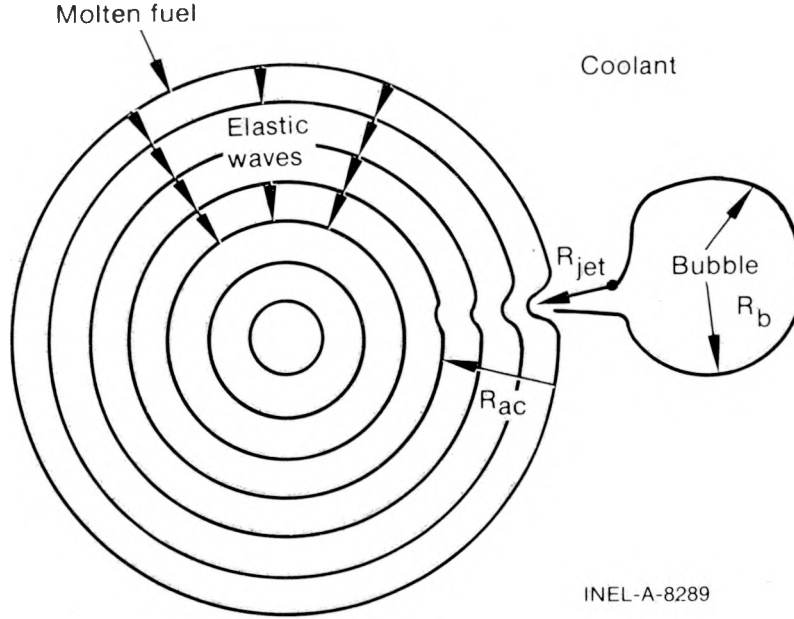


Fig. 11 Illustration of jet collapse mechanism.

is assumed to be generated in the molten fuel, with an associated acoustic energy (E_{ac}) per unit mass of

$$E_{ac} = \frac{1}{2} \left(\frac{\Delta p}{\rho_f c_0} \right)^2 \left(\frac{R_j}{R_{ac}} \right)^2 \quad (19)$$

where

R_{ac} = the distance of wave travel in the molten fuel

R_j = the jet radius^[100]

c_0 = the velocity of sound in the molten material.

As opposed to the maximum potential energy of the vapor bubble, the acoustic energy associated with jet impingement is essentially independent of the bubble size. As shown in the last two columns of Table V, the energy deposition in the fuel due to collapse impingement is only a small fraction of the bubble work and much less than that required to account for fine-scale fragmentation. However, it is felt here that this estimate of the energy transmitted to the fuel is more realistic than that assuming 100% conversion of the

maximum thermodynamic bubble work potential at the calculated departure radii. Thus, because of particle size to bubble radius considerations, it is felt here that the problem has yet to be treated in a realistic manner, and as such, the problem remains to define how much of the boiling energy is imparted to the fuel^[a].

A somewhat different approach to the bubble growth and collapse concept, which considers the additional effect of surface solidification during quenching, has been formulated by Benz, Frohlich, and Unger^[82-84]. Basically, the approach taken is to calculate the heat removal rate from the molten surface assuming a nucleate boiling heat transfer mode, where the bubble growth rate is calculated as

$$R_b(t) = 0.5 \left[0.234 \left(\frac{k}{\rho L} \right) \left(\frac{\rho \sigma}{\mu^2 \psi} \right)^{0.55} Pr^{0.33} \right]^{0.69} (T_w - T_\infty)^{0.69} t^{0.69} \quad (20)$$

where

σ = surface energy

μ = viscosity

ψ = bubble detachment angle

T_w = surface temperature

Pr = Prandtl number.

The other symbols are as previously defined. Equation (20) is based on Beer's^[101] curve fit of experimental bubble growth rate data from a hot plate. Bubble collapse is considered to occur when the inertial forces are overcome. Assuming that some fraction (η) of the maximum bubble potential energy is used in the creation of new surface area upon bubble collapse, the increase in surface area (F_s) can be expressed as

$$F_s = \frac{4\pi\eta(\Delta P)R_b^3}{3\sigma} \quad (21)$$

An iterative calculation is made for each bubble growth-collapse period, during which time an assessment is made of the heat transfer process associated with solidification of the molten material. As illustrated in Figure 12, such a process is exponentially increasing with respect to surface area generation (F_s/F_o) and exponentially decreasing with respect to the solidification process (illustrated as T_{sm}). Such a model, however, is somewhat parametric in nature due to the necessity of assessing such parameters as η and fraction of heat flux for

[a] It should be noted that the bubble growth rate is maximum during the initial stages of inertia-controlled growth; thus, the boiling forces imparted to the molten sample may be greater during the time of initial bubble growth rather than during collapse.

