ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

A THERMOHYDRODYNAMIC MODEL
FOR MOLTEN UO_2 -Na INTERACTION,
PERTAINING TO FAST-REACTOR
FUEL-FAILURE ACCIDENTS

by

August W. Cronenberg

Reactor Analysis and Safety Division

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NOMENCLATURE →

NOMENCLATURE

<u>Symbol</u>		<u>Units</u>
A	Cross-sectional area of coolant channel	cm ²
a	Outside radius of spherical fuel particles	cm
C	Circumference of heat-transfer surface	cm
c _p	Specific heat of liquid	cal/g-°C
D _e	Equivalent diameter of coolant channel	cm
D _n	Diameter of coolant-channel sections, obtained from volumetric displacement	cm
f	Blasius coefficient of friction	
g	Acceleration due to gravity	cm/sec ²
H	Enthalpy of sodium	cal
h	Heat-transfer coefficient	cal/sec-cm ² -°C
$\bar{h}$	Specific enthalpy of sodium	cal/g
KE	Kinetic energy	cal
Ke	Resistance coefficient for expulsion	
k	Thermal conductivity	cal/cm-sec-°C
L ₁ '	Length of upper slug	cm
L _{1,2,3...}	Lengths of coolant-channel sections	cm
M	Mass of liquid plugs	g
m	Mass of sodium in interaction region	g
Nu	Nusselt number for flowing sodium through annular coolant channel	
n _s	Number of fuel particles	
P	Pressure	dyne/cm ²
PE	Potential energy	cal
Q	Heat input to interaction region	cal
$\dot{Q}$	Volumetric heating rate to liquid plugs	cal/cm ³ -sec
Re	Reynolds number	
r	Radius within fuel particles	cm
S	Fuel-particle surface area	cm ²
T	Temperature	°C
t	Time	sec
V	Volume of sodium in the interacting region	cm ³
v _c	Sonic velocity	cm/sec

<u>Symbol</u>		<u>Units</u>
W_{by}	Work done by the sodium in the interacting region on the surroundings	cal
We	Weber number	
ΔX	Length of interaction zone	cm
x	Distance moved by liquid plugs from time of interaction	cm
$\dot{x}$	Velocity of liquid plugs	cm/sec
$\ddot{x}$	Acceleration of liquid plugs	cm/sec ²

Subscripts

c	Condensation
exp	Expansion losses
f	Fuel
fm	Film
frc	Friction losses
i	Inside (radius)
l	Liquid
m	Coolant
n	Plenum number (1 = test section)
o	Outside (radius)
pg	Gas plenum
s	Sphere
v	Vapor or vaporization
w	Wall

Greek Symbols

α	Thermal diffusivity	cm ² /sec
α_p	Thermal-expansion coefficient	°C ⁻¹
β_T	Isothermal compressibility	cm ² /dyne
γ	Surface tension	dyne/cm
ϵ	Conversion efficiency	
λ	Latent heat of vaporization	cal/g
μ	Thermal decay constant	sec ⁻¹
ξ	Distance into liquid slug from liquid-vapor interface	cm
ρ	Density	g/cm ³

<u>Greek Symbols</u>		<u>Units</u>
σ	Film thickness	cm
π	Ratio of circle circumference to diameter	
τ	Time	sec
ϕ	Equilibrium sodium temperature in interaction region	$^{\circ}\text{C}$
χ	Thermal pressure coefficient	$\text{dyne}/\text{cm}^2\text{-}^{\circ}\text{C}$

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ABSTRACT

As part of the liquid-metal fast-breeder-reactor (LMFBR) safety program, the consequences of molten-fuel release into sodium coolant must be evaluated in order that design constraints might minimize the safety hazard of such an event. The work presented here is the first attempt to compare the voiding rates obtained from an in-pile, fuel-failure experiment with theoretical results of a fuel-coolant interaction (FCI) model.

The theoretical approach taken was to seek a coupled solution to the energy and momentum equations of a single bubble which expands against an upper and lower liquid slug. During the initial contact period fuel fragmentation is assumed to occur as a result of violent boiling. The resulting active region contains fuel, liquid sodium, and sodium vapor. Within the bubble, finely divided fuel particles interact with sodium, resulting in vaporization and subsequent bubble growth. A thin liquid-film layer is assumed to adhere to the intact portions of the pin and test section, thus allowing for condensation at these surfaces. The model used represents the first analytic treatment of the energy exchange process at all boundaries of the expanding interaction zone. Parametric calculations were made considering the effects of particle size, condensation, and initial fuel-liquid-vapor volume fractions.

I. INTRODUCTION

The possibility of overheating, melting, and subsequent interaction of fuel with contiguous coolant in nuclear power systems has been a concern from the time reactors were first considered. This problem, however, is not unique to the nuclear industry in the sense that almost all mechanical systems and industrial processes may involve a sequence of events leading to destructive overheating and interaction with the surroundings. However, by their nature reactors contain highly toxic radioactive material, which if released may cause as much or more damage than that due to chemical and/or mechanical effects. This requires that the licensing of any reactor be preceded by an assessment of the various initiating accidents and an in-depth analysis of the phenomenology involved. From such studies, design constraints are established to insure a minimum probability of occurrence and a maximum probability of accident confinement.

The technical feasibility of building and operating safe reactors of various types has been demonstrated many times over. The design of each reactor system has been accompanied by extensive experimentation and analysis into the causes, consequences, and prevention of both major and minor accidents. The research and development program pertaining to the liquid-metal fast-breeder reactor (LMFBR) is no exception to this rule. The degree of emphasis placed on the safety aspects of the LMFBR was demonstrated at both the 1958 and 1964 Geneva Conferences (Refs. 2 and 3). To assess safety problems associated with fuel-coolant interaction in any reactor system one must first identify the various kinds of situations which may lead to fuel-element failure. One method of categorization is to divide the problem into probable and hypothetical accidents.

Since there are as many as 10^5 fuel pins in a reactor core, manufacturing defects, local coolant blockage, or minor localized power and coolant transients may initiate failure of individual pins. An analysis of the dynamics involved should therefore define both design constraints to insure against damage propagation and, perhaps, instrumentation for failure location. Confinement against propagation is likewise important from an economic standpoint, since, in general, single-element failure should not require reactor shutdown.

Other incidents which may lead to fuel-coolant interaction are the less probable single-subassembly blockage and the hypothetical whole-core loss-of-flow and power-exursion accidents. In each case, the modeling of coolant dynamics during the initial stages of expulsion (e.g., from intact geometries) is well under way; however, a satisfactory postfailure analysis is still lacking. Since the sequence of events leading to failure may be quite different depending on accident type, the initial conditions of the fuel-coolant interaction analysis may likewise vary. This results in sizeable differences in the ultimate work potential and rate processes involved. Such factors as reactor design, power level, previous operating history, and type and extent of the initiating accident will effect the outcome of the interaction. For example, the question of whether boiling occurs before fuel-element failure for single-subassembly blockages depends on such factors as fuel enrichment, lifetime, power generation, and extent of blockage. If boiling should occur before failure, the extent

and time sequence of the interaction may be quite different from that of fuel dispersal into an intact geometry of subcooled liquid. For this reason, one must clearly define the conditions under which a certain model will pertain. Indeed, this fact has been previously illustrated by the number of analytic models proposed for calculating the expulsion of sodium from intact channels. Their difference is due, in part, to the various flow regimes which may result as a consequence of the different types of accidents and reactor conditions.

The model proposed here attempts to describe the thermohydrodynamics of UO_2 -Na interaction following molten-fuel dispersal into liquid sodium. As will be explained, this situation is thought to result as a consequence of fuel-element failure, initiated by an autocatalytic power excursion. Although such an accident is highly improbable, nonetheless it must be considered in any safety analysis of fast reactors. This is due to the fact that unlike thermal reactors, LMFBRs have a relatively short prompt-neutron lifetime, a small delayed-neutron fraction for mixed uranium-plutonium fueled cores, and the potential for a positive reactivity feedback depending upon extent and location of coolant voiding. Thus, little time is available for mechanical control of prompt critical excursions. Although safety features, namely, the Doppler effect and axial fuel expansion, are designed into the system, the probability of a runaway excursion, although small, is finite. In order to contain such an accident satisfactorily, the amount of energy released either as heat or coolant kinetic energy must therefore be determined. The adaptability of this model to other accidents will be discussed in the results section of this thesis.

MacFarlane *et al.*⁴ have shown that for oxide cores, a ramp reactivity insertion rate of 50 cents/sec may lead to fuel melting and element failure before coolant boiling. In such a situation, molten-fuel dispersal in liquid sodium may result in a rapid rate of energy exchange and pressure buildup.

The objects of this work are twofold, namely, to derive a theoretical model which describes the dynamics of fuel-sodium interaction following this type of failure, and to compare the theoretical results with experimental results obtained from in-pile fuel-failure experiments. From such a study, it is hoped that insight into the actual phenomenology involved in fuel-sodium interactions might be gained.

II. LITERATURE SURVEY

A. Experiments

The complexity of fuel-coolant interaction is illustrated by the extensive number of published articles in areas relating to fuel failure and reactor safety. The problem is compounded by the fact that there are many different types of reactor systems, using various materials and operating under different conditions. For example, if it is desired to estimate the amount of energy release associated with fuel-element failure one must investigate not only the heat-transfer process but also the possibility of a chemical reaction between the fuel and coolant. In both reactions, not only the types of fuel (e.g., U-metal, UO_2 , and U-alloy) and coolant (e.g., H_2O , NaK, and Na) are important, but also the thermophysical state of each. Likewise, the effects of a cladding-fuel and/or a cladding-coolant chemical and/or heat-transfer interaction must be evaluated. Each area is also attended by unique problems that must likewise be investigated. Under such conditions, it becomes difficult to formulate meaningful conclusions which pertain to all reactor systems.

During the 1950's and early 60's, much of the work on the interactions between fuel and coolant was associated with water-cooled thermal reactors. As more research data accumulated, the full complexity of the problem became evident. To this date, there are still many unanswered questions concerning the reaction mechanisms involved. Although only a portion of the thermal reactor studies are directly applicable to fast reactors, some of this work is reviewed here since many of the research areas presently being investigated in the context of fast-reactor fuel failure, have been defined by experience gained from the water experiments.

Early industrial experience showed that thermal explosions often result during the accidental spillage of molten metals onto damp surfaces. Long⁵ has reviewed accidents which led to his molten aluminum-water experiments. One such incident he describes resulted when molten steel slag was accidentally spilled into an open trough containing water. The resultant explosion caused extensive damage: 17,000 sq ft of iron roofing and 3000 sq ft of steel window sash were blown from the building. Epstein⁶ also documented other examples of liquid metal-water explosions. In one case, the loading of wet scrap aluminum into a furnace produced an explosion causing six deaths, 40 injuries, and approximately \$1,000,000 in property damage. Although these two cases resulted in severe damage, many smaller accidents have been reported involving molten metals and paper smelt⁷ (fused sodium carbonate).

In view of such explosions, Long⁵ conducted a series of experiments in which he poured 50 lb of molten aluminum into a tank of water. He attributed the resultant explosion to a rapid rate of vaporization which occurred as a consequence of fragmentation of molten aluminum. Furthermore, he suggested that the fragmentation was initiated by the vaporization of a thin layer of water trapped under the sudden rush of molten metal. This explanation is commonly referred to as the entrapment theory, since it was observed that only when water was trapped between the molten metal and the container surface did breakup occur. Further evidence to

support this theory was obtained by coating the container with grease. This prevented water from being trapped by the molten particles, therefore eliminating both fragmentation and subsequent vapor explosions. Higgins⁸ conducted similar experiments with molten zirconium and water. He observed that peaking pressures occurred about 1-3 ms after initial contact. Based on kinetic theory, Epstein⁹ concluded that such rapid chemical reaction rates are highly improbable and not in agreement with consistent experimental observations. The results of this work strongly indicated that rapid heat transfer and subsequent vapor generation might be the principal causes of the molten metal-water explosions.

As part of the nuclear-reactor safety program both in- and out-of-pile experiments have been conducted. Likewise, a number of destructive reactor experiments were carried out to investigate the effects resulting from overpower fuel-failure transients.

One of the first indications of a metal-water interaction occurring in a nuclear reactor was obtained as a result of the core-meltdown accident of the NRX test reactor (1952).¹⁰ During a low-power experiment, failure occurred in the shutdown-rod system owing to a concurrence of mechanical defects and operating errors. Although the accident resulted in fuel failure and damaging pressure buildup, it was unclear what the individual effects of the possible destructive mechanisms were, that is the nuclear-energy release, the metal-water interaction, and/or the hydrogen-oxygen reaction. Hurst¹¹ 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 and not nuclear or chemical in nature. Following the NRX incident, the first successful set of destructive reactor experiments were performed with the BORAX reactors.^{12,13} As described by Dietrich,¹² "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 the mechanical damage indicated that the peak pressure was at least as high as 6000 psi, and was probably higher than 10,000 psi." Dietrich also concluded that there was no evidence of any significant chemical reaction.

During an experiment with the NaK-cooled EBR-I, a misunderstanding of instructions resulted in the first core meltdown with a coolant other than water.¹⁴ Upon investigation, it was observed that a porous structure formed in the meltdown region. From its composition no chemical reaction was possible; thus Kittel¹⁵ postulated that vaporization of NaK entrained in molten fuel might have formed the sponge-like material.

The first fatal power-reactor accident occurred on January 3, 1961 as a result of the explosion of the SL-1 boiling water reactor (a prototype reactor, designed for use at remote military installations as a power and heat source). Although other causes have been postulated, it seems certain that the accident resulted primarily from the withdrawal of a control rod (during the installation of newly designed control-rod drives), leading to a nuclear excursion, fuel-element failure, and violent interaction between molten metal and water, the reaction being largely non-chemical in nature.¹⁶ Postaccident examination of the reactor pressure vessel indicated that during the transient the vessel rose approximately

9 ft above its normal position, shearing off all piping in the process. 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 fuel-coolant interaction.

Results of the controlled destructive experiments with the SPERT reactors indicated that a conventional rather than nuclear explosion occurred.¹⁷ Similar to that observed in the EBR-I meltdown, "approximately 20 kg of spongy metallic debris, ranging in particle size from a few inches to less than 0.003 in. in diameter, was recovered from the reactor tank."¹⁸ Results of chemical analysis indicated that a maximum of 10% of the total energy developed resulted from a chemical reaction; the reaction times for such a process would be of the order of seconds^{19,20} rather than the observed 0.5-ms time of peak pressure.¹⁸ Considering the heat-transfer characteristics of such a process, Zivi²¹ estimated an average required heat flux of 3.0×10^7 Btu/hr-ft². For film boiling, a heat-transfer coefficient approximately 200 times greater than for conduction through a 10^{-2} -cm-thick vapor film would be required. Although Zivi's calculations seemed to discredit the arguments of a vapor-explosion process initiated by rapid heat transport, Judd²² proposed a mechanism other than classical film boiling which might account for such a high rate. He suggested that the explosion might be due to water coming in contact with molten fuel in a finely divided form, transferring heat before significant vapor blanketing. Recent work by Farahat,²³ in which a hot sphere was immersed in stagnant coolant (water or sodium), indicated that as the sphere temperature was increased and the bath temperature decreased (below saturation), the heat flux sustained in the transition region and onset of nucleate boiling was increased. If Farahat's results can be extrapolated to the melting point of UO_2 (2800°C), then the high fluxes estimated by Zivi might have occurred in the transition or nucleate region rather than the film boiling regime.

Other fuel-failure experiments involving coolant reactions include the TREAT²⁴ tests. A good review of these experiments and out-of-pile studies is given in ANL-7125.²⁵ Results indicate that the chemical reaction of UO_2 and steam is endothermic, whereas the uranium metal-water reaction is exothermic. If the fuel is clad in aluminum, zirconium, or stainless steel, chemical reaction of these metals with water will occur. The amount of fragmentation and thermophysical state of the materials are also important parameters that effect the rate and extent of reaction. However, in most cases, both the slow chemical rates and the relatively low energy yields failed to explain the rapidity of the observed explosions. From these studies it was concluded that heat transfer must play an important role in any explosive energy release following fuel failure.

A program similar to that carried out for thermal reactors is presently being pursued on the behavior of fast reactor materials. To date, however, the main body of work consists of laboratory experiments and in-pile studies, rather than destructive transients imposed upon entire reactor cores. From experience gained in the studies of thermal-reactor material, it was evident that experiments should be conducted to determine the possible physical or chemical nature of interactions between fast-reactor material and sodium coolant.

Swift and Pavlik²⁵ conducted some of the earliest laboratory experiments at Argonne in which heated samples were dropped into liquid sodium. The first series of tests consisted of cladding-sodium interaction studies. No evidence of a chemical interaction was found in any of the zirconium, vanadium, nickel, tantalum, or stainless steel experiments. These tests also showed that the materials, when in a solid state, were simply quenched by sodium, whereas, the molten samples fragmented, the extent of breakup increasing with both sample and sodium temperature. Similar results were obtained with stainless steel-potassium experiments,²⁶ giving further support to the physical nature of the interaction process. Follow-on sodium experiments with molten uranium metal²⁶ and molten UO_2 ²⁷ also indicated that fragmentation occurs with these fuel materials, and that the proportion of fines (200 to 1000 μ) increases somewhat with sodium temperature. Again there was no evidence of a uranium-sodium chemical reaction. Thus, more emphasis was placed on research into the mechanisms of heat transfer and fragmentation.

To test for mechanical breakup, dropping experiments into both sodium and water were conducted^{25,26} with molten stainless steel, aluminum, uranium, and zirconium. The principal finding of these experiments was that fragmentation occurred with sodium but not water, independent of the dropping height. To test the hypothesis that oxide-film formation (with water) prevented fragmentation, experiments with noble metals (gold and silver) were carried out. Again fragmentation occurred in sodium but not in water, indicating that breakup resulted from the difference in physical properties between water and sodium. To account for these findings, Swift and Pavlik²⁵ first stated the violent-boiling theory of fragmentation. Although their arguments are less defined than in the present discussion, the conclusions drawn are essentially the same. An explanation of the lack of breakup in water while fragmentation occurred in sodium can be interpreted in terms of the classical boiling curve. It was postulated

T_{cr} = CRITICAL TEMPERATURE

that breakup might result from the turbulence occasioned by the formation and collapse of vapor bubbles during coolant boiling at the surface of the molten metal. Since it is well known that the transition region is hydrodynamically the most violent of the boiling mechanisms, followed by nucleate vaporization, with film boiling being relatively quiet, fragmentation will most likely occur in the transition or perhaps nucleate regions. Under equilibrium conditions Westwater²⁸ showed that nucleate boiling occurs below the fluid critical temperature. Therefore, fluids with relatively low critical temperatures, such as water ($T_{cr} \approx 373^\circ\text{C}$) would tend to quench the molten material in the quiet film region, with metal solidification taking place before transition or nucleate boiling

occurs. On the other hand, molten metals dropped into a sodium bath which has a high critical temperature ($T_{cr} \approx 2300$ to 2700°C), may be subjected to the violence of transition boiling before the solidification temperature

is reached, thus resulting in metal fragmentation. The observed lack of fragmentation in water while breakup occurred in sodium seems to validate this theory. To test this hypothesis further, experiments with molten tin and bismuth were conducted, since their melting points are below the critical temperature of water. Breakup did occur with these materials; thus the postulated fragmentation theory seemed valid. As will be seen in the review of analytic models of fuel-coolant interaction, the violent-boiling hypothesis for fragmentation is a critical premise which may significantly alter the results of models developed to date. However, the boiling mechanism of fragmentation would also be subject to the subcooling effect demonstrated by Farahat.²³

The dynamics of fragmentation were also studied under isothermal conditions, with mercury being dropped into a water bath at room temperature.²⁹ Above a critical dropping distance or contact velocity, breakup occurred due to inertial forces overcoming the surface tension of the drop. The ratio of these two forces is commonly called the Weber Number ($We = \rho DV^2/\sigma$; where ρ , D , and σ are the drop density, diameter, and surface tension, respectively, and V is the drop velocity at contact). Hinze³⁰ demonstrated that when the inertial forces exceeded the surface tension by approximately an order of magnitude, the molten globule fragmented into a smaller, more stable size. Thus it may be true that in water systems the Weber effect may be the primary cause of fragmentation, while with sodium violent boiling may initiate fuel breakup. Therefore, in the case of the SPERT (water-cooled) reactor inertial forces caused by the sudden bursting of the fuel pins might have caused fuel fragmentation (since the fuel temperature was well above the critical point of water), whereas fuel breakup in the EBR-I may have been due to boiling during the initial contact period. If this is true, then it follows that destructive nuclear transients imposed on water-cooled reactors would of necessity have to be more severe to cause sudden explosion of the fuel pins. This would not be necessary in sodium systems to cause fuel fragmentation.

Additional experiments have been and are presently being conducted. A good review of the present state of the art, with respect to fragmentation, is given by Witte *et al.*⁷

A parallel effort concerning the phenomena associated with fuel-element failure is being conducted in a series of in-pile experiments, the main body of which are being carried out in the TREAT irradiation facility. Basically, these experiments have supplied data on the threshold and mode of fuel-element failure, movement of fuel during transient heating, swelling, melting, and postfailure effects of fuel-coolant interaction. Some of the more interesting results were obtained by photographing meltdown experiments in a transparent container.^{31,32} Although these experiments provided visual information on fuel failure and dispersal, all were performed in a dry environment, thus yielding no information on fuel-sodium interactions. Results of other TREAT experiments have been described in a series of articles appearing in Nuclear Safety.³³⁻³⁶

The most significant work performed in TREAT with respect to the fuel-coolant interaction problem involved the stagnant sodium-autoclave experiments described by Barghusen *et al.*³⁷ An estimate of the thermal-energy transfer from the molten-oxide fuel to the sodium coolant was

determined by following the motion of a piston located in the coolant plenum above the fuel elements. The work done in accelerating the piston was of the order of 1 J for a 5-pin cluster. The conversion of the estimated heat energy of the fuel to mechanical work was only about 0.005%. This percentage is small compared to the 2.8% conversion reported by Martinson³⁸ for a UO_2 -water test. A comparison between these results leads to the interesting conclusion that the energy-transfer process and subsequent vapor expansion may be significantly less for sodium than for water, for a given fuel energy. One explanation for this occurrence might be as follows. Since it could be expected that molten UO_2 undergoes considerably more fragmentation in sodium than in water, one would expect a higher rate of energy transfer for the UO_2 -sodium interaction. However, this initial high rate of vapor generation might result in only the first portion of the fuel interacting with the coolant, the rest being blanketed due to vapor formation. With water, however, the initial fragmentation, heat transfer, and vapor-generation rates may be slower, so that the total amount of fuel that comes in intimate contact with the water coolant is much greater, causing a larger fraction of interaction, although somewhat delayed. As will be discussed further, the difference in the rate of film condensation at cold boundaries is also thought to play a role in the net vapor-expansion process.

Although the TREAT experiments have advanced the understanding of fuel-failure mechanisms, very little has been done in the way of post-failure analysis with respect to the transfer of thermal energy to vaporizing coolant, with consequential expulsion and reentry. The need for realistic postfailure analysis was emphasized by Dickerman:³⁶ "As experimental data accumulate, it should be possible for analysis to confirm failure models and build up code modules for the postfailure regimes. The need for such capability is great. For example, the detailed phenomenology and kinetics of postfailure thermal interactions between molten fuel and sodium are not known. In the absence of this information, limiting-case calculations have been relied upon to estimate the severity of the sodium vaporization caused by the heat dump from the molten fuel Presumably a knowledge of the real phenomenology of movement, mixing, and kinetics of heat transfer and an understanding of the role played by structure would permit a calculation much closer to the actual meltdown-experimental results." The work presented here represents a first attempt to compare transient analytical results with data obtained from such experiments.

B. Analytic Models

Although there has been some model development concerning fuel-coolant interaction, results of parametric calculations have not been applied to the transient analysis of in-pile experiments. Two basically different approaches have been adopted in theoretical studies, namely, the thermodynamic models which estimate the maximum work available and the transient models which estimate the rate processes involved.

A limiting-case calculation was developed by Hicks and Menzies³⁹ in which an upper limit on the expansion work of the coolant was determined. This work is taken as 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. Judd⁴⁰ essentially used the same approach to obtain the thermodynamic efficiency of a molten fuel-sodium interaction. However, he used the more realistic Himpan⁴¹ equation of state to determine the sodium pressure at higher temperatures. Since calculations based upon this type of thermodynamic approach do not take into account the transient nature of the heat-transfer and expulsion rates, peaking pressures caused by the time delay between these two rate processes are not obtainable. Since damage to the reactor system will depend upon the severity of the pressure pulse, a transient analysis is essential in evaluating the safety problems of an LMFBR. Recently, a number of models have been proposed which describe the time dependence of the voiding and pressurization rates during a molten fuel-coolant interaction.

Padilla^{42,43} was the first to develop a method which considered the transient dependence between the heat-transport and expansion processes. Since the basic assumptions of his work have been incorporated into other models, a fairly detailed description is given here. Padilla describes the process by assuming that spherical fuel particles are uniformly dispersed and in intimate contact with liquid sodium. The transient temperature history of the sodium is determined by solving numerically the heat-conduction problem in spherical symmetry. If boiling is considered to be suppressed, temperature increase results in thermal expansion of the liquid sodium, governed by its equation of state

$$\frac{dP}{dt} = \chi_v \left. \frac{dT}{dt} \right|_{\text{Na(liquid)}} - \frac{1}{\beta_T V} \frac{dV}{dt},$$

where χ is the thermal pressure coefficient and β_T the isothermal compressibility. The expansion rate of the mixing region (dV/dt) is found by determining the compressibility of the constraining liquid plug due to pressure wave propagation. For one-dimensional wave propagation in a compressible plug of infinite extent, the expansion rate is

$$\frac{dV}{dt} = \frac{A}{\rho_l v_c} \frac{dP}{dt}$$

where A is the cross-sectional area between the interacting region and the liquid plug, ρ_l the density of the liquid plug, and v_c the acoustic velocity in the liquid plug.

These two equations along with that of heat transfer determine the transient nature of the expansion and pressure history. If $P(t)$ and $V(t)$

are known, the energy content of the interacting sodium is found, assuming a closed frictionless thermodynamic system such that

$$[\text{Sodium Energy Content}] = \int P dV .$$

This sequence of calculations is valid up to the time when the calculated sodium pressure falls below the saturation pressure of the heated zone. At this point, onset of boiling occurs, and the energy imparted to the liquid plug is taken to be equal to that calculated above. Parametric calculations with this model result in peaking pressures between 10^3 and 10^4 atm. This results from the fact that during the heating process the only mechanism for pressure release results from the compressibility of the liquid plug above the interacting region. It seems reasonable that both condensable and noncondensable gases would be entrapped in the mixing zone during a fuel-coolant interaction; thus, a two-phase analysis would be required, resulting in a lower pressure buildup. Also, the cutoff criterion for heat transfer is not necessarily conservative, since a significant amount of energy may be imparted to the system during boiling of sodium from the fuel particles.

Unlike Padilla, Duffey⁴⁴ assumed that the expansion process of a fuel-coolant mixture is caused solely by vapor production, with a small contribution due to changes in vapor density. In this model, the rate of heat transfer is specified by a heat flux and fuel surface area, which are given input parameters. This assumption requires that an estimate be made of the heat flux and area involved in such a reaction. Secondly, the constraint is of the inertia type, unlike the acoustic approximation used by Padilla. Thus, the expansion rate of the mixing zone is determined by the expulsion of an incompressible liquid plug whose movement is governed by Newton's second law, considering the effects of friction, gravity, and pressure head. Heat transfers at the vapor-plug interfaces and along the channel walls are not taken into consideration.

As would be expected, the high pressures predicted by Padilla are not calculated with this model. This results from the fact that the heating rate gives rise to coolant vaporization at saturation; thus there is a vapor cushioning effect. The additional effect of condensation at cold boundaries, especially during the later stages of expulsion, when a significant amount of wall film is exposed, would likewise have decreased the pressure even further. By using a defined heat flux and surface area, Duffey avoids the problem of describing exactly what the heat-transfer mechanism is. Since an adequate description of the heat-transfer process has not yet been established, this is not necessarily a bad approach. In fact, empirical relations for the heating rate during a fuel-coolant interaction may eventually be used.

Another approach to the fuel-coolant interaction problem has been developed by Atomics International as a modification to the MARS disassembly code (FISFAX).⁴⁵ The motion of the fuel and sodium is the basis for a reactivity feedback which is used to calculate the change in reactor

power during fuel-coolant interaction. At the position of pin rupture, the fuel is assumed to disperse homogeneously into the coolant channel, the quantity of fuel being an input parameter. Heat transfer is calculated by an arbitrary exponential-decay function. The sodium mass, temperature, and volume define the thermodynamic state. For a pure liquid system, the Himpan equation of state is used to determine the pressure. In the two-phase region, the pressure is calculated from the vapor equation of state. This pressure is then used to calculate the displacement of the interface, assuming incompressible flow of the constraining liquid plug. As the expulsion proceeds, fuel is carried along with the expanding region. The motion of the fuel is determined by considering drag forces on a spherical particle.

The interesting feature of this model is that it accounts for the motion of the fuel particles during the expulsion process and its effects on reactivity changes. Since the magnitude of the pressurization is dependent upon both the rate of heat transfer between the fuel and sodium and upon the inertial constraint of the surrounding liquid plug, the validity of the model is strongly influenced by whether or not the heat-transfer rate can be expressed as an exponential function, using a thermal decay constant. Also, condensation has been neglected in this model.

Cho's analysis^{46,47} is similar in approach to Padilla's work in that he considers an initial phase of thermally induced liquid expansion before vaporization is allowed for. The two major contributions of his work are that the effects of noncondensable gas are included and his analysis is continued past the onset of boiling. In addition, Cho compares the different rates of expansion, assuming either acoustic or inertial constraints, for two different heat-transfer mechanisms. The acoustic approximation is similar to that described by Padilla; the inertial approximation is similar to that of Duffey's model.

By using different heat-transfer mechanisms, Cho attempted to define the various stages of a fuel-coolant interaction, that is, the initial stage of mixing and fragmentation, followed by quasi-steady heat transfer. In the case of instantaneous fragmentation and mixing, the fuel particles (spheres) were assumed to be in intimate contact with the coolant, the rate of heat transfer being controlled only by the thermal resistance of the fuel. The integral method was used to solve this problem analytically. The second approximation attempts to define the reduction in heat transfer (quasi-steady state) resulting from a finite time for mixing and fragmentation. The heat-transfer coefficient in this case is given by k_f/R (k_f is the fuel thermal conductivity and R the particle radius). Although Cho investigated the effects of different heating rates, constraints, and presence of noncondensable gas, the assumption of an initial phase of sodium liquid expansion is the critical premise which determines the extent of pressurization. If, however, an initial volume of sodium vapor were present, then the thermodynamics of expansion would be quite different. Condensation at the boundaries of the interaction zone has likewise been neglected.

In the General Electric evaluation report of the Fast Flux Test Facility (FFTF),⁴⁸ the specialized case of fuel-coolant interaction resulting from sodium reentry into a channel containing molten fuel was

described. The analysis was carried out by assuming the fuel and sodium to be in intimate contact, the geometric configuration being two semi-infinite slabs in perfect contact. Pressure generation resulted from thermally induced liquid expansion similar to that described previously. The cutoff mechanism for energy transfer was the same as that assumed by Padilla. The assumption that the energy-exchange process can be described by lumping fuel and coolant into two slabs in perfect contact may be physically unrealistic. Whether or not a sodium hammer effect is assumed, it seems reasonable that if the fuel is molten then some fuel dispersal into sodium will occur.

In a similar manner, Westinghouse Corporation analytically evaluated fuel-failure propagation for the FFTF.⁴⁹ In this report, the consequences of fission gas and molten fuel release from a failed pin, and the interaction of molten fuel with sodium coolant were appraised with respect to destructive progression to other pins and through the core. Section 6.3 deals specifically with the modeling of fuel-sodium interaction. Again a perfect-contact model is assumed in which the heating rate was similar to that of the GE model, and the pressurization rate was found from the constant-volume approximation of the equation of state. Essentially an iterative calculation was made to determine the time at which the acoustic pressure pulse associated with the thermal expansion of the heated sodium layer fell below that corresponding to the interface saturation pressure. Cutoff of heat transfer was assumed at this time by considering vapor blanketing of the interface. The available energy in this heated layer was found to be small compared to energy required to deform a single fuel pin. After this initial contact period and a calculation of the available energy associated with the postulated acoustic phenomenology, an estimation was made for the expulsion process as the interacting sodium vaporized. The expulsion process during this stage was determined by the movement of the liquid plugs above and below an expanding vapor bubble, considering the plugs to be incompressible and governed by Newton's second law. The heating rate from the fuel was described by an equation of the form

$$Q(t) = Q(0) \left(1 - e^{-t\mu}\right) \left(1 - \frac{P_v}{1000}\right)^{1/2}.$$

Heat loss due to condensation along the wall film was included.

Probably the most significant contribution from this model is that the fuel-coolant interaction problem was divided into two basically different processes: an initial prefragmentation period followed by a post-fragmentation analysis. This is an important point, since heat transfer and pressure generation during fragmentation might be quite different from that after fragmentation has occurred. However, there are a number of questionable assumptions in the characterization of the heating processes during both stages. The arbitrary decay constant and cutoff of heating at vapor pressures above 1000 psi may not be physically realistic. Also,

during the initial contact period, fragmentation might occur as a result of violent boiling²⁵ or sodium entrapment,⁵⁰ so that the assumptions of no vapor formation until the postulated acoustic pressure pulse has been relieved might not be physically correct.

III. FORMULATION OF THE MODEL

A. Geometry

Although the following analysis is based on the description of a single failed fuel element and its associated coolant, the geometry is assumed to apply to subassembly failures as well. The validity of the model is restricted to a postfragmentation analysis, although a postulated characterization of the initial contact period and fragmentation process is described in Appendix A.

Fig. 1.
Model for Fuel-Coolant Interaction.
ANL Neg. No. 900-776.

Consider the mixing volume, shown in Fig. 1, as the active region for fuel-coolant interaction. This mixing zone expands against an upper and lower liquid plug, in a manner similar to that of slug-type ejection. The rates of pressurization, vaporization, and expulsion are determined by the competing effects of the inertia of the liquid plugs and the rate of heat exchange in the mixing zone.

B. Basic Assumptions

- (1) The initial fuel-sodium mixture is uniform in the interaction region.
- (2) The fuel is in the shape of small spheres, the diameter being a variable input parameter.
- (3) The liquid-vapor mixture is assumed to be in thermodynamic equilibrium throughout the expulsion process. The initial

liquid-vapor ratio is an input parameter resulting from violent boiling during the fragmentation process.

- (4) A liquid-film layer is assumed to wet the surface of the fuel particles and the intact portions of the pin, the initial film thickness being defined by the relative amounts of sodium in liquid and vapor form, and fuel in the mixing zone at the time of interaction.
- (5) The thermal resistance of the film layer is neglected; thus, all temperature gradients are determined by the transient-temperature history of the expanding vapor region.
- (6) A uniform pressure within the interaction zone is assumed.
- (7) The only moving component in the interacting region is the vapor, whose inertia is negligible compared to that of the liquid plugs.
- (8) The thermophysical properties of the fuel are considered to be constant; those of the sodium are temperature-dependent and determined from ANL-7323.⁵¹
- (9) Only axial expansion of the reacting region is considered.
- (10) Effects of noncondensable gas in the mixing zone are neglected.
- (11) The expansion of the mixing zone causes the expulsion of incompressible liquid slugs whose motion is described by Newton's second law.
- (12) The forces acting on the liquid slugs are due to gravity, pressure differences, frictional drag, and resistance effects at abrupt area changes.
- (13) The inlet and outlet pressures are unaltered by the expansion process.

C. Discussion of Assumptions

Assumption (2), of small fuel particles between 200 and 1000 μ in diameter, is consistent with observed experimental data.^{27,52} Although such particles are irregular in shape, spherical characterization is as valid as any. In addition, a relatively simple analytic solution to the heat-transport process is obtained with this geometry. The third assumption is consistent with the premise that the ejection occurs as a result of sodium vaporization. This assumption of equilibrium ejection has been validated for sodium-voiding models⁵³ which are similar to the single-bubble analysis used here. As discussed in Appendix A, the assumption of presence of sodium vapor at the start of the analysis is consistent with the hypothesis that molten-fuel breakup results from violent boiling during initial contact.