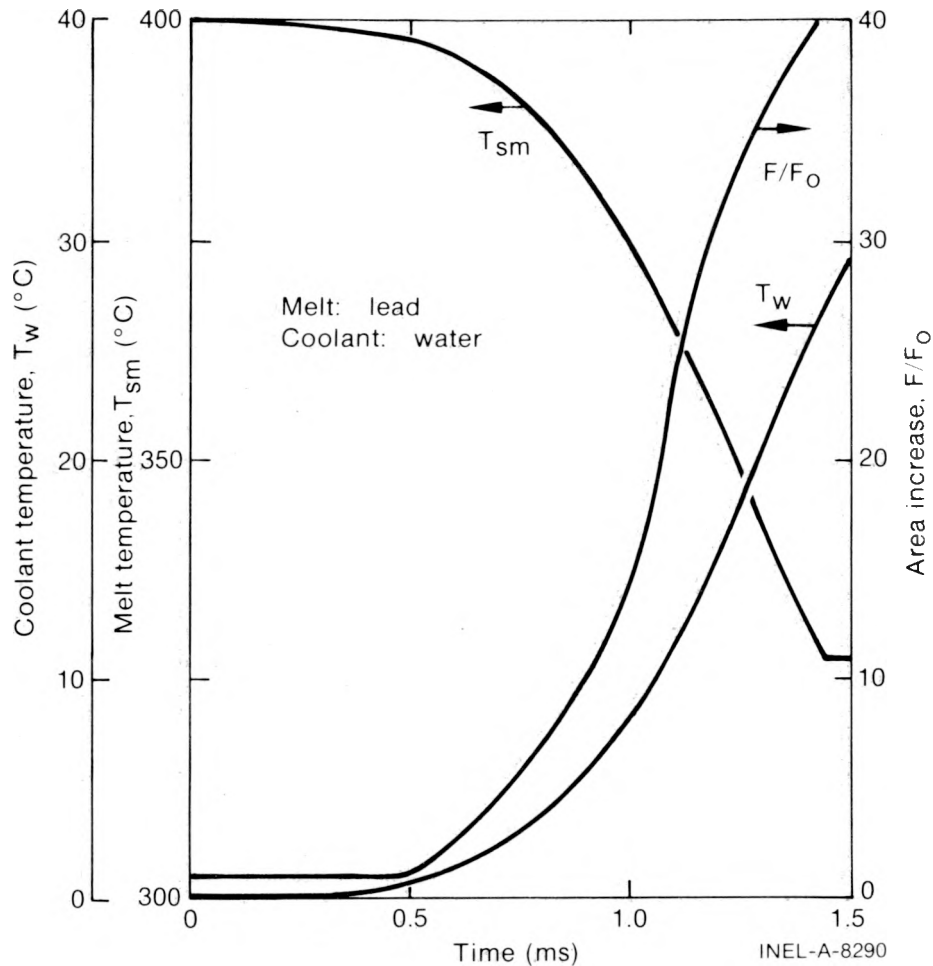


Fig. 12 Illustration of surface area generation (F/F_0), course of melt temperature (T_{sm}), and water coolant temperature (T_w) as a function of time^[82].

surface solidification. Comparison of the initial and final surface areas in controlled dropping experiments may, however, lead to an evaluation of such unknown parameters. An attempt at such an evaluation is presently being pursued, using Frohlich's experimental results^[102]. The basic assumptions of the model, however, are supported by several investigations^[41,88,103] where the extent of fragmentation correlates with the onset temperature for transition boiling and the fragmentation is accompanied by solidification.

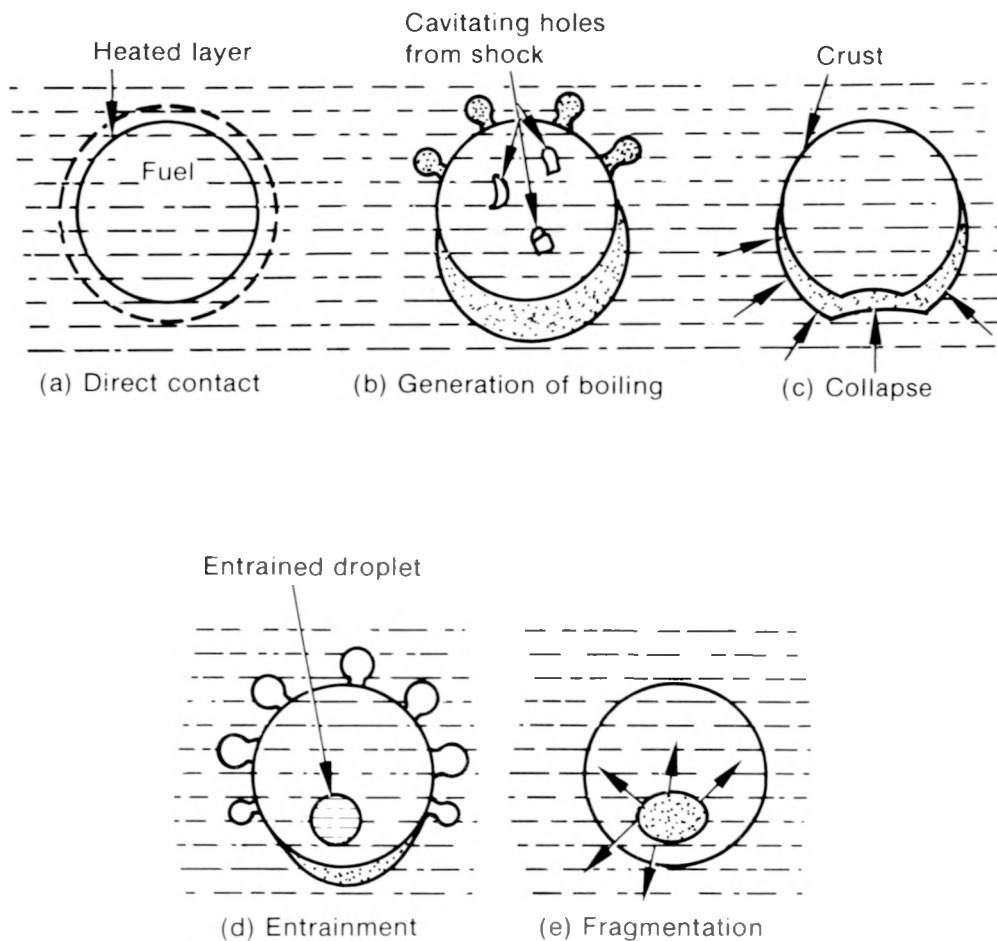
In addition to both hydrodynamic and boiling effects on the fragmentation process, internal pressurization within molten fuel, due to various sources, has also been considered as a potential initiator of fragmentation. A description of the various internal pressurization concepts is discussed in the following section.

1.3 Internal Pressurization Effects

Several mechanisms have been proposed which consider coolant encapsulation by the hot phase as the principal cause of fragmentation. Long's^[2] early experiments and those of

Hess and Brondyke^[104] indicated that small amounts of cold liquid were confined by the hot phase, resulting in an explosive molten aluminum-water interaction. Similar results were reported by Sallack^[105] with molten smelt and water and by Brauer et al^[106] with various molten metal-water systems. Sallack^[105], however, considers that a solid shell may form during encapsulation, with shrinkage having an additional stress effect.

Based on such experimental observations, Schins^[107] proposed a sequence of events which might lead to such encapsulation and fragmentation. Although a mechanistic description of events is proposed, no quantitative analysis of the fragmentation process is given. The hypothesized sequence of events is depicted in Figure 13 and can be described sequentially as:



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Fig. 13 Descriptive illustration of the Schins boiling model for fragmentation^[107].

- (1) Direct liquid-liquid contact, which results in a rapid temperature increase of the adhering coolant layer
- (2) Incipience of transition boiling, which imparts a shock to the molten fuel surface

- (3) Collapse of the vapor film, which initiates cavitation of bubbles within the molten droplet
- (4) Entrainment of coolant in such cavitated fuel
- (5) Fragmentation caused by explosive vaporization of entrained droplets.

Although such a sequence of events may occur, the question remains whether the process is sufficiently energetic to cause fine, coherent fragmentation, and whether the kinetics of events simulate experimental results. Until a quantitative model development has been made, such questions cannot be answered.

Besides the model concept of Schins, Kazimi^[108] proposed a cavitation-induced fragmentation process as depicted in Figure 14. As illustrated, internal acoustic cavitation

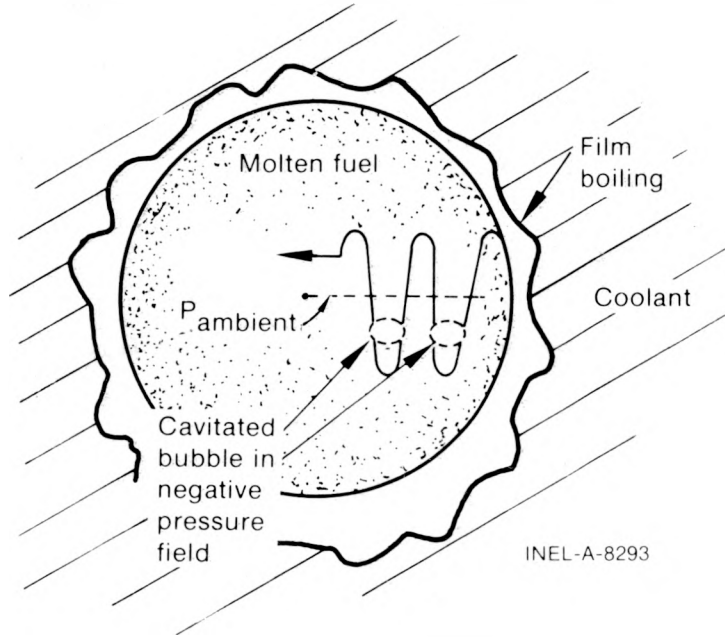


Fig. 14 Descriptive illustration of the acoustic cavitation model for fragmentation.

within the molten material is assumed to be induced by fluctuating pressure waves generated in the melt as a result of surface boiling and attendant film collapse. Two conditions necessary for fracture by cavitation are bubble inception and continued growth. In Reference 109 the minimum negative threshold pressure (P_{th}) for homogeneous cavitation is given as

$$P_{th} = \left[\frac{9.06 \sigma^3 / kT}{\ln \left(\frac{1.45 \rho N^2 \sigma^2}{P_{th} M^{3/2} RT} \right) - \frac{L}{kT}} \right]^{1/2} \quad (22)$$

where

- k = Boltzmann's constant
- N = Avogadro's number
- M = molecular weight
- L = latent heat of vaporization
- R = gas constant.

The other symbols are as previously defined. This condition was not satisfied in parametric calculations performed by Kazimi^[108]. However, it was postulated^[108] that due to the presence of impurities, cavitation may occur in laboratory experiments or under reactor conditions. An alternate criterion, suggested in Reference 110, is to consider the presence of small amounts of gas in the molten droplet. For this condition, the threshold pressure can be calculated based on the assumption of equilibrium between pressure and surface tension forces, and is given by^[111]

$$P_{th} = \Delta P + \frac{4\sigma}{3\sqrt{3} R_{gn}} \left(1 + \Delta P \frac{R_{gn}}{2\sigma} \right)^{-1/2} \quad (23)$$

where

- ΔP = difference between system and vapor pressure
- R_{gn} = radius of the gas nuclei (2.0×10^{-5} cm^[111]).

For molten UO_2 at a system pressure of 1 atm, P_{th} is approximately 20 atm, which is about the order of magnitude of the internal pressure amplitudes calculated by Kazimi^[108]. Thus, such cavitation may occur in molten UO_2 if extraneous gas is present. However, even if such a cavitated bubble could nucleate, it must survive and grow in a fluctuating pressure field, such that the rate of growth must be greater than the rate of collapse to achieve a sufficient buildup of bubble energy to cause fragmentation. Since no assessment of either the work potential to cause fragmentation or the growth kinetics was made, the validity of the model is difficult to assess, other than to say it does not satisfy homogeneous cavitation requirements.

Other general variations of the internal pressurization concept are the violent gas release model proposed by Epstein^[112,113] and the impulse-initiated gas release mechanism of Buxton and Nelson^[114,115]. As illustrated in Figure 15, Epstein's model assumes that dissolved gases are present in the molten sample. During rapid quenching it is assumed that the liquid becomes supersaturated, such that violent gas release causes

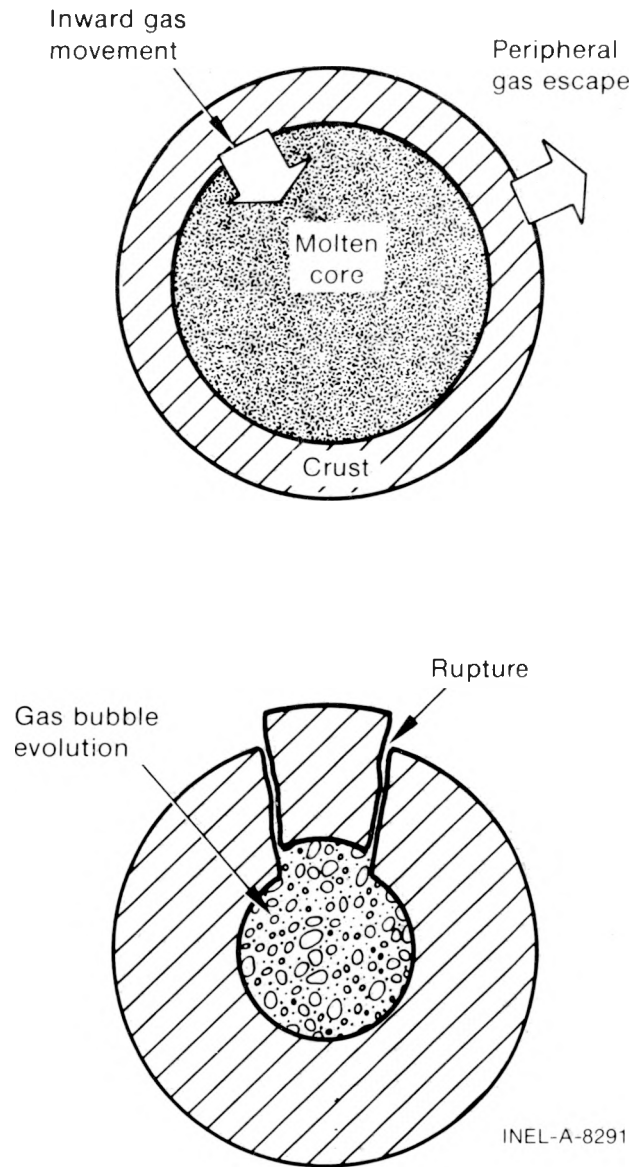


Fig. 15 Illustration of gas evolution model^[113].