Assumption (4) is based on results of voiding experiments which have shown that liquid film adheres to the test-section walls during the expulsion process.⁵³⁻⁵⁵ Although the stability of this film is dependent upon many parameters (e.g., heat flux, physical surface condition, vapor velocity, and hydraulic diameter), experiments indicate that this film remains on the wall for a significant portion of the expulsion time. For surfaces cooler than the vapor temperature, this film serves as a site for condensation. The description of a liquid film wetting the fuel particles is essentially a bookkeeping method. In actuality, it is thought that some combination of Leidenfrost, transition, and/or nucleate boiling (see Fig. 2) occurs; once the liquid within the initial interaction region vaporizes,

Fig. 2.
Boiling-heat-transfer Mechanisms.
ANL Neg. No. 900-784.

the fuel heat transport is essentially terminated. In order to describe such a process, a film layer is assumed to adhere to a defined fuel fraction and particle size, which represents the net volume-to-surface ratio associated with intermittent contact between fuel and liquid sodium. Assumption (5), of negligible film thermal resistance, is valid for liquid metals since the thermal boundary layer is equal to or larger than the film thickness within a short period of time.

Conditions (6) and (7) are common to most single-bubble models,⁵⁶⁻⁵⁸ and have been validated by good agreement between experimental and theoretical results for relatively short channels.⁵⁸ However, for longer channels with significant axial dependence of the vaporization and condensation rates, the assumption of uniform bubble pressure may not be valid,⁵⁹ and the effect of vapor inertia may cause wall-film breakup.⁶⁰ In the case of fuel-coolant interaction, however, the bubble pressure is significantly higher than the system pressure such that any pressure differential within the bubble can be neglected as far as it effects the expulsion process. The restrictions owing to conditions (8), (9), and (10) can be altered if a greater degree of sophistication is desired.

Since the propagation time associated with acoustic effects ($2L/v_c$) is small compared to that associated with the expulsion process, the expansion of the bubble is essentially controlled by the inertia of the liquid slugs. Likewise, since the vapor within the mixing region cushions to a great extent pressurization, assumptions (11), (12), and (13) are made. Additional assumptions entailed in the analysis will be stated as the model is developed.

D. Theoretical Development

The problem to be solved is that of the addition of heat to an expanding two-phase equilibrium mixture. The basic solution, as developed, is quite general and can be applied to a variety of energy-transfer problems. An approach similar to that developed here was used in the analysis of single-bubble expulsion from a heated channel.⁵⁷ The results of that analysis are briefly illustrated in Appendix B.

The generalized macroscopic energy balance for a two-phase mixture is determined by applying the differential form of the first law of thermodynamics to the sodium:

$$\frac{dQ}{dt} - \frac{dW_{by}}{dt} = \sum_{\ell, v} \left(\frac{dH}{dt} \right) + \frac{d(KE)}{dt} + \frac{d(PE)}{dt}, \quad (1)$$

where Q refers to the overall heating rate to the sodium coolant, and W_{by} is the work done by the sodium excluding flow work which is required to push mass into or out of the region; H is the enthalpy of the sodium (liquid and vapor), KE is kinetic energy, and PE is potential energy. If a steady-flow frictionless process is assumed during the time increment, then

$$\frac{dW_{by}}{dt} = -v \frac{dP}{dt} - \frac{d(KE)}{dt} - \frac{d(PE)}{dt}. \quad (2)$$

Thus, the overall differential macroscopic energy balance on the sodium is

$$\sum_{EES} \left[\frac{dQ}{dt} - m_{\ell} \frac{\partial \bar{h}_{\ell}}{\partial t} \right] - \sum_{EES} \left[\bar{h}_{\ell} \frac{\partial m_{\ell}}{\partial t} \right] + \left[v \frac{dP}{dt} \right] = \left[\frac{\partial (m_v \bar{h}_v)}{dt} \right], \quad (3)$$

where the first term on the left-hand side of Eq. 3 represents the rate of heat transport at each energy-exchange surface (EES) minus the energy storage within its associated liquid-film layer. The second is due to the change in the mass of the liquid at each surface resulting from vaporization or condensation (Eq. 13), and the third is the work. The heat-transfer rates at each energy-exchange surface are:

Spheres (Fuel Particles)

The heat-transfer rate across the fuel particles, neglecting the heat of fusion, is

$$\frac{dQ_s}{dt} = n_s k_f S \left. \frac{dT_s(r,t)}{dr} \right|_{r=a} . \quad (4)$$

The time-dependent solution for the temperature gradient is found by solving the transient heat-conduction equation, assuming concentric isothermal surfaces within a sphere whose properties are constant. The form of this equation is

$$\rho c_p \frac{\partial T(r,t)}{\partial t} = k \left(\frac{\partial^2 T(r,t)}{\partial r^2} + \frac{2}{r} \frac{\partial T(r,t)}{\partial r} \right) . \quad (5)$$

If the surface temperature is determined by the transient-pressure history within the vapor space (assuming vapor-liquid equilibrium) and the initial temperature distribution is a constant, then a solution can be found by applying the following boundary and initial conditions:

$$T(r,0) = T_0; \quad T(a,t) = \phi(t); \quad \left. \frac{dT(r,t)}{dr} \right|_{r=0} = 0 .$$

The solution to Eq. 5 and the above boundary conditions is similar to that derived in Ref. 61 (p. 200), and results in a temperature gradient whose solution is

$$\left. \frac{dT_s(r,t)}{dr} \right|_{r=a} = \frac{2\pi}{a^3} \sum_{n=1}^{\infty} n(-1)^n \exp[-\alpha_f n^2 \pi^2 t/a^2] \left\{ -T_0 \frac{a^2}{n\pi} (-1)^n - \alpha_f n \pi (-1)^n \int_0^t \phi(\tau) e^{\alpha_f n^2 \pi^2 \tau/a^2} d\tau \right\} . \quad (6)$$

Intact Walls

The heat-transfer rate across physical boundaries (intact fuel pin or test vessel) is given by

$$\frac{dQ_w}{dt}(t) = h_{fm} C \int_{x=\xi_2}^{x=\xi_1} [T_w(x,t) - \phi(t)] dx , \quad (7)$$

where C is circumference, ξ_1 and ξ_2 are the positions of the upper and lower plug interfaces, and h_{fm} is the film-heat-transfer coefficient, defined as

$$(\text{vaporization}) \quad h_{fm} = k_{Na}(T)/\sigma ;$$

$$(\text{condensation}) \quad h_{fm} \leq k_{Na}(T)/\sigma ,$$

where

$$\sigma(\text{wall}) = 0.015 \text{ cm} ; \sigma(\text{particles}) = f(D_s, \%V) .$$

Slug Interfaces

The heat transfer across the upper and lower slug interfaces is

$$\frac{dQ_I(t)}{dt} = k_{Na} A \left. \frac{dT(\xi, t)}{d\xi} \right|_{\xi_1, \xi_2=0} . \quad (8)$$

As in the case of the fuel particles, the temperature gradients at the interfaces are found by solving the transient-heat-conduction equation for slab geometry, assuming isothermal surfaces parallel to the interfaces. The form of this equation is

$$\alpha \frac{\partial^2 T(\xi, t)}{\partial \xi^2} + \frac{\dot{Q}(\xi, t)}{\rho_l c_p} = \frac{\partial T(\xi, t)}{\partial t} , \quad (9)$$

subject to

$$T(\xi, 0) = F(\xi) ; \quad T(0, t) = \phi(t) ; \quad T(\infty, t) = \infty .$$

The solution for the interface temperature gradient was derived by Cronenberg:⁶²

$$\begin{aligned} \left. \frac{dT(\xi, t)}{d\xi} \right|_{\xi=0} = & - \int_0^t \frac{1}{\sqrt{\pi\alpha(t-\tau)}} \frac{d\phi(\tau)}{d\tau} d\tau - \frac{\phi(0)}{\sqrt{\pi\alpha t}} \\ & + \int_0^\infty d\xi \int_0^t \frac{\xi}{2k\sqrt{\pi\alpha(t-\tau)^3}} \exp \left[\frac{-\xi^2}{4\alpha(t-\tau)} \right] \dot{Q}(\xi, \tau) d\tau \\ & + \int_0^\infty \frac{F(\xi)}{2\alpha} \frac{\xi}{\sqrt{\pi\alpha t^3}} \exp \left[\frac{-\xi^2}{4\alpha t} \right] d\xi , \end{aligned} \quad (10)$$

where $\dot{Q}(\xi, \tau)$ is the equivalent volumetric-heat-input rate from the intact fuel element to the liquid slug, which is given by

$$\dot{Q}(\xi, \tau) = \frac{h_m}{D_e} \left[T_{cl}(\xi, \tau) - T_m(\xi, \tau) \right] ; \quad (11)$$

h_m is the heat-transfer coefficient determined from the Nusselt number calculated for the flow of sodium through annular channels:⁶³

$$Nu = 0.8 \left(\frac{r_o}{r_i} \right)^{0.3} \left[5.1 + 0.028 P_l^{0.8} \right] . \quad (12)$$

The equilibrium temperature, $\phi(t)$, not only determines the rate of heat transfer but also the saturation pressure $P(t)$ and the enthalpies $h_2(t)$ and $h_v(t)$. The variation in the mass of the liquid on the fuel particles and along wall surfaces is

$$\frac{dm_l}{dt} = \frac{1}{\lambda} \left[\frac{dQ}{dt} - m_l c_p \frac{dT_{fm}}{dt} \right] , \quad (13)$$

where $\frac{dQ}{dt}$ is the heat-transfer rate at each surface and T_{fm} is the film temperature which equals $\phi(t)$. If the change in liquid mass from Eq. 13 and the change in vapor mass from Eq. 3 are known, the volumetric rate of expansion of the interacting region is calculated as

$$A \frac{d\Delta x}{dt} = \frac{1}{\rho_l(t)} \frac{dm_l}{dt} + \frac{1}{\rho_v(t)} \frac{dm_v}{dt} . \quad (14)$$

Equation 14 may be solved providing $\phi(t)$ is a known function of time. This is accomplished by coupling the energy equation to the momentum equations of the constraining plugs. The coupling parameter used here is $\phi(t)$, which determines the saturation pressure within the vapor space. If this pressure is known, the momentum equation (assuming incompressible plug flow) is integrated by a fourth-order Runge-Kutta routine to obtain the position x , the velocity $\dot{x}$, and the acceleration $\ddot{x}$ of both the upper and lower plug interfaces.

The forces acting on the liquid slugs during expulsion are due to gravity, pressure differences, frictional drag, and expansion losses at the channel-plenum junctions. The resistance coefficient at each junction is calculated from

$$K_{e_n} = \left[1 - \frac{D_{n-1}^2}{D_n^2} \right]^2 , \quad (15)$$

so that the total pressure loss due to expansion effects is given by

$$\Delta P_{\text{exp}} = \sum_{n=2,3,4\dots} K_{e_n} \frac{\rho \dot{x}_{n-1}^2}{2} . \quad (16)$$

The frictional drag is estimated from the Blasius relation, where the friction factor is given by

$$f_n = 0.316 \text{Re}_n^{-0.25} , \quad (17)$$

so that the total pressure drop due to friction losses is

$$\Delta P_{\text{frc}} = \sum_{n=1,2,3\dots} \frac{f_n L_n \dot{x}_n^2}{2 D_e} , \quad (18)$$

where L_n is the length of the liquid plug in each region and D_e is the equivalent diameter within the respective regions.

The resulting force balance on the upper slug is therefore

$$\sum \text{Forces} = (P_v - P_{gp}) - \Delta P_{\text{frc}} - \Delta P_{\text{exp}} - \left(L'_1 + \sum_{n=2,3,4\dots} L_n - x \right) \rho g . \quad (19)$$

The inertia of the column is given in terms of the acceleration of the interface within the test section ($n = 1$):

$$\sum M\ddot{x} = \left(L'_1 + \sum_{n=2,3\dots} \frac{D_1^2}{D_n^2} L_n - x \right) \rho \ddot{x} . \quad (20)$$

The acceleration of the interface is obtained by equating Eqs. 19 and 20:

$$\ddot{x} = \frac{(P_v - P_{gp}) - \Delta P_{\text{frc}} - \Delta P_{\text{exp}} - \left(L'_1 + \sum_{n=2,3,4\dots} L_n - x \right) \rho g}{\left(L'_1 + \sum_{n=2,3\dots} \frac{D_1^2}{D_n^2} L_n - x \right) \rho} . \quad (21)$$

A similar equation is obtained for the bottom slug which, however, also considers the momentum of the liquid leg between the pump and the coolant channel inlet as well as the pump head.

The volumetric expansion rate calculated from the energy equation is then compared with that calculated from the momentum equation. If they do not agree within a specified error tolerance, a new value of $\phi(t)$ is chosen, and the iteration continued until the error criterion is satisfied. The calculation then proceeds to the next time step.

For a two-phase sodium mixture, the above solution is used. However, if only a small amount of initial vapor is present, then the possibility exists that complete vapor collapse will occur, due to both liquid expansion and vapor condensation. For a pure liquid the equation of state relating P , V , and T is written as

$$V = V(P, T) \quad (22)$$

or⁶⁴

$$\frac{\partial V}{\partial t} = -\beta_T V \frac{dP}{dt} + \alpha_p V \frac{dT}{dt}, \quad (23)$$

where

$$\beta_T \equiv -\frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_T \quad (24)$$

is the isothermal compressibility, and

$$\alpha_p \equiv \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_p \quad (25)$$

is the thermal-expansion coefficient. Both α_T and β_T are determined from polynomial expansions in temperature,⁶⁵ based upon tabulated values in ANL-7323.⁵¹ If heat losses to the walls and cold plugs are neglected, the rate of temperature rise of the hot sodium liquid plug is

$$\frac{dQ_s}{dt} = m_l c_p \frac{dT}{dt},$$

where dQ_s/dt is given by Eq. 4 and m_l equals the mass of the sodium liquid in the interaction zone at the time of vapor collapse. If the temperature rise during a time increment is known and iteration is carried out for pressure, the equation of state and the momentum equation are continuously solved until the calculated pressure falls below the saturation pressure.

At this time, vaporization is reestablished, and Eqs. 14 and 21 are again used to calculate the expansion and pressure history.

E. Description of the Computer Code

Since this work is basically a model-feasibility study, a relatively simple computational approach was used. If the model proves successful, then it may be incorporated into a more sophisticated accident-analysis code, such as the SASIA.⁶⁶ With this approach in mind, a computer program was written in modular form, such that relatively easy coupling should be possible. In fact, the initial temperature distributions at the time of pin failure were calculated from a modified version of SASIA called SASIA-Ash,⁶⁷ and used as input data. The code was written in Fortran-IV for the CDC-3600 digital system, in the form of a driver program and a number of subroutines. All input data are read in by the driver and stored in common blocks, facilitating easy transfer to appropriate programs and subroutines. Control is transferred to a main program which executes the solution scheme outlined in Fig. 3. The solution printout is likewise executed from the main program.

All input parameters should be in cgs units, since internal computations are made in this system. The analysis is carried out considering the cladding-bond interface of the fuel element to be adiabatic from the

Fig. 3. Block Diagram for Numerical Solution.
ANL Neg. No. 113-1619.

time of failure. In this manner, the initial conditions for the fuel-element heat-transport analysis during the interaction calculation are the axial temperature profiles at both the cladding-bond and cladding-coolant surfaces and the mixed mean coolant temperature profile. Likewise, channel dimensions, material properties (except for sodium), system pressures, fuel-particle size, initial volume fractions and film thicknesses, spacial mesh size, and time step are all read in as input data.

Although the axial node size does not effect the numerical stability of the problem, the accuracy of the solution is somewhat dependent upon mesh length, since the heat transport within each axial location is considered constant. A mesh length of 4.0 cm was found to be satisfactory. Some degree of compromise must, however, be made in the selection of the time interval to insure stability and convergence. This is especially true during the first few milliseconds when there is a high initial heat-transfer rate counteracted by the low momentum of the constraining liquid plugs. A time increment of 0.00002 sec for the first 50 time steps and a 0.00020-sec increment for the remainder of the problem were found to be satisfactory. Typical running times for the CDC-3600 were about 10 min per problem.

IV. DISCUSSION OF THE FUEL-FAILURE EXPERIMENT

A. Description of the TREAT Reactor and the Mark-II Loop

As evidenced in the literature survey, there have been several parallel approaches used in studies of the fast-reactor fuel-failure problem. However, because of the varied and complex phenomena involved, emphasis has been placed on experiments which give the best simulation of actual reactor accident conditions. To date, such studies have centered around the in-pile TREAT experiments.

Basically TREAT^{24,68} illustrated in Fig. 4, is a pulsed, graphite-moderated, thermal testing reactor, specifically designed to evaluate

Fig. 4. Cutaway View of TREAT Reactor.²⁴
ANL Neg. No. 112-771.

fast-reactor fuels and structural materials. The principal design criterion was to maximize the integrated neutron flux without damaging the core. This was accomplished by using a highly enriched fuel ($U_3O_8 \sim 93\%$ enrichment, average particle diameter = 17μ) dispersed in a graphite matrix. The high inherent heat capacity of graphite not only serves as a sizable heat sink during the power excursion, but also generates a negative reactivity feedback, which ensures termination of the transient. Since a maximum core-averaged flux of approximately 3.0×10^{15} nt/cm² sec

is obtainable,³³ test elements which do not contain graphite will reach their melting temperatures while the core remains relatively cool ($\sim 400^\circ\text{C}$, peak).²⁴

Within the reactor core, space was provided for the placement of a self-contained capsule within which meltdown experiments could be performed. The most recent of such vessels is the Mark-II^{69,70} integral-sodium-test loop. This capsule was developed as a high-temperature, high-pressure hydraulic loop, which provides a flowing-sodium test environment. As shown in Fig. 5⁶⁹ this loop is a self-contained package employing a U-tube geometry. The test leg is instrumented at the inlet and outlet for flow, pressure, and temperature. The opposite leg consists of an in-line annular induction pump for coolant circulation. The loop is enclosed within a hermetically sealed stainless steel container, equal in size to two TREAT subassemblies (4×8 in.). The loop was designed to withstand a static pressure rating of 340 atm at a temperature of 538°C .⁷⁰ Mockup of sodium flow conditions is achieved by adjusting the pump power, while energy simulation is obtained by altering the reactor neutronics.