fragmentation. To account for breakup by this mechanism requires that the melt be capable of dissolving gas without forming a stable phase and that the solubility decreases substantially at quenching temperatures. Although some low melting point materials may exhibit favorable solubility characteristics and disruption of molten steel (due to deoxygenation) has been observed experimentally^[116], most fragmentation metal-water experiments have been conducted in an inert atmosphere (He, Ar) where relatively low solubilities can be expected^[117]; yet extensive fragmentation still occurred. With respect to UO_2 , it has also been demonstrated by Gunnerson and Cronenberg^[118] that for the gases present in a reactor environment (for example, He-bond; Ar-cover gas; Xe and Kr fission products), solubility characteristics would not favor such a fragmentation mechanism.

Buxton and Nelson^[114] also proposed a variation of such a gas release mechanism by considering the internal bubble nucleation process to be impulse initiated. The principal characteristics of the model are:

- (1) Achievement of a large quantity of dissolved gas in the molten phase
- (2) Supersaturation of such dissolved gas as the melt is quenched by surface coolant boiling
- (3) Bubble nucleation by an applied impulse trigger
- (4) Rapid bubble growth resulting in fragmentation.

The concept that bubble nucleation can be impulse initiated certainly helps trigger such a gas release phenomenon. Impurities in the melt will also help initiate a bubble nucleation process. However, many experiments have been conducted in inert or evacuated environments with short heating times, in the absence of known impulse triggers, yet extensive fragmentation occurred. Likewise, since solubility characteristics are primarily controlled by the chemical nature of the gas-melt system and vary accordingly, a marked difference in the extent of fragmentation should be expected in accordance with solubility trends. However, as listed in Reference 7, the large body of fragmentation experiments does not lead to such a correlation, but rather leads to the conclusion that thermal versus chemical effects appear to govern fragmentation. Thus, although solubility and surface oxidation^[116,119] effects may contribute to breakup^[a], they are not considered here to be controlling factors that govern a wide range of metal-water or oxide fuel-sodium systems.

1.4 Solidification Effects

In the models described previously it is generally assumed that prior to and during fragmentation the quenched materials remain in the molten state. However, several experimenters^[63,67,69,106,120] have noted that rapid quenching leads to surface solidification. Such solidification may result in a thermal stress-initiated fragmentation process. Variations of thermal stress models are given in References 121-123.

To assess, in a quantitative manner, the potential for fragmentation by shell solidification, Hsiao et al^[121] analyzed the case of initially molten aluminum quenched in water. In Reference 122 such analysis was extended, considering the effects of temperature-dependent properties, compressibility of the inner molten core, various modes of surface heat transfer, and comparison with a UO₂-Na system. In Reference 122 it was found that the assumed heat transfer condition is of primary influence. For the Al-H₂O case, assuming

[a] It should be noted that surface oxidation may also influence the heat transfer process for particular systems (for example, copper quenched in water^[120]), which, in turn, may influence the extent of fragmentation.

perfect contact, the generated surface tensile stress was estimated to exceed the yield strength, demonstrating that surface rupture can be expected. However, for a film boiling heat transfer mode, surface fracture is not predicted. Qualitatively, this compares favorably with experiments in which molten aluminum was forcibly injected into water, with the probability of metal-coolant interaction and consequent fragmentation^[124], whereas dropping experiments with initial film boiling produced little breakup^[68]. For UO_2 fuel (with a much lower conductivity and, thus, a larger surface temperature gradient), the thermal stresses are considerably higher^[122] for equivalent quenching conditions. The effects of thermal shock-induced crack generation have been studied by Knapp and Todreas^[123]. It was again demonstrated that rapidly quenched ceramic fuels, such as UO_2 , would lead to crack formation; thus, the possibility for coolant encapsulation and further fragmentation.

Zyszkowski^[120,125] also considers that thermal interaction for copper-water systems are influenced by the solidification process of the molten copper. According to his hypothesis, an interaction will occur when the molten metal solidifies and some undefined internal mechanism in the metal causes fragmentation. Such a concept is based on experimental results where a thermocouple, which penetrated the copper drop at the time it reached the base of the container vessel, indicated a temperature of about 1300°C prior to explosive-type vaporization. However, violent interactions only occurred when the molten copper was heated in air, forming an oxide layer. Such an oxide layer may have a destabilizing effect on film boiling; thus influencing the interaction process. To test Zyszkowski's hypothesis further, a wide range of materials with very different melting temperatures would be needed. However, since the fuel surface temperature at the time of interaction is an important parameter in any discussion of MFCI events, his experimental technique is most pertinent.

The fact that the thermal energy is directly deposited in the form of stress within the hot phase, versus the boiling models where a significant fraction of the energy is imparted to the coolant upon bubble collapse, lends support to the stress-induced fragmentation concept. Likewise, some experimental evidence^[63,69] exists for such a mechanism for ceramics; however, most metals undergo plastic rather than brittle deformation so that many of the metal-water fragmentation experiments cannot be accounted for by such thermal stress models. In addition, an order of magnitude comparison^[51] of one-step mixing energy requirements ($E_{\text{mix}} \simeq 3\rho V^2/8t^2 R$; where V = initial volume, t = mixing time, and R = fragmented radius) with the elastic energy stored in a thermally stressed shell ($E_e \simeq \sigma_f^2 V/2Y$; where σ_f = fracture stress and Y = Young's modulus) indicates that intermixing cannot be accounted for by the stress mechanism alone^[a]. However, nucleate boiling with attendant rapid heat transfer may lead to both sufficient thermal stress and vapor production, such that the latter effect can sufficiently reduce the mixing energy requirements; thus, thermal stress may initiate breakup, whereas vapor production leads to intermixing.