B. The H-2 Experiment¹

In this experiment, a single, prototypical Fast Flux Test Facility (FFTF) fuel element was taken to failure in the Mark-II loop during a flowing-sodium, pulsed overpower transient. Although the prime objective was to determine the mode and threshold of failure, the relatively simple geometry facilitated the analysis of postfailure coolant dynamics. Figure 6 illustrates a blowup view of the sodium loop and test section; Fig. 7 shows a closeup view of the test element within the adiabatic (Dewar) holder.

The test pin consisted of mixed-oxide nonpreirradiated fuel (25% PuO_2 -75% UO_2 , 88% and 65% enrichment, respectively) clad in a stainless steel jacket. The cold-clean dimensions were 0.493-cm OD for fuel and 0.038-cm-thick cladding with a nominal diametrical gap of 0.015 cm. The steady-state (at zero reactor power) loop conditions were a sodium temperature of 427°C , a gas plenum pressure of 2.53 atm, and a test-section flow velocity of 400 cm/sec. The conditions at failure were an element OD of approximately 0.596 cm and a flow velocity of 670 cm/sec, the fuel being approximately 0.519 cm in diameter at this time.

C. Geometric and Thermohydrodynamic Simulation of the Experiment

Before experimental and theoretical results can be compared, suitable mockup of the test conditions must be made. The following analysis achieves this objective. In each of the plenum regions above the test element, the flow area is obtained by simply subtracting out the volumetric displacement of the fixtures used to hold the test pin. In this manner, the frictional pressure losses in each of the upper plenum regions are estimated from the diameters associated with their respective flow areas. However, along the test element, an annulus is used to determine both the heat transfer and frictional losses at both the walls of the fuel pin and adiabatic holder. Figure 8 illustrates this equivalent channel mockup; in Table I are listed the pertinent dimensions and initial conditions.

Fig. 5. Layout of the Mark-II Integral-Sodium Test Loop.⁶⁹ ANL Neg. No. 112-6766.

Fig. 6. Sodium Loop and H-2 Test Section.⁷³
ANL Neg. No. 900-436.

Fig. 7. H-2 Test Element within Dewar Vessel.⁷³ ANL Neg. No. 900-783.

Fig. 8. Equivalent Coolant-channel Mockup of Test Section.
ANL Neg. No. 900-789.

TABLE I. Dimensions and Initial Conditions for H-2 Experiment

Flow-area Diameters (cm)

D_1	0.561
D_2	2.330
D_3	2.654
D_4	2.936
D_5	1.310
D_6	1.910

Section Lengths (cm)

L_1	60.00
L_2	16.00
L_3	11.27
L_4	13.65
L_5	1.43

Fuel-pin Diameter (OD) (cm)

D_f	0.5954
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Inside Diameter of Dewar Wall (cm)

D_{w1} (section L_1)	0.825
D_{w2} (section L_2)	2.408

Pressures (atm)

P_1	3.660
P_2	2.544
P_3	2.530

At the time of failure, the pressure at the top of the sodium column (P_3) was taken to be equal to the cover-gas plenum pressure (2.53 atm). Likewise, since it was assumed that the sodium expelled during the interaction empties through the coolant overflow (see Figs. 5 and 8), P_3 is assumed to remain constant throughout the analysis. The pressure P_1 at the test-section inlet is taken to be the sum of the exit pressure P_3 , the static pressure head between the gas plenum and the D_2/D_1 junction (0.014 atm), and the dynamic pressure drop calculated from SAS1A-ASH⁶⁷ across the fuel pin just prior to failure (1.116 atm). In this manner, P_1 was found to be 3.660 atm. Since a constant power was supplied to the pump throughout the transient, the test-section inlet pressure was assumed to remain fixed at this value, because the pump characteristics were such that the pressure head developed in the region of operation was essentially the same as that when the flow rate approached zero (or reversal).^{*} Also

^{*} At the time of failure, the coolant velocity in the test section ($D_1 = 0.561$ cm) was 670 cm/sec, which corresponded to a volumetric flow rate of 2.62 gal/min. As seen in Ref. 71 (Fig. 7), the difference in pump heat at this flow rate and zero (or reversal) was negligible.

since the velocities in the elbow connecting the pump and test section were small (relatively large cross-sectional area compared to the test section), frictional losses were neglected.

In addition to defining the geometric and pressure characteristics of the loop, the temperatures along the walls of both the fuel pin and Dewar vessel must be specified, as well as that of the coolant. These temperature profiles were calculated from the SASIA-ASH code. To check the accuracy of the code, Agrawal⁷² made a comparison (see Fig. 9) between the data obtained from the thermocouple nearest the top of the fuel column,

Fig. 9. Comparison of Measured Coolant Temperatures with Temperatures Calculated from SASIA-ASH Code.⁷² ANL Neg. No. 900-423.

during a checkout transient, with the calculated coolant temperatures at this point. As indicated, the measured temperature lagged the calculation by about 40 msec; however, the thermocouple response time accounted for about 20 msec. Thus, it was concluded that the heat-transfer characteristics of the code are fairly accurate. For the power conditions of the actual failure transient, the calculated cladding and coolant temperatures⁷² are plotted in Figs. 10 and 11. At the time of failure, the wall temperature of the Dewar vessel was defined as equal to that of the coolant. If these temperatures are used as initial values, the transient heat transfer within both the cladding and adiabatic holder can be determined by making use of a simplified set of finite-difference equations. The analysis is carried out considering both the cladding-bond interface of the fuel pin and the inner wall-vacuum interface of the Dewar vessel to be adiabatic during the interaction process. Knowing this information, calculational simulation of the experiment is possible.

D. Analysis of the Experimental Data

The test data for the destructive transient are given in Fig. 12.⁷³ These data include the test-section inlet and outlet coolant velocities, the inlet pressure, and the coolant temperatures measured at the test section inlet and at positions 1.0 in. below and 7.0 in. above the top of the fuel column. The flowmeters were of the emf type; fast-response chromel-alumel thermocouples were used. Fuel failure is indicated by both

Fig. 10.
Axial Cladding-temperature
Profiles at Time of Failure,
Calculated from SAS1A-ASH Code.
ANL Neg. No. 900-775.

Fig. 11.
Axial Mixed-mean Coolant-
temperature Profile at Time
of Failure, Calculated from
SAS1A-ASH Code.
ANL Neg. No. 900-770.

Fig. 12. Test Data during Failure Transient.⁷³
ANL Neg. No. 900-409.

flow and pressure anomalies at approximately 1.47 sec. The thermocouple data, when corrected for a response time of approximately 20 msec, also indicate a failure time at approximately 1.47 sec.

Since the model attempts to describe the heat transfer within the mixing zone, a desirable parameter for analysis would be the transient temperature history within this region. Although the thermocouple nearest the top of the fuel column is presumably within the mixing zone, it is uncertain exactly what temperature is being recorded. As shown in Fig. 12, a rapid temperature rise is indicated at about 1.47 sec, with the recorder shortly going off scale. Most likely this rise is due to hot molten fuel fusing with the thermocouple, destroying it in the process. Any attempt to interpret the data quantitatively therefore seems questionable. The rapid temperature rise of the thermocouple, however, does indicate that molten fuel must have entered the coolant in this area. The preburst temperature reading of this thermocouple, from time 1.2 to 1.47 sec, is also consistent with the SASIA-ASH calculations, indicating that temperature profiles obtained from this code, at failure, are reliable. Any analysis of the coolant temperatures at the inlet and outlet transducers would be meaningless with respect to the fuel-coolant interaction problem, since these readings pertain to the cold liquid plugs above and below the interaction zone.

Changes in dynamic pressure measured at the lower transducer are, likewise, of little use in determining the experimental pressurization rate in the mixing zone, since the transient effects of compressibility and pressure losses within the liquid plugs were difficult to determine quantitatively. Therefore, of the experimental data available for analysis, the flow rates measured at the upper and lower meters were chosen as the basis for comparison with theory.

The measured flow rates and their corresponding velocities with respect to the test section are shown in Figs. 13 and 14. As indicated by the flowmeter readings, the coolant behavior is quite complicated, although a number of somewhat defined anomalies occur. This series of events is thought to result as a consequence of a time-delayed sequence

Fig. 13. Coolant Velocities Obtained from Upper Flowmeter.
ANL Neg. No. 900-780.

Fig. 14. Coolant Velocities Obtained from Lower Flowmeter.
ANL Neg. No. 900-779.

of ruptures occurring along the axial length of the pin. Although a complete description of the entire interaction process would be desirable, only the first series of anomalies will be analyzed, those between 1.47 and 1.55 sec. The flow rates were first averaged to the same steady-state velocity of 666 cm/sec in the test section, as indicated in column 3 of Tables II and III. The incremental displacement of the fluid (column 4) was then calculated; the time-integrated movement is given in column 5. Up to approximately 1.47 sec, the inlet and outlet flow rates were about the same. However, past this time the velocity measured at the upper flowmeter increased, while that at the lower meter decreased, indicating

TABLE II. Fluid Velocity and Movement Obtained from Upper Flowmeter

Time (sec)	Velocity in Test Section (cm/sec)	Averaged Test- section Velocity (cm/sec)	Incremental Fluid Movement (cm)	Integrated Movement (cm)
1.400	+ 717.0	+ 666.0	0.00	0.00
1.425	+ 717.0	+ 666.0	+16.65	+ 16.65
1.450	+ 717.0	+ 666.0	+16.65	+ 33.30
1.460	+ 717.0	+ 666.0	+ 6.66	+ 39.90
1.470	+ 845.0	+ 794.0	+ 6.66	+ 46.62
1.480	+1015.0	+ 964.0	+ 7.93	+ 54.55
1.490	+ 717.0	+ 666.0	+ 9.62	+ 64.17
1.500	- 170.0	- 221.0	+ 6.66	+ 70.83
1.505	- 127.0	- 178.0	- 1.10	+ 69.73
1.510	+ 760.0	+ 709.0	- 0.89	+ 68.84
1.515	+2955.0	+2904.0	+ 3.54	+ 72.38
1.520	+4980.0	+4929.0	+14.51	+ 86.89
1.525	+2530.0	+2479.0	+24.64	+111.53
1.530	-1265.0	-1316.0	+12.41	+123.94
1.535	-2110.0	-2161.0	- 6.59	+117.35
1.540	- 422.0	- 573.0	-10.81	+106.54
1.545	+ 422.0	+ 371.0	- 2.86	+103.68
1.550	+ 506.0	+ 455.0	+ 1.86	+105.54
			+ 4.55	+110.09

TABLE III. Fluid Velocity and Movement Obtained from Lower Flowmeter

Time (sec)	Velocity in Test Section (cm/sec)	Averaged Test- section Velocity (cm/sec)	Incremental Fluid Movement (cm)	Integrated Movement (cm)
1.400	+ 615.0	+ 666.0	+ 0.00	
1.425	+ 595.0	+ 646.0	+16.65	+16.65
1.450	+ 575.0	+ 626.0	+16.15	+32.80
1.475	+ 425.0	+ 476.0	+15.61	+48.41
1.500	0.0	+ 51.0	+11.90	+60.31
1.505	- 215.0	- 164.0	+ 1.275	+61.585
1.510	- 425.0	- 374.0	- 0.820	+60.765
1.515	- 515.0	- 464.0	- 1.870	+58.895
1.520	- 640.0	- 589.0	- 2.230	+56.575
1.525	-1490.0	-1439.0	- 2.945	+53.630
1.530	- 900.0	- 849.0	- 7.195	+46.435
1.535	- 215.0	- 164.0	- 4.245	+42.190
1.540	+ 220.0	+ 271.0	- 0.820	+41.370
1.545	+ 340.0	+ 391.0	+ 1.355	+42.725
1.550	+ 680.0	+ 731.0	+ 1.955	+44.680
			+ 3.655	+48.335

that coolant displacement must have occurred. By assuming slug flow, the displacements of the upper and lower liquid plugs were obtained (see Fig. 15). Each curve was divided into four sections representing the sequence of events prior to, during, and following a molten fuel-coolant interaction. From 1.40 to 1.47 sec, the velocities at both ends of the test section were the same, indicating that fuel-coolant interaction had not yet occurred. At 1.47 sec, the relative displacement between the upper and lower plugs indicates that either a sodium bubble has formed due to boiling or that sodium has been displaced due to fuel-element failure. From both the SASIA-ASH calculations and the measured thermocouple data, sodium boiling (without fuel-coolant interaction) could not have occurred, since the coolant is well below saturation at all axial positions within the channel. Therefore, the displacement of coolant must have been due to the entrance of fuel, cladding, and/or bond gases. The SASIA-ASH calculations also indicate that the failure criterion is satisfied at this time and that over half the cross-sectional area of the fuel pin has reached the fuel melting temperature⁷² (2800°C for UO₂). Thus, it may be assumed that pin failure occurred at this time.

The overall accuracy of the voiding curve is limited by a number of factors. Since the displacement was obtained from the measured velocity, the accuracy of the curve depends not only upon errors associated with the experimental instrumentation but also upon the accuracy of the data reduction. The measurement errors are due to electronic-recording and calibration uncertainties. These errors were estimated to be approximately 10%, which corresponds to the difference between the two flowmeter readings recorded at steady state. The accuracy of the data reduction is limited by the ability to read the velocity graphs. Although an attempt was made to interpret the velocity curves to the third significant figure, only the

Fig. 15. Coolant Motion as Determined from the Flowmeter Data Relative to Test Section. ANL Neg. No. 900-777.

first two can be read with assurance. The error associated with the data reduction should therefore not exceed $\pm 10\%$. Thus, the accumulated maximum error is approximately 20%.

Currently, it is thought that essentially two different types of energy processes occur during the interaction. Initially, fuel, cladding, and inert gases enter the coolant channel. During this initial period, the molten fuel fragments into smaller particles, mixing with the coolant and transferring heat in the process. The energy and momentum transport during these first few milliseconds may be quite different from that after fragmentation has occurred. Therefore, a proper analysis of the prefragmentation period is crucial. Although there has been some analytic characterization of this initial contact period, all work has been based on the assumption of strictly heat conduction (no boiling) during this period. This assumption, however, has not been validated by experiments. On the contrary, there is strong indication, as discussed in the literature survey and Appendix A, that vapor generation may be the actual cause of fuel breakup. Of the four fragmentation theories reviewed by Witte *et al.*,⁷ that is, the entrapment, violent boiling, shell, and inertia (Weber Number) theories, all but the last consider vaporization as the initiating mechanism of breakup of molten material. However, the Weber Number effect has been shown to be important mainly with materials at a much lower

temperature range than that of molten UO_2 . Thus, vaporization during fragmentation is assumed to occur.

In order to account (in a rough way) for the vapor generated during fragmentation and the displacement of coolant by fuel, a mixing period was assumed from the time when voiding first started to the time when rapid expulsion commenced. As shown in Fig. 15, this period lasted from approximately 1.47 sec to 1.51 sec. Once a significant amount of fuel breakup has occurred, a much larger surface area is available for heat transfer, and thus rapid expulsion.

Before the calculational mockup of the expulsion process can be made, the initial position from which the vapor slug grows must be located. Both the results of the SASIA-ASH calculations and the neutron hodoscope system⁷⁴ (a bank of 334 neutron detectors focused axially and radially along the pin, which determines the fuel density based on neutrons emanating from the test element: Ref. 75) indicate that failure initiated near the top of the fuel column. As shown in Fig. 10, the axial cladding-temperature profiles are quite steep, the top of the fuel column having an average cladding temperature of 1000°C . Based on an evaluation of the fuel expansion, hoop stress, and inner and outer cladding temperatures, Agrawal⁷⁰ estimated that approximately the upper 5.0 to 10.0 cm of the fuel pin failed at the time of the flow anomalies. Likewise, analysis of the hodoscope data indicated that extensive fuel movement occurred in the top third of the fuel column prior to this time.⁷⁴ Therefore, it was reasoned that initial failure occurred in the top of the fuel column, with an approximate failure zone of 10.0 cm. Table IV gives the lower-interface position starting from a distance 5.0 cm below the top of the fuel; Table V gives the upper-interface position starting from a distance of 5.0 cm above the top of the fuel. When the data indicate that the top slug has reached the plenum junction, the calculated displacement was based upon the velocity within the plenum section. Figure 16 shows the voiding curve based upon the above-mentioned analysis.

In Fig. 17⁷³ a cutaway view of the failed pin and adiabatic holder is shown. As can be seen, the final destruction was quite extensive. Information concerning the time sequence of failure along the axial length of the test element cannot, however, be obtained from this picture. In view of the complicated coolant behavior and extent of failure, a description of all but the initial process would be difficult, if not impossible.

TABLE IV. Interface Position of Lower Slug during Postfragmentation Expulsion

Time (sec)	Velocity in Test Section (cm/sec)	Incremental Displacement in Test Section (cm)	Interface Position (cm)
1.510	- 374.0		+35.00
		-1.870	
1.515	- 464.0		+33.130
		-2.320	
1.520	- 589.0		+30.810
		-2.345	
1.525	-1439.0		+27.865
		-7.195	
1.530	- 849.0		+20.670
		-4.245	
1.535	- 164.0		+16.425
		-0.820	
1.540	+ 271.0		+15.605
		+1.355	
1.545	+ 391.0		+16.960
		+1.955	
1.550	+ 731.0		+18.915

TABLE V. Interface Position of Upper Slug during Postfragmentation Expulsion

Time (sec)	Velocity in Test Section (cm/sec)	Plenum Velocity (cm/sec)	Incremental Displacement (cm)		Interface Position (cm)
			Test Section	Plenum	
1.510					+45.00
	+ 709.0	+ 41.06	+ 3.54	+0.205	
1.515					+48.540
	+2904.0	+168.37	+14.52	+0.842	
1.520					+60.177
	+4929.0	+285.88	+24.65	+1.429	
1.525					+61.606
	+2479.0	+143.90	+12.41	+0.719	
1.530					+62.325
	-1316.0	- 76.39	- 6.58	-0.382	
1.535					+61.943
	-2161.0	-125.34	-10.81	-0.627	
1.540					+61.316
	- 573.0	- 33.23	- 2.86	-0.166	
1.545					+61.150
	+ 371.0	+ 21.52	+ 1.85	+0.108	
1.550					+61.258
	+ 455.0	+ 26.39	+ 2.28	+0.132

Fig. 16. Experimental Voiding Curve Resulting from Molten UO_2 -Na Interaction.
ANL Neg. No. 900-778.

H-2

Fig. 17. Cutaway View of Failed Fuel Element and Adiabatic Holder.⁷³ ANL Neg. No. 900-730.

V. DISCUSSION OF RESULTS

Results of parametric calculations are compared with the experimental voiding curve in Figs. 18 through 31. The initial conditions for each calculation are summarized in Table VI. A uniform dispersion of fuel within the mixing zone is assumed, the initial fuel temperature being taken as the melting point (2800°C). For a defined set of initial conditions, the number of particles and the associated film thickness were determined in a manner exemplified in Appendix C. The thermophysical properties of the fuel, cladding, Dewar vessel, and sodium are given in Appendix D.

Problems A and B

As discussed in the literature survey, the instantaneous mixing models of Padilla^{42,43} and Cho^{46,47} have received considerable attention. A series of calculations was therefore made involving the basic dynamics of such models, the results of which were compared with the TREAT experiment. For the sake of consistency with other calculations presented, the only difference in this series is the assumption of no initial vapor presence. Figures 18 and 19 illustrate the results for two different fuel fractions. As indicated, the theoretical calculations overestimate the experimental voiding rate, especially during the initial stages. Essentially two competing processes are involved, thermally induced liquid expansion counteracted by the inertia of the constraining plugs. During the early period of high heat flux and a relatively low rate of expulsion, pressurization occurs. As the transient heating rate decreases with time and the momentum of the plugs increases, the pressure relaxes until it falls below that of saturation, thus initiating vaporization (~ 0.2 ms later).

If the critical conditions of instantaneous mixing and an initial period of perfect fuel-coolant contact are correct, then the main discrepancies between the theoretical and experimental voiding rates would be due to either the assumed constraint or to the rate and quantity of heat transferred. A reduction in heat exchange, in the context of this model, is accomplished by either assuming that only a small amount of fuel entered the mixing region and fragmented or that a large amount entered but fragmentation does not occur. In the TREAT experiment fragmentation did occur; thus the latter assumption would be incorrect. Figure 18 (problem B) shows the voiding rate considering only a 15% fuel interaction with a relatively high coefficient of condensation. Even under these fairly conservative conditions, the experimental voiding rate is overestimated. Thus, it seems that the heat-transfer process assumed in the instantaneous mixing models may not adequately describe that due to molten fuel release into liquid sodium, unless only a very small amount of fuel interacts with the coolant.

The second condition which may account for the overestimate of the expulsion rate depends upon the assumption of an inertial constraint. In reality, the expansion of the heated volume produces compression waves which propagate through the liquid plugs, such that the velocity, head, and pressure terms in the equation of motion are dependent variables in

TABLE VI. Initial Conditions for Computational Simulation of H-2 Experiment

Mixing-zone height (L) 10.0 cm

Mixing-zone volume (V) 2.47 cm³

Initial wall film thickness
on surface of test pin and
inside wall of Dewar vessel

$[\sigma(t = 0)]$ 0.015 cm

Heat-transfer coefficient
for film vaporization

$h_v = k_{Na}(T)/\sigma(0)$ ~ 6.6 (cal/cm² sec °C
at 1000°C)

Curve Nomenclature	Problem Label	Initial Conditions
	EXPERIMENTAL	
_____	A	$d_s = 500 \mu$ $V_l = 50\%$ $n_s = 18,700$ $V_f = 50\%$ $h_c = 1.5$ $V_v = 0\%$
—•—•—•—•—•—•—	B	$d_s = 500 \mu$ $V_l = 85\%$ $n_s = 5661$ $V_f = 15\%$ $h_c = 3.3$ $V_v = 0\%$
-----	C	$d_s = 500 \mu$ $V_l = 50\%$ $n_s = 5661$ $V_f = 15\%$ $h_c = 3.3$ $V_v = 35\%$
—•—•—•—•—•—•—	D	$d_s = 500 \mu$ $V_l = 50\%$ $n_s = 9440$ $V_f = 25\%$ $h_c = 1.5$ $V_v = 25\%$
-----	E	$d_s = 500 \mu$ $V_l = 50\%$ $n_s = 9440$ $V_f = 25\%$ $h_c = 6.6$ $V_v = 25\%$
_____	F	$d_s = 500 \mu$ $V_l = 50\%$ $n_s = 3776$ $V_f = 10\%$ $h_c = 0.00$ $V_v = 40\%$
—•—•—•—•—•—•—	G	$d_s = 500 \mu$ $V_l = 50\%$ $n_s = 1887$ $V_f = 5\%$ $h_c = 0.00$ $V_v = 45\%$

TABLE VI. (contd.)

Curve Nomenclature	Problem Label	Initial Conditions
	EXPERIMENTAL	
.....	H	$d_s = 1000 \mu$ $V_l = 50\%$ $n_s = 1180$ $V_f = 25\%$ $h_c = 3.3$ $V_v = 25\%$
-----	I	$d_s = 1000 \mu$ $V_l = 50\%$ $n_s = 708$ $V_f = 15\%$ $h_c = 1.5$ $V_v = 35\%$
-----	J	$d_s = 500 \mu$ $V_l = 50\%$ $n_s = 1887$ $V_f = 5\%$ $h_c = 1.00$ $V_v = 45\%$

space and time. Such an equation under these conditions is difficult to solve. However, within a short time ($t > 2L/v_c$; for a 30-cm column, $2L/v_c \approx 0.0003$ sec) the effects of compressibility begin to dissipate due to the reflection of pressure waves from the end of the column. As indicated in Ref. 47, the inertial approximation results in peak pressures that are too large, and pulse widths that are too short, compared with pressures calculated considering compressibility effects in an infinite

Fig. 18. Voided Channel Height vs Time, Assuming No Vapor Present Initially. ANL Neg. No. 900-771.

Fig. 19. Pressure vs Time, Assuming No Vapor Present Initially. ANL Neg. No. 900-781.

column. However, the total impulse, and thus the voiding rate, is probably not severely altered by the assumption of incompressible flow since the integrated pressure histories over the expulsion time tend to equalize.

In view of the above discussion, it appears that some other descriptive model may better describe the events following release of molten fuel from a failed pin. Since the large impulses calculated are a direct consequence of the initial period of thermally induced liquid expansion, an obvious alternative approach would be to introduce some compressibility into the system in the form of condensable sodium vapor or noncondensable fission and/or bond gas. In the following series of calculations, the effects of the initial presence of sodium vapor will be investigated. As mentioned previously and discussed in further detail in Appendix A, this vapor is thought to be generated during the fragmentation process.

Problems B and C

Figures 20 and 21 show that the effect of initial vapor presence on the voiding and pressurization rates is appreciable, especially during the early stages of expansion. The only difference between calculations B and C is the replacement of some liquid with vapor. Not only is there a pressure reduction of approximately an order of magnitude, but also a considerable peaking delay. The decrease in pressure amplitude is the result of the cushioning effect of vapor, bulk condensation, and

Fig. 20. Voided Channel Height vs Time, Comparing the Effects of Vapor Present Initially.
ANL Neg. No. 900-772.

Fig. 21. Pressure vs Time, Comparing the Effects of Vapor Present Initially. ANL Neg. No. 900-782.

condensation at cold boundaries. By cushioning is meant that a substance in the gaseous state is much more compressible than in the liquid state. Bulk condensation would be that amount of condensation needed to keep the gas in saturated equilibrium with the liquid as the system properties (P , V , T) change, whereas condensation at cold boundaries is that which occurs at nonadiabatic surfaces cooler than the vapor. Only the cushioning effect would apply to noncondensable gases (gases well above their critical temperature and pressure). Although the simple addition of some vapor does not completely reduce the calculated voiding rate to that obtained in the experiment, it does lessen it to a somewhat slower rate. A much better prediction of the experimental voiding curve was sought after studying further the various factors which effect the pressurization rate.

Problems D and E

For saturated sodium, cushioning and bulk condensation are dependent upon the initial vapor volume assumed, while condensation at cold wetted surfaces is defined by a heat-transfer coefficient for film condensation (h_c). The effect of the latter mechanism is demonstrated in Figs. 22 and 23 for two different values of h_c . As can be noted, a high condensation rate results in a significant reduction in vapor pressurization, and thus of expulsion rate. During the initial period, a high rate of sodium vaporization occurs from the fragmented fuel. The extent of vapor formation cannot be immediately relieved by the expulsion of the bounding liquid plugs; thus, condensation along relatively cold surfaces becomes an important factor which reduces the magnitude of the vapor buildup. An analogous, although opposite, effect was demonstrated in the context of coolant expulsion from intact channels (see Appendix B), where it was shown that the effect of wall-film vaporization is significant. At this time, the coefficient of film condensation under transient nonisothermal

Fig. 22. Voided Channel Height vs Time, Illustrating the Effect of the Rate of Condensation at Cold Boundaries. ANL Neg. No. 900-787.

Fig. 23.
Pressure vs Time, Illustrating the Effect
of the Rate of Condensation at Cold
Boundaries. ANL Neg. No. 900-788.

conditions cannot be predicted with certainty. However, in general, an upper limit on h_c is the conductance of the film layer (k/σ), although it will normally be lower than this value due to the buildup of a boundary layer of noncondensable gas at the film surface. This gas layer retards the vapor from reaching the film of liquid at the wall where condensation occurs. This effect does not hold true during film vaporization, since the noncondensable gases tend to be carried away with the expanding vapor; thus, h_v is usually defined by the conductance of the film layer. In problem D, the value of h_c was taken as $1.5 \text{ cal/cm}^2 \text{ sec } ^\circ\text{C}$, which corresponds to typical values obtained experimentally⁷⁶ for steady film condensation of sodium vapor. As shown, the calculated voiding rate using this value overestimated the experimental rate. In problem E, the upper limit on the condensation coefficient was used. During the early stages, the calculated voiding history compared favorably with the experimental results, but overestimated the condensation rate in the later stages resulting in reentry. Viewed in terms of a net heating rate (the difference between the rates of vaporization and condensation) it could be said that the overall rate of vaporization between that calculated in problems D and E should result in a fairly close approximation of the experimental voiding history.

Problems F and G

Besides the effect of condensation, two other parameters which will alter the net vaporization rate are the fuel particle size and volume fraction. The calculated results for relatively low volume fractions (5 and 10%) of fuel are shown in Figs. 24 and 25, completely neglecting condensation along the walls of the fuel pin and Dewar vessel. Although agreement with the experimental voiding process was quite good during the initial stages, the theoretical rates were much too rapid during the later portion. This is due to the fact that since wall condensation was neglected, pressurization continues until either vaporization stops (due to dryout of liquid in the mixing zone), or until the liquid plugs have gained enough momentum such that the rate of expansion occurs faster than the corresponding rate of vapor production. Even at the low fuel fraction

Fig. 24. Voided Channel Height vs Time for Two Different Fuel-volume Fractions, Neglecting the Effects of Condensation at Cold Boundaries. ANL Neg. No. 900-769.

Fig. 25. Pressure vs Time for Two Different Fuel-volume Fractions, Neglecting the Effects of Condensation at Cold Boundaries. ANL Neg. No. 900-773.

of 5%, the voiding is overestimated in the later stages. If, however, condensation were allowed for, then its effect would become increasingly important as the expulsion continues, since more wall surface area is exposed. In this manner, a reduction in pressure would occur in a shorter period, thus decreasing the expulsion rate with increased voidage. Therefore, it was reasoned that a fuel-volume fraction and condensation coefficient between that of problems E and F should give a fairly close estimate of the experimental expulsion history. Problem C corresponds to such a condition. In this case, however, the voiding rate was still found to be too rapid during the early stages; thus, a larger fuel-particle size or smaller fuel percentage should be chosen.

Problems H, I, and J

As illustrated in Figs. 26 and 27, the conditions of problems H, I, and J result in expulsion histories similar to that of the experiment. For the larger particles, the decrease in the initial expulsion rate is due to the fact that the resistance to heat conduction is directly related to size.

Fig. 26. Calculated Voiding Histories Similar to Those Obtained in the H-2 Experiment. ANL Neg. No. 900-774.

In problem H, the condensation coefficient was taken as half the upper limit. Although initial simulation is quite good, the calculated re-entry rate is somewhat faster than the experimental collapse. This is due to the fact that a fairly high value of h_c was chosen, which most likely overestimated the actual rate of condensation.

In problem I, a lower value of h_c was chosen equal to the coefficient estimated experimentally during steady film condensation of sodium vapor.⁷⁶ Correspondingly, a lower volume fraction of fuel was used such that the net heating rate to the vapor is similar to problem H, except during the

Fig. 27.
Calculated Vapor Pressures vs Time
which Result in Voiding Histories
Similar to Those Obtained in the
H-2 Experiment. ANL Neg. No.
900-785.

later stages when a large surface area for condensation was exposed. As illustrated, the experimental voiding history is well matched by the calculation under these conditions.

Likewise, the conditions of problem J also resulted in a fairly good estimate of the expulsion process. However, in this case, a lower volume fraction of fuel was used since the smaller particle size results in a quicker rate of heat transfer, the condensation coefficient being equal to 1.00 cal/cm² sec °C in this case. Thus, it can be said that the net heat-transfer rate to the expanding sodium vapor is nearly the same for all problems and that it adequately describes the voiding process, although it is still uncertain whether the condensation rate is overestimated and vaporization underestimated or the inverse is true. Insight into the phenomenology of the model for these problems can be obtained from the following series of curves.

In Figs. 28 and 29, the net energy released to the vapor phase $[\partial/\partial t (m_v h_v)]$ of the expanding mixing region is plotted for problems H, I, and J. As can be seen from Eqs. 3 and 13, the heat-transfer rate from the fuel and surrounding boundaries is reduced by the sensible heat storage taken up by the liquid within the mixing zone. As shown in Figs. 28 and 29, the net heat transfer to the vapor is both positive and negative during the transient, the voiding process being defined by this heating rate.

In region A (see Fig. 28), there is an initial period of vapor collapse. This is due to the fact that, although vaporization from the fuel particles occurs, most of the energy is given up to the liquid in the form of sensible and latent heat, thus resulting in partial vapor collapse. This initial collapse period is a direct consequence of the assumption that although vapor was formed during the fragmentation process, a

Fig. 28.
Calculated Vapor Volume and Expansion Energy vs Time for Problem H, Illustrating the Transient Nature of the Vapor-generation Process.

ANL Neg. No. 900-796.

Fig. 29.
Calculated Vapor Expansion Energies vs Time for Problems J and I. ANL Neg. No. 900-798.

negligible amount of heat was transferred to the bulk of the liquid; thus, its temperature is that of the coolant at the time of failure (which is below that of saturation at the system pressure). However, within a short time, the liquid-vapor equilibrium mixture is heated to a temperature above that of saturation, thus initiating vapor expansion (region B). During this period, vaporization from the fuel occurs at a faster rate than condensation at the walls. Once the liquid associated with the fuel has been completely evaporated, heat transfer from this source terminates. However, the liquid film on the wall (in equilibrium with vapor) which has not gained a significant amount of sensible heat begins to evaporate (region C). This process continues until the vapor pressure falls below the system pressure (since the expulsion is now occurring at a faster pace than the vaporization process); thus, reentry begins (region D) and wall condensation again commences.

In Figs. 30 and 31, the heat-transfer rates at the surface of the fuel particles ($n_s k_s \frac{dT}{dr}|_{r=a}$) are plotted for problems I and J. Comparison of Fig. 29 with Figs. 30 and 31 shows that the net heating rate to the sodium vapor is approximately less by an order of magnitude than the average heat-transfer rate from the fuel particles. As will be shown near the

Fig. 30.
The Transient Rate of Heat
Transfer from Interacting
Fuel for Problem J.
ANL Neg. No. 900-794.

Fig. 31.
The Transient Rate of Heat
Transfer from Interacting Fuel
for Problem I. ANL Neg. No.
900-795.

end of this discussion, the sensible and latent heat given up to the liquid in the mixing zone greatly effects the extent of conversion from thermal to mechanical energy.

Based upon the results of the preceding calculations, it is clear that one of the parameters that should be looked into is the coefficient for film condensation on the wall. If it can be concluded from experiments that the formation of film condensate is small due to the presence of inert gases, then the vaporization process can more easily be predicted. Parametric studies presented here, however, indicate that if film condensation is completely neglected, the calculated voiding history overestimates the experimental results, even at relatively low fuel volume fractions (see Fig. 24). Thus, if the basic characteristics of the model are correct, then some film condensation must have occurred; otherwise the calculated momentum buildup will result in an overestimate of the experimental expulsion rate. It is encouraging to find that the conditions of problem I result in a favorable prediction of the voiding process. The value of h_c used in this problem was based upon a value cited for steady film condensation of sodium vapor, which at this time is the most reasonable value to choose for lack of better data. Likewise, the conditions of problem J are also reasonable, since in fact film condensation may be reduced somewhat by the presence of inert gases released from the failed pin. It is important to note that the sensitivity of the calculation with respect to condensation was magnified by the fact that both the intact portions of the pin and Dewar vessel wall serve as sites of condensation. However, until h_c can be accurately predicted under transient conditions similar to those encountered during reactor accident situations, the problem is indeterminate insofar as the individual effects of condensation and vapor production are concerned.

The other critical parameters of problems I and J are the fuel-volume fractions and particle size. As defined in Table VI, the mixing zone is approximately 2.47 cm^3 ; thus, on a mass basis, the fraction of molten fuel (interacting with liquid at any instant of time to cause vaporization) that correctly predicts the first expulsion event for each problem is

Problem I

% by weight $\approx 0.15 (2.47 \text{ cm}^3) (\sim 9 \text{ g/cm}^3) \approx 3.3 \text{ g}$;

Problem J

% by weight $\approx 0.05 (2.47) (9) \approx 1.1 \text{ g}$.