[a] The concern of energy requirements for intermixing is not limited to the solidification concepts alone, but also applies to the fragmentation models discussed previously.

One of the principal concerns of the shell solidification concept is whether or not crystallization occurs at the quenching surface for the times of interest in MFCI analysis (that is, on the order of several milliseconds). In References 49 and 50 various aspects of crystallization kinetics (that is, the rate of solid crystal nucleation and the rate of growth of solid in its melt) were investigated and compared with the maximum rate of solidification heat transfer for good fuel-coolant contact. Results indicate that for good quenching conditions, surface crystallization of UO_2 commences almost immediately (within 1 or 2 ms). This is of importance not only to fragmentation analysis, but also to overall modeling of phase transformation kinetics, particularly in the context of the spontaneous nucleation model where Volmer's theory is used to describe phase change kinetics in the coolant but has not, to date, been considered with respect to solidification of the fuel in the overall model.

From the discussion of fragmentation models, it can generally be summarized that if either coolant vapor or inert gases blanket the fuel surface, the fragmentation process will be diminished. This has been demonstrated in many experiments where fragmentation is quite limited when various molten materials are quenched in the film boiling regime. From a fragmentation standpoint alone, it would therefore appear that the presence of non-condensable gases or vapor decreases the probability for an energetic interaction. However, Cho^[45,46], in his work on intermixing considerations for vapor explosions, indicated that the presence of vapor or noncondensable gases may actually increase the chances for such violent MFCI-induced vapor explosions. A brief discussion of intermixing considerations is presented in the following section.

2. INTERMIXING

With respect to breakup and intermixing, Cho et al^[45,46] consider that such processes are governed by frictional energy dissipation, with a geometric progression of breakup and a constant mixing velocity during each stage. Based on these assumptions, the minimum mixing energy is found to be

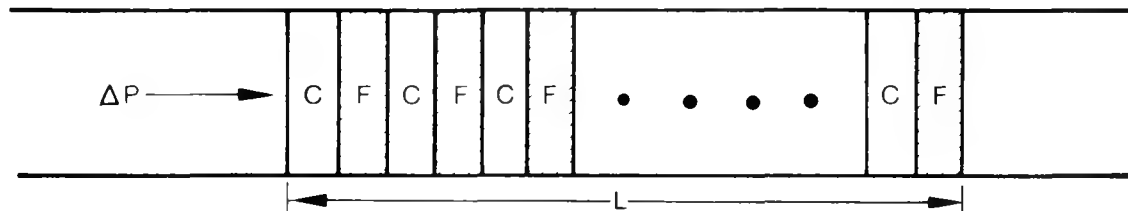
$$E_{\text{mix,min}} = 1.81 \rho V_f \left(\frac{V_f^{2/3}}{t_m^2} \right) \left(1 - \frac{R^2}{V_f^{2/3}} \right) \ln \left(\frac{V_f^{1/3}}{R} \right) \quad (24)$$

where

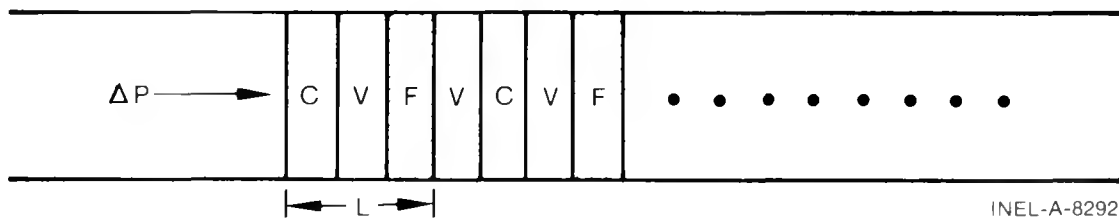
- ρ = coolant density
- V_f = initial volume
- t_m = mixing time
- R = fragmented particle size.

If this mixing energy is less than some fraction of excess thermal energy of the fuel ($E_f = \rho C_p V_f \Delta T$; where ΔT is the temperature of fuel above that of the coolant), it can be said that the energy requirements for rapid fine-scale intermixing are satisfied.

As illustrated in Figure 16, two different one-dimensional cases are considered by Cho et al^[45]. For a coarse mixture of molten fuel and coolant in the absence of vapor (Case a),



(Case a) No vapor layer between fuel (F) and coolant (C) layers.



(Case b) Vapor (V) layer between fuel (F) and coolant (C) layers.

ΔP = pressure differential
 L = reaction zone length

Fig. 16 Illustration of fuel-liquid and fuel-vapor-liquid mixing geometries.

the two fluids cannot effectively begin to accelerate (or mix) until the disturbing force is relieved at the end of the fuel-coolant column. However, if the fuel and coolant layers are separated by a compressible vapor (Case b), then they can accelerate immediately after disturbance relief in the vapor region. Consideration of these two situations indicates that the existence of a compressible layer reduces the effective mass to be accelerated, thus resulting in a much finer "localized" intermixing. This suggests that film boiling prior to a pressurization would result in a more effective intermixing process, which in turn could result in violent explosive interaction. An examination of the SPERT-ID test^[19] supports such arguments. The results of such experiments indicate that a vapor explosion is accompanied by a fragmentation process, resulting in particle sizes of approximately 100 μm in radius (R) and a mixing time (t_m) of a few milliseconds or less. If a mixing time of 5 ms is assumed, and if it is assumed that 1% of the excess fuel sensible heat is used in the intermixing process, the energies can be compared. As illustrated in Table VI, the volume of each of the fuel elements for the SPERT-ID^[19], BORAX-I^[17], and SL-1^[18,126] reactors are small enough so that intermixing energy requirements necessary for a vapor explosion are satisfied.