The results of the SAS1A-ASH calculations indicate that approximately 35% of the fuel mass was in the molten state in the upper regions of the pin at time of failure.⁷² For the estimated 10.0-cm failure zone this corresponds to approximately 19 g of fuel, 6.65 g being in the molten state. Thus, approximately 1/6 to 1/2 of the molten fuel within the postulated failure zone interacts with the sodium during the first expulsion event. However, as was shown, only a small percentage of the heat content within this fuel mass actually is used to expand the vapor. It also should be realized that to speak only of the mass fraction of fuel which interacts with the sodium is misleading, since it is really the surface area that

determines the transient nature of the expulsion process. For 500- μ particles the interaction ratio on a molten-mass basis is 1/6. This is thought to be reasonable since not all the molten fuel in the failure zone would be released at once. Thus, some vapor blanketing of the fuel ejected at a later time would occur. Likewise, the assumption that the vaporization process occurs as some combination of Leidenfrost, transition, and/or nucleate boiling during the intermittent contact between fuel and liquid necessitates that only a fraction of the total fuel that actually enters the mixing zone interacts at any instant of time. Support for this assumption of intermittent contact is given by recent observation of hot metal particles being suspended above a cool liquid surface by vapor generation, the effect being referred to as the inverse Leidenfrost phenomenon,⁷⁷ analogous to the well-known effect of a liquid droplet being suspended above a hot surface.⁷⁸ The observations were made by heating metal foils under water with a laser beam. When their temperatures exceeded 1500°C, the particles dispersed and were found to bounce repeatedly from the bubble walls in which they shortly became entrapped, generating vapor at the wall interface. This process continued until the particles finally came to a quasi-stable position above the base of the bubble. As is the case with Leidenfrost boiling, only a portion of the fuel-surface area interacts with the liquid. Hall *et al.*⁷⁷ believe that such a phenomenon might occur during the thermal interaction of high temperature debris with liquid. Although the model presented here assumes that both liquid and fuel intermittently collide with one another within an expanding vapor bubble, the point is that only a fraction of the total fuel which may be released from a failed pin interacts at any instant of time.

Although particle sizes of 500 and 1000 μ are somewhat larger than the average diameter obtained from dropping experiments of molten UO₂ into sodium (mean diameters: 250 μ ²⁷ and 510 μ ⁵²), they are still within the range of the size distribution collected from such experiments. It also has been reported⁷⁹ that for a given energy density the fraction of smaller particles is greater in dropping experiments than obtained from a number of in-pile fuel-failure experiments. The radial temperature distribution within the pin (colder outer edge) is thought to play a role in limiting the breakup of the released fuel. Thus, the particle sizes used in the calculations presented here are thought to be reasonable.

In order to design for containment when fuel-coolant interaction occurs, the thermal-to-mechanical-energy-conversion efficiency must be specified. In the method outlined by Hicks and Menzies³⁹ an upper limit of a 10% conversion efficiency was calculated. A comparison between the amount of energy deposited in the pin at failure and the energy used in the first expansion event of the vapor (which results in a voiding history similar to that obtained in the H-2 experiment) is determined as follows. At the time of failure the energy deposited in the fuel pin was estimated to be 1375 J/g.¹ For a cold-clean fuel diameter of 0.493 cm and a height of 34.3 cm, the approximate total mass of fuel within the pin was 71 g. Thus, the total fuel energy at failure was 9.75×10^4 J (2.33×10^4 cal). As can be determined from Fig. 29, the theoretical net average heating rate to the expanding sodium vapor is approximately 775 cal/sec (average value of problems I and J, which includes the rate of sensible heat addition, $m_v \bar{h}_v / \partial t$, to the vapor, which is small compared to $\bar{h}_v \partial m_v / \partial t$), with a vapor growth period of about 0.036 sec (1.548 sec - 1.512 sec). Thus,

the net thermal energy given to the vapor by the fuel during the first vapor-expansion process was approximately 28.0 cal. This corresponds to a vapor conversion efficiency of

$$\epsilon(\%) = \frac{28.0(100)}{2.33 \times 10^4} = 0.12\% .$$

Although only a fraction of this energy is available for mechanical work, the value is of interest since it demonstrates the extent of the vapor-generation process. However, a more realistic estimate of the potential for mechanical damage can be obtained by simply determining the maximum recorded velocity of the ejected liquid slugs. Some typical values are

$$\epsilon \approx 0.002\% (1900 \text{ J/g})^{80}$$

$$\epsilon \approx 0.030\% (940 \text{ J/g})^{37}$$

$$\epsilon \approx 0.070\% (1250 \text{ J/g})^{37}$$

$$\epsilon \approx 0.010\% (1375 \text{ J/g; H-2 experiment})^{81}$$

The last value not only includes the maximum kinetic energy of the liquid plugs, but also the work done by the pump.

The energy released by the interacting fuel for problems I and J can be estimated from Figs. 30 and 31. In each case, the heat transfer was evaluated by dividing the exponential curve into two sections and determining the respective decay constants (μ) and zero intercepts (A).

Problem J

$$\mu_1 = 268.0 \text{ 1/sec (t = 0.000 to 0.006)}$$

$$\mu_2 = 63.0 \text{ 1/sec (t = 0.006 to 0.04)}$$

$$A_1 = 5.0 \times 10^4 \text{ cal/sec}$$

$$A_2 = 1.5 \times 10^4 \text{ cal/sec}$$

Problem I

$$\mu_1 = 525.0 \text{ 1/sec (t = 0.000 to 0.003)}$$

$$\mu_2 = 59.3 \text{ 1/sec (t = 0.003 to 0.0156)*}$$

* Time for film associated with fuel particles to be completely vaporized.

$$A_1 = 1.2 \times 10^5 \text{ cal/sec}$$

$$A_2 = 3.1 \times 10^4 \text{ cal/sec}$$

The energy released during the vapor-expansion process is calculated as

$$E_f = A_1 \int_0^{t_1} e^{-\mu_1 t} dt + A_2 \int_{t_1}^{t_2} e^{-\mu_2 t} dt$$

$$E_f \text{ (problem J)} \approx 300 \text{ cal}$$

$$E_f \text{ (problem I)} \approx 410 \text{ cal}$$

Therefore, it was estimated that the approximate energy released by the fuel during the first interaction event of the H-2 experiment was 355 cal, for a heat-transfer conversion efficiency of

$$\epsilon(\%) = \frac{355(100)}{2.33 \times 10^4} = 1.52\% .$$

This is greater by about an order of magnitude than the energy contained within the vapor, but less than the 10% theoretical upper limit for the mechanical-conversion efficiency calculated by Hicks and Menzies.³⁹

The difference between the heat released by the fuel (355 cal) and the energy given up to the vapor (28 cal) is due to a number of factors. A significant portion of the initial energy released is given up as sensible heat to the liquid associated with the fuel particles. Although this liquid is eventually vaporized, the energy stored within it does have a delaying effect on the rate of heat transfer to the vapor, and thus to the rate of momentum buildup in the liquid plugs. An even greater effect, which occurs over the entire expulsion event, is that due to the formation of condensate at the cold boundaries. Not only is the sensible heat addition to the wall film significant, but also the heat transferred to the physical structure. In terms of safety, it can be said that these heat sinks significantly reduce the extent of mechanical-energy conversion. Although the calculated results apply only to the first expulsion event, this initial incident was the most violent insofar as coolant expulsion was concerned, and thus was the most important for estimating the damage potential of the vapor-expansion process.

One of the more puzzling questions concerning the general problem of fuel-coolant interaction is that due to the discrepancy between the conversion efficiencies obtained during the interaction of molten UO_2 with water versus that between UO_2 and sodium. Listed below are typical values obtained during autoclave pin-failure experiments in water:

$$\epsilon \approx 2.8\% (2750 \text{ J/g})^{38}$$

$$\epsilon \approx 0.01\%; 0.2\% (1000 \text{ J/g}; 1740 \text{ J/g})^{82}$$

$$\epsilon \approx 0.4\% (2400 \text{ J/g})^{83}$$

$$\epsilon \approx 1.9\%, 2.5\% (205 \text{ J/g}; 193 \text{ J/g})^{84}$$

Although the range of conversion efficiencies is rather widespread, on the average the water experiments result in a conversion ratio higher by an order of magnitude than in the sodium experiments. The results of the analysis presented in this work suggest a reasonable explanation for this phenomenon.

As was discussed in the context of the H-2 experiment, the effects of condensation and sensible heat storage at the liquid film layer adhering to the structural confines is thought to reduce appreciably the net amount of fuel energy released to the expanding vapor. This results in a reduction in the conversion efficiency. In the case of the water experiments, however, the effects of condensation at surfaces covered by liquid film would be less.* Therefore, for equivalent vaporization rates from the interacting fuel, the extent of vapor expansion would be greater in the case of $\text{UO}_2\text{-H}_2\text{O}$ experiments than for the $\text{UO}_2\text{-Na}$ interaction; thus a higher conversion efficiency could be expected. The fact that the results of the Spert tests⁸³ indicate that the extent of fragmentation (most probable particle sizes range from 685μ at 2400 J/g to 8600μ at 1550 J/g : Ref. 83, p. 68) is, in general, no greater than that due to a $\text{UO}_2\text{-Na}$ interaction (250 to 500μ based on dropping experiments; cleanup data for various TREAT experiments indicate even a smaller average particle size; however, significant breakup occurs during the screening process) also lends support to the idea that the difference in conversion efficiencies may be due to a difference in condensation. A better comparison, however, could be made if failure experiments were performed with both sodium and water coolant under similar fuel heating and geometric conditions. Transient analysis for these two coolants and comparison with the experimental results would then yield insight not only into the effects of condensation and vaporization, but also the difference in the thermodynamics of the two coolants.

* A rough comparison between the condensation rates for water and sodium vapor can be made by comparing the coefficients for film condensation (h_c). Typical values for pure water vapor lie in the range from 0.25 to $0.60 \text{ cal/cm}^2 \text{ sec } ^\circ\text{C}$ based on Nusselt film theory,⁸⁵ while for sodium $h_c = 1.5 \text{ cal/cm}^2 \text{ sec } ^\circ\text{C}$ based on experimental values obtained for steady film condensation.⁷⁶

VI. RECOMMENDATION FOR FUTURE WORK

A. Experimental Setup

As stated previously, the test-section geometry, loop conditions, and instrumentation were designed primarily to obtain experimental data concerning the mode and threshold of fuel-element failure. However, the various geometries of the test-element holding fixtures, for example, introduce uncertainties into the hydraulic characterization of the coolant. If a simple uncluttered geometry, with a minimum of dimensional changes were used, such uncertainties could be eliminated which would facilitate the testing of theoretical expulsion models pertaining to fuel-coolant interaction.

Figure 32 illustrates a simple in-pile experiment, employing a U-tube geometry, which might be used. Once the testing of the model has been accomplished under controlled conditions, the theory can be applied to more realistic reactor conditions. The only major changes in the Mark-II loop would be the removal of the induction pump, which would be replaced by a straight, constant-diameter pipe section. For the geometry illustrated, the cover pressure in both legs would be equal. To insure that vapor collapse and reentry will occur before the liquid plugs have been completely expelled from the test section, a larger sodium flow area and longer axial length than that of the H-2 experiment should be used. A better estimate of the breach size could be obtained if only a small section of the pin actually contained fuel (approximately 5 cm in length). Likewise, the complications introduced by the possibility of multiple mixing zones resulting from more one failure site would be eliminated. If the insulating plugs were designed such that failure would occur only in the fuel section, then the complicating effects of inert gas entering the coolant during failure could be eliminated. Other variations of the U-tube experiment might also be devised for the testing of theoretical models of FCI. However, whichever version is chosen, it should remain simple in geometric design, thus reducing to a minimum the introduction of possible uncertainties into the calculational simulation of the experiment.

With such a simplified experiment, comparison between experimental and theoretical results for both a fuel-sodium and fuel-water test might also lead to a better understanding of the differences between these two interaction processes.

B. Model Improvements

Cho⁴⁶ demonstrated that a peak-pressure reduction of 6% could be accomplished by the introduction of 1% by volume of noncondensable gas (fission, bond, and/or cover gas) into the mixing zone, assuming the gas behaves in a polytropic manner. Although the additional cushioning effect of inert gases in a system containing condensable vapor would, of necessity, be smaller than that due to the combined effects of sodium vapor condensation and compressibility, nevertheless, a more thorough model should include its presence.

Fig. 32. Sketch of Proposed Experiment for Analytic Model Testing.
ANL Neg. No. 900-786.

If we assume that the inert gas behaves as an ideal gas, and that expansion and contraction can be considered as a frictionless, adiabatic process, then the volume change in the noncondensable gases is determined from

$$P(t)^{1/n} V_{Ng}(t) = P(0)^{1/n} V_{Ng}(0) ,$$

where n is the polytropic exponent, $P(0)$ is the initial pressure, and $V_{Ng}(0)$ is the initial volume of noncondensable gas. Then

$$\begin{aligned}\frac{dv_{Ng}(t)}{dt} &= P(0)^{1/n} v_{Ng}(0) \frac{d}{dt} \left(P(t)^{-1/n} \right) \\ &= - \frac{v_{Ng}(0)}{n} \left(\frac{P(0)^{1/n}}{P(t)^{1+1/n}} \right) \frac{dP(t)}{dt}.\end{aligned}$$

This volume change of the inert gas is then simply added to Eq. 14 to obtain the total change of the mixing zone.

C. Additional Applications of Model

As discussed in the introduction, a number of postulated situations may lead to fuel-element failure. Although the model proposed was developed in the context of multiple-pin failures resulting from an autocatalytic power excursion, it is thought that with minor adjustments the model might also apply to single-pin failures resulting from localized malfunctions.

Since there are as many as 10^5 fuel elements within a reactor core, the failure of individual pins is one of the problems that must be considered. The initiation of single-element failure may arise as a consequence of manufacturing defects; localized, fission-gas pressure buildup; local flow or power irregularities; etc. Although failure under such conditions will probably result in solid rather than molten fuel release, nonetheless significant heat transfer from hot fuel to coolant may occur. If the effects of noncondensable gas are included in a manner described above, and the fuel size and thermophysical properties are adjusted to represent the conditions at failure, then the general approach taken here might also describe the thermohydrodynamics of mild single-element failures as well. In a manner similar to that observed in sodium-expulsion experiments from an intact channel, the description of a liquid-film layer adhering to the solid-fuel particles may be physically correct in this situation.

D. Supporting Information Needed

As mentioned previously, experiments should be performed to determine the coefficient of film condensation. Until such data are available, the individual effects of vaporization from interacting fuel and condensation at cold boundaries cannot be evaluated accurately. Likewise, although the violent-boiling mechanism for molten-fuel fragmentation has received some experimental verification²⁵ with reactor materials and sodium coolant, further investigation is certainly needed. Also, basic experiments should be designed to study the effects of heat transfer once fragmentation has occurred. One such experiment might be to evaluate the heat fluxes obtained due to Leidenfrost boiling of sodium from a surface at temperatures greater than 2000°C.

VII. SUMMARY AND CONCLUSIONS

The ability to reduce in-pile fuel-failure data to a workable form and to simulate the test-loop hydraulics, such that a comparison between the actual coolant-expulsion history and that calculated from a theoretical analysis of the fuel-coolant interaction process, has been demonstrated in this work. It is encouraging to find that the postulated analysis correctly predicts the experimental voiding history and that a relatively low interaction process is involved. A conversion efficiency of approximately 0.12% (ratio of the calculated vapor-expansion energy during the first expulsion event to the total energy contained within the pin at failure) indicates that this interaction is considerably less violent than that predicted by the well-known Hicks and Menzies maximum-work calculation.³⁹ In addition, it was shown that the core structure (cladding, assembly cans, wire wrap, etc.) and the associated liquid-film layer which adheres to it serves as a sizable heat sink, depending on the extent of vapor condensation at these surfaces. Likewise, it is thought that the difference in film condensation for sodium and water vapor may well explain the difference in conversion efficiencies determined from fuel-failure experiments with these two coolants. However, until the coefficient for film condensation is evaluated under conditions simulating a vapor-expansion process initiated by fuel-coolant interaction, the individual effects of vaporization and condensation cannot be determined with certainty.

The calculations presented in Appendix A also indicate that the assumption of fuel fragmentation resulting as a consequence of violent boiling is certainly reasonable. This mechanism has also been supported by the experiments conducted by Swift and Pavlik.²⁵ Therefore, to be consistent with this mechanism of fuel breakup, it is assumed that prior to rapid expulsion there exists within the mixing zone not only sodium liquid but also sodium vapor. It has been shown that this initially present vapor reduces, by approximately an order of magnitude, the extent of peak pressurization obtained with the instantaneous-mixing models.^{42,46,47} In addition, the model developed is the first to take into account the energy-exchange process not only between the fuel and sodium but also at the constraining boundaries, that is, at both the liquid-vapor slug interfaces and at the structural confines.

APPENDIX A

Fuel Fragmentation

The discussion presented in this appendix is not meant to be an in-depth analytic study or review of all the possible events and situations that may arise during or following the release of molten fuel, cladding, and bond and/or fission gases from a failed fuel element. Rather, it is meant to be an outline of one plausible sequence of events which support the assumption of initial vapor presence proposed in Ch. III. Other fuel-coolant interaction scenarios might also be postulated, which may result in an entirely different set of initial conditions. Indeed the instantaneous-mixing models might well be more realistic in the light of a reentry situation, if coolant voiding should occur before fuel failure. Likewise, new information concerning the mechanisms of fuel release and fragmentation might also invalidate some of this discussion. However, it is hoped that within a few years experimental and analytic research will have been developed to a point such that the speculative approach taken here will not be necessary.

The postulated sequence of events following fuel failure is divided essentially into three major processes. This division is based on a conception of the dynamics involved during each stage, rather than say the time associated with the different events. The three areas chosen are:

- (1) molten-fuel release from the failed element (initial contact period);
- (2) fragmentation of fuel;
- (3) postfragmentation analysis.

The initial conditions for the postfragmentation analysis are obtained in view of the discussion of the first two processes.

1. Release of Molten Fuel

Although situations may arise where pinhole-type failures occur, resulting in breakup of molten fuel due to the turbulence associated with the streaming of a jetlike spray from a small hole, in-pile experiments (in TREAT) have shown that with significant fuel melting the rupture size is rather large. Likewise, if fuel melting takes place, there is no reason to believe that only a small hole would be burnt in the clad. Therefore, it is assumed that for fuel-element failure the molten fuel is released in rather large globular particles (compared with the final fragmentation size of ~ 100 to 1000μ in diameter) and the fragmentation occurs due to interaction with liquid sodium.

2. Fragmentation of Fuel

The basic question associated with this process is what initiates the breakup. Essentially, three mechanisms have been postulated: fragmentation resulting from inertia forces generated as the fuel is suddenly

released into the sodium, effects due to a thermally induced acoustic pulse associated with initial fuel-sodium contact, and the various boiling mechanisms discussed in the literature survey. If the energy associated with the first two processes is large enough to cause fragmentation, then the instantaneous-mixing model proposed by Padilla^{42,43} may very well be valid for the fuel-failure problem. In order to determine whether or not fragmentation will occur, the energy of each process is estimated and compared with the surface energy (commonly known as surface tension) associated with the cohesion forces (the attraction of like molecules) of the molten fuel. If the energy of a particular mechanism is larger than this surface tension, then it is assumed that the necessary, but perhaps not sufficient, condition for fragmentation has been met.