TABLE VI

COMPARISON OF MIXING ENERGY REQUIREMENTS WITH AVAILABLE SENSIBLE HEAT OR FUEL
AT TIME OF VAPOR EXPLOSION IN THREE DIFFERENT WATER COOLED REACTORS

	SPERT-ID	BORAX-I	SL-1
Considered cause of reactor damage	Vapor explosion	Vapor explosion	Vapor explosion
Fuel element design	Plate	Plate	Plate
Fuel dimensions in active core	0.02 x 2.45 x 23.5 in.	0.021 x 2.5 x 2.36 in.	0.05 x 3-7/8 x 26 in.
Fuel volume	1.15 in. ³ (18.25 cm ³)	1.24 in. ³ (20.3 cm ³)	5.04 in. ³ (82.55 cm ³)
Fuel type	U-Al alloy	U-Al alloy	U-Al alloy
$E_{\min, \max}$ [Equation (24)]			
$R = 100 \mu$ (0.01 cm)	8.05 cal	9.16 cal	102.9 cal
$t = 2$ ms			
ρ_f		$\sim 3.10 \text{ g/cm}^3$	
$C_{p,f}$		$\sim 0.225 \text{ cal/g-}^\circ\text{C}$	
$T_{\text{melt}, f}$		$\sim 940^\circ\text{C}$	
ΔT		$\sim 900^\circ\text{C}$	
E_f (at 1%)	1.18 cal	131 cal	518 cal
Comparison		E_f (at 1%) $> E_{\text{mix}, \min}$	
Potential for vapor explosion	Yes	Yes	Yes

Although such calculations can only be considered first-order estimates, the fuel rod bundle concept appears to satisfy the initial dispersal requirements for vapor explosions. A more detailed calculation might include kinetic energy requirements for fuel particle movement through the coolant and fragmentation energy requirements considering such phenomena as bubble growth and collapse or thermal-stress-induced breakup.

V. NUCLEAR REACTOR CONSIDERATIONS

As indicated from the previous discussion, most recent vapor explosion research has centered primarily on obtaining an understanding of the necessary conditions for explosive vaporization. Although, in a general sense, some consensus of opinion is emerging on defining such necessary conditions, there appears to be little agreement on the details of the underlying phenomena. Thus, any discussion of vapor explosion potential in nuclear reactor systems is subject to a somewhat limited knowledge of the problem. Nevertheless, some general remarks can be made concerning accident initiators and preventive measures. It should be noted, however, that present knowledge indicates that the necessary conditions appear to be difficult to meet in reactor systems and, because of redundant safety features, vapor explosions have never occurred in commercial power reactors and their probability of occurrence is low^[8].

1. ACCIDENT INITIATORS

Initially, severe transient overpower (TOP) accidents were of primary interest relating to the MFCI vapor-explosion problem as applied to LWR systems, where such accidents must have a sufficiently high reactivity rate (several $\$/s$) to cause fuel melting and rod failure prior to significant voiding of liquid coolant from the core. Indeed, as discussed, the SPERT-ID and BORAX-I experiments and the SL-1 accident were of this type. However, with present-day power reactor designs calling for low reactivity worth of both individual fuel bundles and control rods, the probability of initiating such reactivity excursion accidents is insignificant. However, various loss-of-flow (LOF) scenarios can be hypothesized which result in the potential for MFCI-induced explosive vaporization. Such LOF accidents could lead to fuel overheating and failure, where subsequent reflooding of the reactor core might result in coolant being forced into contact with molten fuel. If such intimate contact between molten fuel and coolant were to occur, the potential for a vapor explosion could exist (as demonstrated by Wright's water-hammer-type experiments with molten aluminum^[71]).

With respect to LMFBRs, both TOP (because of a potential positive void coefficient) and LOF accidents are of interest. In addition, the core of a large fast reactor is not in its most critical configuration, such that there is the added concern of a recriticality and coolant reentry problem^[127], which could lead to an explosive MFCI situation. However, as discussed previously, the conditions for the occurrence of a true vapor explosion in either reactor system appear difficult to meet, based on the present understanding of phenomena associated with thermal vapor explosions. Likewise, knowledge gained to date suggests that certain reactor design steps might be given serious consideration as preventive measures. Indeed, the present practice of limiting single control rod worth below 1 \$, so as not to cause a prompt critical situation, can be partially attributed to the knowledge gained from the analysis of the SL-1 explosion. Other preventive measures of a thermal-hydraulic nature, which might be considered in view of present knowledge, are discussed in the following section.

2. PREVENTIVE FACTORS

Although numerous criteria must be considered when assessing various nuclear reactor designs, the following discussion is based on the thermal vapor explosion hazard only, where an attempt is made to clarify what measures might be considered to diminish the potential for explosive vaporization resulting from a severe hypothetical reactor core meltdown event.

Since intimate molten fuel contact with liquid coolant appears to be an important criterion necessary for initiating a vapor explosion, factors which tend to separate fuel from coolant should diminish the potential for such an explosion. The presence of non-condensable gases can lead to such separation, in addition to the effect of damping out pressurization. Thus, it would appear that the probability of such an event is somewhat less likely for irradiated fuel than for fresh elements, due to the presence of gaseous fission products that are released from the fuel matrix. Trends of the TREAT fuel experiments^[128-133] indicate such an effect, although none of these experiments underwent a true vapor explosion, but rather milder MFCI-induced coolant voiding. Likewise, fuel element designs calling for a gaseous bond, such as He, would appear to be safer than concepts calling for metallic bonded fuel elements or sandwich-type designs used for low-power LWRs (for example, fuel clad directly to an outer metallic sheath, similar in design to the SPERT-ID, BORAX-I, or SL-1 fuel designs). For similar reasons, vented fuel elements would not appear to be safer than designs calling for a gaseous plenum region within the fuel element itself, although such vented elements might be more desirable when considering normal swelling behavior or less severe off-normal events such as localized overheating. In addition, single-phase liquid coolant reflooding, approaching a hammer-type situation, with a partially molten core should be avoided.

With respect to the spontaneous nucleation concept, several factors might be considered which would diminish the probability of explosive vaporization, if such a concept actually applies to reactor systems. As pointed out by Fauske^[29], the presence of radiation, gaseous fission products, solid particulate matter, and other nucleation aids tends to cause heterogeneous nucleation prior to reaching the temperature limit at which rapid change-of-phase would occur, thus initiating mild MFCI rather than a true vapor explosion.

With respect to the pressure detonation model, elimination of an initial trigger pressure pulse would essentially eliminate the possibility of a vapor explosion based on this model concept; thus, the presence of noncondensables would again be advantageous. Also, designs which eliminate rigid, long-tube geometries would be desirable.

VI. SUMMARY

As a result of knowledge gained from recent research efforts, it can be summarized that a vapor explosion is characterized by the following factors^[a]:

- (1) A period of stable film boiling
- (2) Destabilization of film boiling by either thermal or pressure-induced means, or both
- (3) Intimate contact between molten fuel and coolant
- (4) Extensive fuel fragmentation and intermixing with liquid coolant, resulting in a large effective heat transfer area causing rapid coherent coolant vaporization
- (5) Sufficient system constraint to cause severe shock pressurization.