Although the surface tension is usually a complex function of the physical state and chemical structure of the liquid, Eötvös derived an expression which is based on the critical temperature and "molecular free surface energy" of the liquid. Eötvös' Law⁸⁶ is

$$\gamma (\text{dyne-cm/cm}^2) = k_e (T_c - T) / (Mv)^{2/3}, \quad (\text{A.1})$$

where T_c is the critical temperature and T is the temperature of the liquid at which the surface tension is to be evaluated, both in °K, Mv is the molecular volume in cm^3/mole , and k_e is a constant and equal to 2.0 for most liquids. For UO_2 at 2800°C , calculations give

$$\gamma_{\text{UO}_2} = 1200 \text{ dyne-cm/cm}^2$$

for

$$(Mv) = \frac{270 \text{ g}}{\text{mole}} \frac{\text{cm}^3}{8.74 \text{ g}} = 30.8 \text{ cm}^3/\text{mole},$$

$$T_c(\text{UO}_2) \simeq 9000^\circ\text{K};^{87}$$

$$T(\text{UO}_2) \simeq 2800 + 273 = 3073^\circ\text{K}.$$

However, the surface energy of the liquid sodium is approximately 110 dyne-cm/cm² near its boiling point,⁸⁸ so that the surface energy at the UO_2 -Na interface (γ_I) was taken as the difference between the two:

$$\gamma_I \simeq 1090 \text{ dyne-cm/cm}^2.$$

For lack of good experimental measurements of γ_I , this value will be used as the basis for comparison.

The inertial (kinetic) energy associated with a fuel particle traveling through sodium is calculated as

$$E_{\text{inertia}} = \rho DV^2/2g_c \text{ (dyne-cm/cm}^2\text{)} , \quad (\text{A.2})$$

where ρ is the sodium density, D is the diameter of the unfragmented fuel, V is its velocity, and g_c is the conversion factor. Based on the ejection studies in Ref. 49 (p. 62), a breach diameter of 0.25 cm will result in a molten-fuel ejection velocity of 20 ft/sec (609 cm/sec). If the unfragmented particle size equals this breach size and if the sodium density is defined for the temperature at the position and time of failure in the H-2 experiment (920°C), the inertial energy is calculated to be

$$E_{\text{inertia}} = \frac{(0.73)(0.25)(37.16 \times 10^4)}{2(980)} = 35 \text{ dyne-cm/cm}^2 .$$

This value is lower by more than an order of magnitude than the surface energy, so that fragmentation could not have occurred under the assumed conditions. Even if the initial particle size were larger by an order of magnitude than that used and the particles traveled at the same velocity, the initial energy still would not be sufficient to overcome the surface tension. Furthermore, it has been shown in dropping experiments^{29,30} that the inertial forces must exceed the surface tension by at least an order of magnitude before fragmentation occurs. Therefore, it seems reasonable that some other mechanism initiated fuel breakup in the H-2 experiment.

The following analysis, which is essentially the same as in Ref. 49, was used to test the hypothesis that pressurization, resulting from the thermal expansion of a heated sodium layer in contact with fuel, might cause fragmentation. Unlike as in dropping experiments, fission and/or bond gases are probably released prior to and along with molten fuel from a failed pin. Although the presence of this gas would tend to prevent perfect fuel-sodium contact, an estimate of the maximum heating rate to the coolant is made by assuming that the heat-transport process can be described by two semi-infinite slabs with negligible resistance at the plane of separation. The solution to a conduction problem of this type is given in Ref. 61 (p. 70). The resultant temperature equations for the fuel, sodium, and interface are

fuel ($x < 0$)

$$T_f(x,t) = T_m(x,0) + \phi \left(T_f(x,0) - T_m(x,0) \right) \left[1 + \frac{k_m/\sqrt{\alpha_m}}{k_f/\sqrt{\alpha_f}} \operatorname{erf} \left(\frac{|x|}{2\sqrt{\alpha_f t}} \right) \right]; \quad (\text{A.3})$$

sodium ($x > 0$)

$$T_m(x,t) = T_m(x,0) + \phi \left(T_f(x,0) - T_m(x,0) \right) \left[\operatorname{erfc} \left(\frac{x}{2\sqrt{\alpha_m t}} \right) \right], \quad (\text{A.4})$$

where

$$\phi = \frac{k_f / \sqrt{\alpha_f}}{k_f / \sqrt{\alpha_f} + k_m / \sqrt{\alpha_m}} ;$$

interface ($x = 0$)

$$T_I(0, t) = \frac{T_m k_m / \sqrt{\alpha_m} + T_f k_f / \sqrt{\alpha_f}}{k_m / \sqrt{\alpha_m} + k_f / \sqrt{\alpha_f}} . \quad (\text{A.5})$$

Two interesting features of this problem are that the interface temperature is constant for all time and the complementary error function decreases rapidly for arguments greater than one. For all practical purposes, therefore,

$$\text{erfc}(x/2\sqrt{\alpha_m t}) \approx 0 \text{ at } (x/2\sqrt{\alpha_m t}) = 2 .$$

In this manner, the thickness of the heated sodium layer at any time t is given by

$$x_h = 4\sqrt{\alpha_m t} , \quad (\text{A.6})$$

with an average temperature equal to

$$\begin{aligned} T_h &= T_m(x, 0) + \phi \left(T_f(x, 0) - T_m(x, 0) \right) \left[\frac{\int_0^{x/2\sqrt{\alpha_m t}} \text{erfc}(\epsilon) d\epsilon}{x/2\sqrt{\alpha_m t}} \right] \\ &= T_m(x, 0) + \phi \left(T_f(x, 0) - T_m(x, 0) \right) \left[\frac{1}{2} \int_0^2 \text{erfc}(\epsilon) d\epsilon = \frac{0.488}{2} \right] . \quad (\text{A.7}) \end{aligned}$$

Note that although the heated layer thickness increases with time, its average temperature remains constant.

If the conservative assumption is made that the system is completely rigid (constant volume), then the pressure wave set up by the expansion of this heated layer is given by

$$P_h = \frac{\alpha_P}{\beta_T} (T_h - T_{\text{ambient}}) + P_{\text{ambient}}, \quad (\text{A.8})$$

where

$$\alpha_P \text{ (thermal expansion coefficient)} \equiv \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_P;$$

$$\beta_T \text{ (isothermal compressibility)} \equiv \frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_T.$$

This pulse propagates through sodium at sonic velocity v_c such that the distance traveled by the leading edge is given by

$$x_c = v_c t \quad (\text{A.9})$$

as illustrated below:

The conservative assumption is made that when the average pressure $P_{\text{ave}}(t)$ of the entire pulse over x_c falls below the saturation pressure corresponding to the interface temperature T_I , coolant boiling begins. At this time, the energy contained in the pulse is used to determine the maximum work available. Evaluation of $P_{\text{ave}}(t)$ is by mass averaging the temperatures of both the heated (x_h) and unheated ($x_c - x_h$) lengths of the pressure pulse such that

$$T_{ave}(t) = \frac{\left[x_h(t) T_h(t) \right] + \left[T_{ambient} (x_c(t) - x_h(t)) \right]}{x_c(t)} . \quad (A.10)$$

Thus,

$$P_{ave}(t) = \frac{\alpha_P}{\beta_T} (T_{ave}(t) - T_{ambient}) + P_{ambient} . \quad (A.11)$$

The maximum damage potential of this pulse is determined by calculating the available thermodynamic work, which is given in Ref. 49 as

$$\Delta W_{available} = c_v (T_{ave} - T_{ambient}) - c_v T_{ambient} \ln \left(\frac{T_{ave}}{T_{ambient}} \right) . \quad (A.12)$$

Numerical Results of Initial-contact Model

At the time and position of fuel-pin rupture the sodium temperature was approximately 920°C. Using the following thermal properties:

$$T_m = 920^\circ\text{C} \quad k_m = 0.125 \text{ cal/cm sec}^\circ\text{C}$$

$$\alpha_m = 0.54 \text{ cm}^2/\text{sec}$$

$$T_f = 2800^\circ\text{C} \quad k_f = 0.005 \text{ cal/cm sec}^\circ\text{C}$$

$$\alpha_f = 0.0042 \text{ cm}^2/\text{sec} ,$$

the interface temperature was calculated to be

$$T_I = 1475^\circ\text{C} ,$$

which corresponds to a saturation pressure of

$$P_I = 31 \text{ atm} .$$

The value of other parameters used in the calculation were

$$\alpha_p = 3.15 \times 10^{-4} / ^\circ\text{C}^{49}$$

$$\beta_T = 3.07 \times 10^{-5} / \text{atm}^{49}$$

$$P_{\text{ambient}} = 2.544 \text{ atm}$$

$$v_c = 23.0 \times 10^4 \text{ cm/sec}^{49}$$

$$c_v = 0.29 \text{ cal/gr}^\circ\text{C}^{49}$$

The ambient pressure was taken as the estimated system pressure of the TREAT experiment at the position of failure (see Table I). The following iterative process was then used to determine the average temperature and pressure of the pulse.

Iteration 1

Test to see if P_{ave} has fallen below the interface pressure in 10^{-7} sec.

The compressed layer thickness (x_c) at this time is

$$x_c = v_c t = 23 \times 10^4 (10^{-7}) = 0.023 \text{ cm} .$$

The heated layer thickness is calculated from Eq. A.6:

$$x_h = 4\sqrt{\alpha_m t} = 4\sqrt{0.54 \times 10^{-7}} = 0.00093 \text{ cm} .$$

The average temperature of this sodium layer is given by Eq. A.7:

$$T_h = 920 + \phi(2800 - 920) \left(\frac{0.488}{2} \right) ,$$

where

$$\phi = \frac{k_f / \sqrt{\alpha_f}}{k_f / \sqrt{\alpha_f} + k_m / \sqrt{\alpha_m}} = \frac{0.077}{0.077 + 0.17} = 0.312 .$$

Thus

$$T_h = 920 + 0.312(1880)(0.244) = 920 + 143 = 1063^\circ\text{C} .$$

From knowledge of the temperature and thickness of the heated layer, the average temperature of the entire compressed layer can be determined from Eq. A.10:

$$T_{\text{ave}} = \frac{0.00093 (1063) + (0.0230 - 0.00093)(920)}{0.023} = 925.59^{\circ}\text{C} .$$

The average pressure is calculated from Eq. A.11:

$$P_{\text{ave}} = \left(\frac{3.15 \times 10^{-4}}{3.07 \times 10^{-5}} \right) (925.59 - 920.00) + 2.544 \approx 60 \text{ atm} .$$

Since the average pressure behind the front is still above the saturation temperature of the interface, a longer time for pressure relief is necessary.

Iteration 2

$$t = 5 \times 10^{-7} \text{ sec}$$

$$x_c = 23 \times 10^4 (5 \times 10^{-7}) = 0.115 \text{ cm}$$

$$x_h = 4\sqrt{0.54 \times 5 (10^{-7})} = 0.00208 \text{ cm}$$

$$T_h = 1063^{\circ}\text{C}$$

$$T_{\text{ave}} = \frac{0.00208 (1063) + (0.115 - 0.00208)(920)}{0.115} = 922.586^{\circ}\text{C} .$$

$$P_{\text{ave}} = 10.26 (2.586) + 2.544 = 29.08 \text{ atm} .$$

Since this pressure is below the interface saturation pressure, the compressed layer thickness is taken as 0.115 cm at an average temperature of 922.586°C. The available energy to do mechanical work is calculated from Eq. A.12:

$$\begin{aligned} W_{\text{available}} &= 0.29 (2.586) - 0.29 (920) \left(\ln \frac{922.586}{920.000} \right) \\ &= 0.00105 \text{ cal/g} \\ &= 4.4 \times 10^4 \frac{\text{dyne-cm}}{\text{g}} \Big|_{\text{of sodium}} \end{aligned}$$

$$= 4.4 \times 10^4 \frac{\text{dyne-cm}}{\text{g}} \left(\frac{0.73 \text{ g}}{\text{cm}^3} \times 0.115 \text{ cm} \right)$$

$$= 3700 \text{ dyne-cm/cm}^2 .$$

Thus, the maximum energy associated with the postulated thermally induced acoustic pulse is approximately three times greater than the estimated surface energy of the $\text{UO}_2\text{-Na}$ interface. It was concluded that this mechanism could not account for fuel breakup for the following reasons. As mentioned previously, dropping experiments have shown that the forces applied to the molten globule must be at least larger by an order of magnitude than the surface tension to cause fragmentation. Furthermore, the calculated work is thought to be much larger than that which actually occurs. First of all, the heating rate is the maximum possible for a $\text{UO}_2\text{-Na}$ heat-exchange process by conduction. This results from the fact that not only has the contact resistance been neglected, but also the boundary condition of an infinite sink dictates that a minimum temperature potential buildup occurs in the sodium. Secondly, the conservative assumption of a completely rigid system neglects the cushioning effects of noncondensable gases and the pliability of the system which would absorb some of the energy of the pressure pulse. Thirdly, the tail pressure of the pulse would in reality be lower than the calculated average pressure. The onset time for boiling, therefore, would occur in a shorter period and the total energy transferred to the coolant reduced, which in turn results in a lower value of available work (although higher total percent). For these reasons, it was thought that the energy generated by the acoustic pulse was not sufficient to cause fragmentation.

Swift and Pavlik²⁵ postulated that fragmentation of molten metals might result as a consequence of the turbulence associated with the formation and collapse of vapor bubble during coolant boiling. The results of their quenching experiments strongly indicate that such a mechanism is reasonable. Pressure measurements, high-speed motion pictures, and noise-detection studies indicate that the transition regime is the most violent of the boiling regions, followed by nucleate bubble formation, with film boiling being relatively quiet. Thus, fragmentation would most likely occur due to either transition or nucleate boiling. To compare the forces generated in such a process with the surface energy of the molten fuel, the following analysis was made.

If the pressure can be determined within a bubble of known size located at the surface of the molten- UO_2 unfragmented particle, then the local tension setup in the fuel globule by this pressure force is calculated as

$$\gamma_p (\text{dynes/cm}) = P \frac{\pi D_b^2}{\pi D_b} = P D_b , \quad (\text{A.13})$$

where D_b is the bubble diameter at departure (see accompanying diagram). It should be noted that σ_p is independent of the actual contact area (which may be considerably smaller), since it is the projected area over which the pressure acts to deform the fuel. To obtain an estimate of the pressure associated with boiling from an unfragmented particle, Farahat's²³ sodium-quenching experiment with a solid tantalum sphere was analyzed ($T_{Na} = 720^\circ\text{C}$; $T_{Ta} = 2300^\circ\text{C}$). Although the sphere temperature was somewhat below the melting point of UO_2 (2800°C), the characteristics of vapor-bubble growth of the sodium are probably similar. A sketch diagram of Farahat's experiment is shown in Fig. A.1. If the assumptions are made that there is no pulse attenuation due to acoustic-energy absorption in the system, that constructive and destructive interference of reflected waves cancel on the average, and that the liquid between the sphere and transducer is essentially incompressible

(e.g., $L/v_c < \text{pulse width of 1-2 msec}$), then the measured pressure can be taken as that induced by boiling (the pressure pulse due to the dropping of the sphere into sodium was accounted for). The average pressure pulse recorded was approximately 50 psig at a frequency of 180 pulses/sec, the maximum pulse being about 84 psig. An estimate of the bubble size at departure can be obtained from Zuber's formula,⁸⁹ which accounts for the buoyancy and surface tension of the surrounding liquid medium and the frequency of bubble detachment:

$$D_b = \frac{0.59}{f} \left[\frac{\gamma_{Na} (\rho_l - \rho_v) g}{\rho_l^2} \right]^{1/4} \quad (\text{in cgs units})$$

or, since $\rho_l \gg \rho_v$,

$$D_b = \frac{0.59}{f} \left[\frac{\gamma_{Na} g}{\rho_l} \right]^{1/4} . \quad (\text{A.14})$$

This formula has been validated by experiments for nucleate boiling at relatively low frequencies (1-2 cps) with many liquids, including sodium. For lack of a better correlation at higher frequencies and during transition boiling this formula was used. It should be noted that the experimental frequency pertains to the entire sphere rather than one nucleation site; therefore, a low estimate of D_b and σ_p is made by taking $f = 180$ cps. In reality, there are probably many nucleation sites on the sphere; thus the frequency per site would be less. Based on the following values:

difference in Farahat's experiment was less than that which occurred in the TREAT experiment, it could be expected that initially higher pressures would develop during boiling of sodium from molten UO_2 . Also, the assumption that the measured pressure is the same as the bubble pressure is conservative. In reality, the recorded pressure would be lower than the actual bubble pressure due to some attenuation as the front travels through sodium. Likewise, as previously mentioned, there are probably many nucleation sites, so that the measured frequency pertains to all sites rather than just the one site assumed. Thus, it is expected that the estimated bubble-departure size is small compared to the actual statistical average size that would occur during nucleate boiling. Likewise, the fact that somewhat larger patches of vapor are released during transition boiling compared to bubbles in the nucleate region also indicates that the calculated bubble size, and thus the resultant tension, is probably small.

Although only a very elementary approach was used here, it gives some quantitative indication of the energies associated with the different postulated mechanisms of fragmentation. On comparing these energies, it becomes evident that the boiling process is by far the most severe.

$$E_{\text{UO}_2\text{-Na}} \approx 1090 \text{ dyne-cm/cm}^2$$

$$E_{\text{inertia}} \approx 35 \text{ dyne-cm/cm}^2$$

$$E_{\text{acoustic pulse}} \approx 3700 \text{ dyne-cm/cm}^2$$

$$E_{\text{boiling}} \approx 226,000 \text{ dyne-cm/cm}^2/\text{bubble}$$

Although the energies associated with the first two processes will probably precede boiling, it does not seem likely that they could cause fuel breakup, especially in the light of the fact that the above estimates are probably high, while that for the boiling process is low. Therefore, the assumption of some vapor presence prior to the postfragmentation expulsion process seems reasonable.

APPENDIX B

A Single-bubble Model for Sodium Expulsion from a Heated Channel

A theoretical model, similar to that developed for the problem of fuel-sodium interaction, has been previously applied to the expulsion of sodium from an intact heated channel. The following text is a summary of an article to appear in Nuclear Engineering and Design which presents the results of that work.⁵⁷

Introduction

Of primary importance to LMFBR safety is an improved understanding of the mechanics of sodium ejection in the event of channel blockage, pump failure, or power transients. A reduction of sodium density can result in either a positive or negative reactivity, depending on the location and extent of the vapor void. Therefore, an accurate description of the voiding process with respect to space and time is necessary. The models which have been developed to date can be categorized as multiple-bubble, single-bubble, or annular-flow models.⁹⁰ Recent work by Grolmes and Fauske⁹¹ on the ejection of Freon-11, and by Spiller, Grass, and Perschke⁵³ with liquid potassium indicate, however, that slug-type expulsion with a liquid wall film remaining on the wall occurs during expulsion. A single-bubble model is therefore presented here, which takes into account heat transfer in both upper and lower liquid slugs, as well as the wall film. This model, called "Slug,"⁹² is similar to that of Schlectendahl⁹³ (Blow Code), which, however, neglects the heat transfer in the liquid slugs, and hence may be expected to underestimate the initial stages of void growth. A more recent version of the Blow Code does, however, include the initial stages of spherical bubble growth.⁵⁶

Basically the approach taken is to calculate the heat transfer from the fuel pin to the coolant until at some point in space and time the coolant reaches a certain temperature, corresponding to a specified amount of superheat. At this point inception of boiling occurs. The stages of spherical bubble growth are approximated by a thin bubble assumed to occupy the entire coolant channel area, except for the liquid film remaining at the cladding wall. The coupled solution to the energy and hydrodynamic equations of the coolant, and the heat-transfer equations of the fuel pin are then continuously solved during the voiding process.

Formulation of the Slug Model

Since the principal area under investigation is the hydrodynamics of slug expulsion and not a heat-transfer model for the fuel pin, a simple radial-heat-flow model is employed for the pin, neglecting axial heat flow and angular variations of heat conduction. The channel is divided into a number of axial segments, the rate of heat generation within each segment being constant. The radial temperature distributions are calculated for each of the sections in succession, following the direction of the coolant flow. The steady-state equations are solved directly; the finite-difference method is used to obtain the transient solution. The

thermophysical properties of the fuel, bond, and clad are taken to be constant functions of temperature and space. The sodium properties are taken to be constant up to the time of boiling and temperature-dependent during the expulsion. Table B.I lists the initial conditions for the calculation.

TABLE B.I. Parameters Used in Expulsion Calculation

Characteristics of Reactor Channel

Core length (cm)	100
Upper blanket length (cm)	30
Lower blanket length (cm)	30
Upper plenum length (cm)	20
Lower plenum length (cm)	20
Fuel-rod ID (cm)	0.580
Fuel-rod OD (cm)	0.650
Bond thickness (cm)	0.010
Clad thickness (cm)	0.025
Inlet pressure (atm)	3
Outlet pressure (atm)	3
Power density of peak node (cal/cm ³ -sec)	
High	409
Low	100

Steady-state Conditions

Coolant volume fraction	0.50
Coolant velocity at $t = 0$ (cm/sec)	800
Coolant inlet temperature (°C)	500

Material Properties

Fuel (UO ₂)	
Thermal conductivity (cal/cm-°C-sec)	0.00745
Specific heat (cal/g-°C)	0.08
Density (g/cm ³)	10.90
Bond (Helium Gas)	
Thermal conductance (cal/sec-cm ² -°C)	0.45
Clad (Stainless Steel)	
Thermal conductivity (cal/cm-°C-sec)	0.0575
Specific heat (cal/g-°C)	0.146
Density (g/cm ³)	7.60
Coolant (Sodium)	
Temperature-dependent properties	
Film thickness (cm)	0.015

Consider the transient resulting from an instantaneous loss of flow for the channel configuration as shown in Fig. B.1. The heat-transfer rates within the fuel pin and coolant are solved until the superheat criterion is satisfied, initiating bubble nucleation.

Fig. B.1. Reactor-channel Geometry and Power Profile Used for the Calculations.
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At the instant of bubble nucleation a thin vapor space which occupies the entire channel cross section is assumed. The vapor space is bounded by the upper and lower liquid slug. It is assumed that the pressure and temperature of the vapor are in equilibrium with the surrounding liquid. If the vapor temperature is known, the pressure and other thermophysical properties of the sodium⁵¹ are determined. With this estimate of the vapor pressure, the microscopic momentum equation (similar to Eq. 21 in the text) can be solved to obtain the position of the upper and lower slug interfaces.

Having determined the interface position from the momentum equation, the energy equation for the vapor is then solved. The rate of vapor generation is proportional to the heat transferred by conduction across the slug interfaces and the wall film. Thus the energy equation, neglecting both the pressure work term and the sensible heat of the vapor, which are small, is written as

$$kA \left. \frac{dT(\xi_1, t)}{d\xi_1} \right|_{\xi_1} + kA \left. \frac{dT(\xi_2, t)}{d\xi_2} \right|_{\xi_2} + \frac{dQ_w(t)}{dt} - \sigma C \Delta X \rho_l c_p \frac{dT_{fm}}{dt} = A \frac{d}{dt} (\rho_v \lambda \Delta X) .$$

The temperatures $T(\xi_1, t)$, $T(\xi_2, t)$, and $T_{fm}(t)$ are in equilibrium with the vapor temperature $\phi(t)$. The temperature gradients at the slug interfaces

are given by Eq. 10 in the text, the heat transfer at the walls by Eq. 7.

The variation in wall-film thickness due to evaporation and condensation is calculated by assuming that the energy transfer at the cladding surface equals the latent heat of vaporization plus the sensible heat storage within the film layer. The effects of the shear force generated by the gas flow over the film layer and surface-tension gradients due to temperature fluctuation at the interface are neglected. Thus the change in film thickness is calculated from

$$C\Delta X\rho_{\ell}\lambda\frac{d\sigma}{dt} = \frac{dQ_w}{dt} - \sigma C\Delta X\rho_{\ell}c_p\frac{dT_{fm}}{dt}.$$

The energy and momentum equations are coupled by guessing the equilibrium temperature $\phi(t)$ at each time interval, as discussed in the text.

Results

A. Effect of Wall Film

Figure B.2 illustrates the effect that the presence of wall film has on the voiding rate. It is clear that the vapor contribution from the

Fig. B.2.
Voided Channel Height vs Ex-
pulsion Time, Illustrating the
Effect of the Presence and
Absence of Liquid Wall Film,
and the Rate of Film Condensa-
tion and Vaporization.
ANL Neg. No. 900-332. Rev. 2.

residual film dominates that from the slug interfaces. This effect holds true throughout the expulsion, except during the initial stages of vapor growth. Figure B.3 shows that when a dry wall is considered, the initial superheat pressure quickly drops to the system pressure of 3 atm. With a

Fig. B.3.
Vapor Pressure Within the Bubble
vs Expulsion Time, Illustrating
the Effect of Wall Film on
Pressure. ANL Neg. No. 900-85.

wet wall there is an initial pressure buildup while film vaporization is occurring in the core region due to the heat generation in the fuel, followed by a depressurization due to partial vapor condensation in the blanket region.

The variation in film thickness due to vaporization and condensation is shown in the lower portion of Fig. B.2. The positions of the upper and lower slug interfaces are given at various times after the initiation of expulsion, in addition to the calculated values of the wall-film thickness within each axial node between the interfaces. The initial film thickness at every node is taken to be 0.15 mm, which is the median value as reported by Spiller *et al.*⁵³ for their experiments with liquid potassium. As would be expected, vaporization occurs in the central core region, indicated by the diminishing values of the film thickness, while condensation occurs in the blanket regions. For the chosen conditions film dryout did not occur during the initial voiding of the channel.

B. Effect of Power Density and Superheat

The effects of both power density and superheat when wall film is considered are shown in Figs. B.4 and B.5. For a low power density, superheat is the overriding factor which governs the expulsion rate; for the higher power density the effect of superheat is not as important, although still significant, since the total voiding time for 20°C is about double that for 150°C. In the case of 150°C superheat, the magnitude of the power density is not very significant because of the large amount of energy storage in both the coolant and fuel pin.

In the case of both low superheat and power density, reentry occurred in the blanket region for several reasons. The rates of condensation and vaporization are governed by the temperature gradient between the clad surface and vapor. Although the heat-transfer coefficient used for vaporization is about four times that for condensation, the positive gradient in the core region is much smaller in magnitude than the negative gradient in the blanket region. The fact that the cladding temperature in the

Fig. B.4.
 Voided Channel Height vs Expulsion
 Time, Showing the Effects of Both
 Superheat and Power Density.
 ANL Neg. No. 900-81.

Fig. B.5.
 Vapor Pressure vs Expulsion Time,
 Illustrating the Effects of Both
 Superheat and Power Densities on
 the Pressure History Within the
 Vapor Bubble. ANL Neg. No. 900-86.

blanket region is much lower than the saturation temperature of the vapor results from the specified condition of stagnant coolant during the period from the initiation of the transient up to inception of boiling. Shortly after the interfaces enter the blanket regions, the rate of condensation on the cold walls causes the vapor pressure to fall below the system pressure, resulting in reentry of the upper and lower slugs. As the power density is increased, film vaporization in the core region overrides the rate of condensation in the blanket, resulting in complete expulsion. Expected pressure generation due to complete vapor collapse was not considered in these calculations (hammer effect), as well as vapor condensation in the upper and lower plenums after complete expulsion has occurred.

C. Effect of Heat Capacity of Fuel Pin

In order to demonstrate the effect of the fuel-pin heat capacity on the expulsion rate, the heat-transfer dynamics of the fuel pin are decoupled from the expulsion model. In both cases, the axial power profile is the same. However, in the decoupled case the wall heat flux (q) at each axial location is time-independent and taken to be

$$q = \frac{\dot{Q} D_f^2}{4 D_{cl}}$$

where $\dot{Q}$ is the fuel heat generation ($\text{cal/cm}^3 - \text{sec}$), D_f the outside diameter of fuel (cm), and D_{cl} the outside diameter of cladding (cm).

The results are summarized in Figs. B.6 and B.7. As would be expected, the expulsion rate is faster when the heat capacity of the fuel is neglected; in this case the voiding rate is about twice as fast. As

Fig. B.6. *Voided Channel Height vs Expulsion Time, Illustrating the Effect of Fuel-pin Heat Capacity on the Expulsion Rate.* ANL Neg. No. 900-82.

shown in Fig. B.7, the pressure buildup with a time-independent wall-surface heat flux is extremely rapid, since heat is continuously being transferred into the vapor space, resulting in film vaporization and a rapid pressure rise. In this case condensation can only occur at the upper and lower slug interfaces.

When the heat transfer within the fuel pin is coupled to the expulsion model, the pressure cannot rise as rapidly, since part of the heat generation goes into energy storage of the clad and fuel material.

Fig. B.7.
Vapor Pressure vs Expulsion
Time, Illustrating the Ef-
fect of Fuel-pin Heat Capac-
ity on the Pressure History.
ANL Neg. No. 900-87.

Conclusion

Some interesting physical features of the sodium-expulsion process are indicated by these calculations. The growth of the vapor slug is dominated by heat conduction from the liquid slugs in the early growth period ($\Delta X/D_e \ll 1$) and by heat conduction from the exposed walls in the late growth period ($\Delta X/D_e \gg 1$), provided, in the later case, that the exposed wall is covered by an adhering film of residual liquid. The nature of the expulsion and reentry will therefore depend strongly on whether or not liquid film is present. Chugging will most likely occur for an accident condition involving a sudden loss of flow if there exists a long blanket or plenum region, since the cladding temperature in these regions will then be below the saturation temperature. Reentry may occur if film vaporization in the core region ceases due to film breakup or dryout.

Superheat is also an important parameter which affects both the time to initiate boiling and the rate of voiding. The superheat effect is most pronounced for low heat fluxes and at the beginning of the voiding process. For large superheats the power density appears to be of little significance; for lower superheats the power density affects the rate of voiding.

A similar model to that presented here has been used in the study of the isothermal depressurization of Freon-113 in a 0.72-cm-dia glass tube.⁵⁸ For this case it was thought desirable to take into account the variation in the thermal boundary layer of the wall film, which depends upon the age of the liquid surface as a function of axial distance. Figure B.8⁵⁸ shows the experimental interface position as a function of time for a superheat of 109°F compared to the theoretical solution computed in the manner described above. It will be noted that the agreement is quite good over the entire expulsion history. Similar agreement was obtained with several different superheats.

It is rather interesting that this model agrees well with experimental data, even during the early stages of ejection, despite the

Fig. B.8.
 Voided Channel Height vs Time
 for Slug Expulsion on Freon-113
 at Constant Plenum Pressure.
 ANL Neg. No. 900-84.

assumption of a disc of vapor filling the tube cross section. This early growth period accounts for an appreciable portion of the total ejection time. An alternative approach proposed by Schlechtendahl⁵⁶ employs a spherical-bubble geometry in the early growth stages.

The ability of the model to predict the effective delay time before rapid expulsion commences is encouraging and implies that the assumption of a slug geometry, even during the early stages of vapor growth, approximates the surface-volume relationship of the vapor region satisfactorily at all times.

APPENDIX C

Sample Calculation of Initial Conditions

The following sample calculation is based on the initial conditions for Problem D.

Defined Parameters

Mixing zone height (L)	10.0 cm
Wall film thickness on surface of test pin and inside wall of Dewar vessel (σ)	0.015 cm
Flow-area diameter (D_1)	0.561 cm
Diameter of fuel particles (D_s)	500 μ
Volume percent of fuel	25%
vapor	25%
liquid	50%

Calculated Parameters

Mixing volume = $\pi D_1^2 / 4 \times L = 0.785 (0.561)^2 \times 10 = 2.47 \text{ cm}^3$
 Fuel volume = $0.25 (2.47) = 0.6175 \text{ cm}^3$
 Liquid volume = $0.50 (2.47) = 1.2350 \text{ cm}^3$
 Vapor volume = $0.25 (2.47) = 0.6175 \text{ cm}^3$
 Number of fuel particles (n_s)

$$n_s \frac{\pi D_s^3}{6} = 0.6175 \text{ cm}^3$$

$$n_s = 0.6175 \frac{6}{\pi} \frac{1}{0.05^3} = 9440$$

Volume of liquid = film on Dewar wall + film on fuel pin + liquid associated with fuel particles

$$\text{Volume film on pin} = \sigma (\pi D_1) L = 0.015 (\pi 0.5954) 10 = 0.2804 \text{ cm}^3$$

$$\text{Volume film on Dewar wall} = \sigma(\pi D_{w1})L = 0.015 (\pi 0.825) 10 \\ = 0.3888 \text{ cm}^3$$

$$\text{Volume of liquid associated with fuel particles} = 1.235 - 0.2804 - 0.3888 \\ = 0.5658 \text{ cm}^3$$

Thickness of film associated with
one fuel particle, $\sigma_s = R_b - R_s$

where R_b (see accompanying figure) is obtained from volume of liquid associated with fuel particles

$$\frac{0.5658 \text{ cm}^3}{9440} = \frac{4\pi}{3} [R_b^3 - R_s^3]$$

$$R_b = 0.031 \text{ cm}$$

$$\sigma_s = R_b - R_s = 0.031 - 0.025 = 0.006 \text{ cm} = 60 \mu$$

To test the assumption that the thermal resistance of the film layer can be neglected, the approximate time for the thermal boundary layer to reach the outside edge of the film is estimated to be

$$\sigma = \sqrt{\alpha_{Na} t}$$

$$t = \sigma^2 / \alpha_{Na}$$

where, at 1000°C,

$$\alpha_{Na} = \frac{k}{\rho c_p} \sim \frac{0.125}{0.758 (0.3)} = 0.55 \text{ cm}^2/\text{sec}$$

$$t_{\text{particle film}} = (0.006)^2 / 0.55 \sim 0.655 \times 10^{-4} \text{ sec}$$

$$t_{\text{wall film}} = (0.015)^2 / 0.55 \sim 0.41 \times 10^{-3} \text{ sec}$$

Since these times are short compared to the estimated experimental expulsion time of (1.51 sec to 1.55 sec) 0.04 sec, the assumption is valid.

APPENDIX D

Thermophysical PropertiesSodium

$$\rho, k, \bar{h}, P_{\text{sat}} = f(T) \quad (\text{Ref. 51})$$

$$c_p = 0.305 \text{ cal/g-}^\circ\text{C} \quad (\text{Ref. 51})$$

$$\alpha_p = 0.21968 \times 10^{-3} + 0.81226 \times 10^{-7} T$$

$$+ 0.97135 \times 10^{-11} T^2 + 0.68998 \times 10^{-15} T^3 \text{ 1/}^\circ\text{K} \quad (\text{Ref. 65})$$

$$B_T = (VT\alpha_p^2/c_p) + 0.69651 \times 10^{-5} + 0.26741 \times 10^{-7} T$$

$$- 0.14891 \times 10^{-10} T^2 + 0.82082 \times 10^{-14} T^3 \text{ 1/atm} \quad (\text{Ref. 65})$$

Fuel (UO₂ at 2800°C)

$$c_p = 0.11 \text{ cal/g-}^\circ\text{C} \quad (\text{Ref. 48})$$

$$k_f = 0.005 \text{ cal/sec-}^\circ\text{C-cm} \quad (\text{Ref. 48})$$

$$\rho_{\text{UO}_2} (\text{liquid}) = 8.74 \text{ g/cm}^3 \quad (\text{Ref. 94})$$

$$\rho_{\text{UO}_2} (\text{solid}) = 11.0 \text{ g/cm}^3 \quad (\text{Ref. 63})$$

$$T_{\text{critical}} = 9000^\circ\text{K} \quad (\text{Ref. 86})$$

$$\alpha_f = 0.0042 \text{ cm}^2/\text{sec}$$

Cladding and Dewar Vessel (Type 316 Stainless Steel at 1000°C)

$$\rho = 7.6 \text{ g/cm}^3 \quad (\text{Ref. 63})$$

$$c_p = 0.146 \text{ cal/g-}^\circ\text{C} \quad (\text{Ref. 63})$$

$$k = 0.0575 \text{ cal/sec-}^\circ\text{C-cm} \quad (\text{Ref. 63})$$

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