At the present time, however, there appears to be little consensus of opinion as to the details of the actual physical phenomena involved in such processes. For example, there appears to be little agreement on the actual mechanism of fragmentation, the rate at which it occurs, and the ultimate particle size that can be expected. Likewise, the question of the energy transfer mechanism between fuel and coolant is still unanswered. On one hand it has been proposed that rapid phase-transformation by spontaneous nucleation is a necessary condition for obtaining a vapor explosion, whereas others have postulated that a nucleate-type boiling process from finely divided fuel intermixed with coolant can equally produce vapor at a sufficient rate to obtain shock pressurization of the system. In spite of such uncertainties, it appears that some of the basic phenomena associated with vapor explosions can be characterized at this time. As fundamental research continues on the subject, a reevaluation of the pertinent phenomena may be necessary. Until such time, the following features are suggested for incorporation into simplified parametric calculations.

1. FRAGMENTATION-INTERMIXING PROCESS

As discussed previously, current research efforts have centered primarily on a determination of the principal mechanisms involved in fragmentation, rather than on an assessment of the kinetics of such breakup and the resultant particle size distribution that can be expected for a defined set of initial conditions. However, both in-pile fuel-failure tests and out-of-pile molten metal dropping experiments indicate that the process is

[a] The first two factors may be inappropriate for "water-hammer" impact-type conditions.

primarily thermal in nature, with hydrodynamic influences having an added effect. Nevertheless, because no one model has yet been accepted which enables the user to estimate the rate of breakup and expected particle sizes, one must resort to empirical evidence for parametric calculation.

Mizuta's^[69] correlation for the particle size distribution appears appropriate, since it is based on an extensive compilation of data from simulant materials, as well as UO_2 fuel quenched in both sodium and water. Such data include in-reactor UO_2 -Na and UO_2 - H_2O results, laboratory induction-heated and thermite-reaction UO_2 into Na, and data from the SPERT-ID destructive test. The particle size distributions from such experiments show remarkable consistency and normal Gaussian distribution when displayed on a logarithmic scale. Mizuta's distribution function for the fines is

$$f(\log D) = 58.1 \exp \frac{-(\log D - 2.27)^2}{0.944} \quad (25)$$

where D is the particle diameter (μm), the most probable mean-mass size being $\simeq 200 \mu\text{m}$, with a maximum bound of $\simeq 2500 \mu\text{m}$. It is cautioned that this correlation is based primarily on fragmentation data obtained from controlled small-scale experiments (some of which cannot be considered vapor explosion events), rather than the situation of a large-scale vapor explosion for a nuclear reactor; thus, such a correlation is subject to questions of prototypicality. The large-scale UO_2 -Na French experiments^[134,135] should help in clarifying such uncertainties.

As discussed by Cho^[44,45], an appropriate breakup and intermixing time, based on the results of parametric calculations^[46] and the results of the SPERT-ID^[19] destructive experiments, is on the order of a few milliseconds. Further evidence that such mixing and fragmentation occurs on a millisecond time scale can be found in numerous out-of-pile dropping experiments and also in the analysis of the H-2 in-pile fuel failure experiment^[132,133] where the total time for cladding expansion and rupture, fuel release from the interior of the rod, breakup, and intermixing was found to be no greater than 40 ms. A time for breakup and intermixing alone of several milliseconds is therefore suggested.

2. HEAT TRANSFER-PRESSURIZATION PROCESS

Besides the condition of a rapid fragmentation-intermixing process, it is generally agreed that intimate fuel-coolant contact occurs, resulting in rapid vaporization and shock pressurization. However, there is little agreement with respect to the mechanics involved in the heat transfer-vaporization process. On one hand, several authors^[29,35] consider a heat transfer-vaporization process, asserting that if the instantaneous contact temperature between a large mass of fuel and coolant exceeds the spontaneous vapor nucleation temperature, a vapor explosion will occur. Others^[33,38,52,53,75,77,83] consider a progressive process where continued fragmentation/heat transfer-pressurization can lead to explosive vaporization. With respect to the spontaneous nucleation model, it has been

argued that a vapor explosion can occur for a fuel-water system, but not for the large-mass fuel-sodium case (because the instantaneous contact temperature is below that for homogeneous nucleation of sodium). The progressive models, however, predict that vapor explosions can occur for many fluid systems (including $\text{UO}_2\text{-Na}$) under favorable hydrodynamic conditions (which require a rather detailed analysis). For this reason, present research efforts have concentrated on identifying the basic criteria and mechanisms involved. Until such issues are settled, a unified heat transfer-vaporization-pressurization model, which is capable of predicting the important state variables necessary for estimating work potential (that is, specific volume and pressure), cannot be established with any degree of confidence at this time.

VII. CONCLUSIONS

At the time a previous review paper^[1] was published (1973), very little in the way of overall modeling of the vapor explosion problem existed, other than the simplified equilibrium thermodynamic approach of Hicks and Menzies^[27] and the liquid thermal expansion concept of Cho and Wright^[136,137]. Neither of these approaches, however, addressed the problem of assessing the criteria for and transient phenomena involved in rapid vaporization-induced shock pressurization (that is, a true vapor explosion). Since that time, several overall mechanistic type models have been developed which attempt to describe the actual mechanisms involved and the kinetics of such processes, the most significant concepts being the spontaneous nucleation approach of Fauske^[29,30] and Henry^[35-37] and the pressure detonation model of Board and Hall^[38,52]. Although each of these approaches has its supporters, neither has gained wide acceptance in the engineering community as an acceptable description of the actual phenomena involved or as encompassing all possible scenarios that could lead to explosive vaporization. It is the opinion here that the spontaneous nucleation model is one mechanism by which vapor explosions can be accounted for; however, it alone may not be considered the basic criterion upon which vapor explosion potential should be judged. An 'a priori' conclusion that a vapor explosion will not occur in a reactor system if the instantaneous contact temperature between fuel and coolant is below the spontaneous nucleation temperature or if the system pressure is greater than the critical pressure of the working fluid, cannot suffice if it can be demonstrated that progressive fragmentation-heat transfer-pressurization models can lead to explosive vaporization. The work of Board and Hall is an attempt at such an approach; however, as discussed previously, serious questions arise as to the original hydrodynamic assumptions and associated fragmentation dynamics; thus, further investigation of this concept appears warranted. The work of Anderson and Armstrong^[33], Sharon and Bankoff^[59], Patel and Theofanous^[57], and Williams^[58] should help clarify some of these questions.

The fact that extensive investigations with simulant fluid experiments appear to support the interface-spontaneous nucleation concept, indicates a cautioned validity of the arguments presented by Fauske and Henry. However, it is emphasized that most simulant fluid experiments have been carried out to test particular model assumptions rather than to assess all-encompassing conditions which could lead to shock-type explosive vaporization. For example, the water-hammer experiments of Wright and Humberstone^[71] produced vapor explosions with molten aluminum impacted upon water (which satisfies the contact interface-nucleation criterion); however, such experiments have not been conducted for molten UO_2 impacted upon sodium (which would not satisfy the contact interface-nucleation criterion), yet explosive vaporization under such conditions appears possible. Therefore, $T_I > T_{SN}$ is not considered to be a necessary condition for explosive vaporization, but rather, just one mechanism by which rapid vaporization can be accounted for. Further experimental verification of required conditions is thus deemed necessary before either the pressure detonation concept or other plausible scenarios can be completely discounted in reactor safety assessment.

An overview of vapor explosion conditions for various models is illustrated in Table VII and indicates that some commonality of thought exists in that they all attempt to attribute some necessary trigger criterion to account for explosive vaporization. The detonation concepts require pressure- or thermal-induced film boiling destabilization and fragmentation, and the spontaneous nucleation concept requires a quantum jump in vapor nucleation rate at a temperature condition considered to be the spontaneous nucleation temperature. Considering the ideas presented in these model concepts and experimental results, it appears to the authors that destabilization of quiescent film boiling, due to either pressure or thermal conditions, or both, resulting in rather violent nucleate-type boiling and fragmentation into a large surface heat transfer area, satisfies the conditions for explosive vaporization. The fact that the predicted homogeneous nucleation temperature is not that different from a thermodynamic prediction of the minimum film boiling temperature^[39,42,138] (Leidenfrost point) and that contact-wetting conditions affect both, indicates that experiments which have been interpreted in light of a spontaneous or homogeneous nucleation temperature^[35,37] may also be explained by a film boiling destabilization temperature. In addition, pressure effects have been shown to also cause film boiling collapse. The recent work of Lienhard^[139], Dhir^[140], Gunnerson and Cronenberg^[40,42,138], and Bankoff et al^[141] with respect to understanding the conditions for film boiling stability should help in understanding vapor explosion criteria.

Several new approaches to the fragmentation process have also been developed. In a general sense, the violent boiling-collapse mechanisms appear promising, although significant questions remain as to an adequate modeling of the collapse process and associated energy imparted to the hot material. In addition, most of this work has not considered the role of solidification on the breakup process; yet it has been shown that the molecular crystallization theory^[49,50] would predict the commencement of surface solidification within times less than a millisecond for oxide fuels which undergo the large heat transfer quenching rates for good contact conditions. The work presented in References 82 and 83 attempts to couple such boiling concepts with surface solidification; thus, it appears to be a consistent approach. The mixing and vapor blanketing effects discussed by Cho^[43,46] also deserve further consideration and should be incorporated into modeling efforts.

The fact remains, however, that an all-encompassing fragmentation mechanism has not been widely accepted; indeed, the situation of many conflicting model concepts exists. The problem is complicated by the fact that certain concepts (surface solidification, gas release . . .) may describe a particular material and experimental system (UO₂ in Na, Ag in H₂ . . .), but may not be relevant to the vapor explosion problem. This is not to say that an understanding of fragmentation is unimportant; indeed it is, since it is the one necessary condition that is generally accepted. However, it appears desirable to first understand the overall nature of the phenomena involved in explosive vaporization and, at that point, relate the details of fragmentation to the problem.

Besides some of the suggestions given in Reference 53, further research efforts might include:

TABLE VII

COMPARISON OF VAPOR EXPLOSION CONDITIONS FOR VARIOUS MODELS

Vapor Explosion Conditions	Fauske-Henry	Board-Hall	Anderson-Armstrong	Cronenberg-Gunnerson	Universal Model
1. Initially stable film boiling, so that vapor film separates the two liquids and permits coarse premixing without excessive energy transfer	Consistent	Consistent	Consistent	Consistent with all model concepts	Consistent with all model concepts
2. Breakdown of film boiling	Due to thermal or pressure effects	Due to pressure effects	Due to pressure effects	Due to thermal effects	Due to thermal or pressure effects
3. Fuel-coolant contact upon breakdown of film	Liquid-liquid contact	Liquid-liquid contact	Liquid-liquid contact	Liquid-liquid or solid crust-liquid contact	Liquid-liquid or solid crust-liquid contact
4. Rapid vapor production, causing shock-pressurization	Due to spontaneous vapor bubble nucleation (assessed from kinetic theory) and fine-scale fragmentation-intermixing	Due to a large effective heat transfer surface as a result of fine-scale fragmentation and intermixing	Due to a large effective heat transfer surface as a result of fine-scale fragmentation and intermixing	Due to a large effective heat transfer surface as a result of fine-scale fragmentation and intermixing	Large effective heat transfer surface due to fragmentation and intermixing; possible, but not necessary, spontaneous nucleation of vapor
5. Adequate physical and inertial constraints to sustain a shock wave	Consistent	Consistent	Consistent	Consistent	Consistent with all model concepts

- (1) Injection or entrapment experiments to provide the conditions for triggering vapor explosions
- (2) Large-scale experiments to demonstrate the effects of geometry, size, mass ratio, and ambient pressure effects on the pressure detonation model
- (3) Shock wave experiments to measure the number of fragments as a function of the pressure pulse and energy
- (4) Further theoretical development of fragmentation and inter-mixing models based on the pressure wave initiator concept
- (5) Clarification of the effect of transient solidification, of the molten material during quenching, on the fragmentation process and its influence on the spontaneous nucleation model
- (6) Experimental and theoretical studies on dynamic surface tension between suddenly contacting materials as applied to the spontaneous nucleation model
- (7) Experimental and theoretical studies to assess the temperature and pressure conditions for destabilization of film boiling.

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