MECHANISMS OF VAPOR EXPLOSIONS

Technical Progress Report

Oct. 1976 - Mar. 1977

NOTES
This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research and Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

S. G. Bankoff	Principal Investigator	(15%)
A. Sharon	Doctoral Candidate	(50%)
M. Maeshima	Visiting Scholar	(50%)
A. Inoue	Visiting Scholar	(100% from 3/1/77)

Chemical Engineering Department
Northwestern University
Evanston, Illinois 60601

Prepared for the U.S. ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION under
Contract No. EY-76-S-02-2512-*000

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

MASTER

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

ABSTRACT

Several studies are being performed related to destabilization of film boiling in liquid-liquid and liquid-solid systems due to local pressurization, in view of the key role of this step in initiating and propagating vapor explosions. A study of the destabilization of Leidenfrost boiling of single pentane drops on a hot silicone oil surface shows that pressure increases of less than one atm. are effective in producing vapor collapse with slow pressurization (rise time ~ 0.5 sec.). For a given drop size the stability boundary in the ΔP vs. T_h plane shows two branches: a low-temperature branch which is independent of T_h , and a higher-temperature branch showing a nearly linear dependence of ΔP vs. T_h . The corresponding critical Weber numbers for droplet coalescence are $\sim 10^3$, compared to $\sim 10^2$ for free-falling drops and ~ 10 for droplet breakup due to inertial effects. Another study of film boiling destabilization with a rise time of $\sim 10^{-2}$ sec. shows that collapse occurs after only ~ 1 -2 atm. pressure rise, and that contact is made even when the heating surface is well above the critical temperature. Finally, in contradiction to a recently published study, boundary layer stripping in a UO_2 -Na mixture is found to produce negligible breakup, and hence cannot escalate into a shock wave.

1. Introduction

The present research program consists of an analytical and experimental study of mechanisms leading to vapor explosions in metal-water and fuel-sodium thermal interactions. Previous work^{1,2} has theoretically demonstrated the vanishingly small probability of a Board-Hall³ type thermal detonation wave, based upon Taylor instability⁴ or boundary-layer stripping⁵ as the breakup mechanism. A "splash" theory^{6,7} has also been proposed for the mixing step in vapor explosions, based upon empirical correlations of our data on free fall of volatile drops onto hot liquid surfaces.⁸ This is based on the concept that random liquid-liquid contacts produce local pressurized regions due to rapid vapor formation, which drives the mixing by a splash (potential flow) mechanism. Another theoretical study² of breakup of UO_2 drops entering a sodium pool indicates rapid fracture of the UO_2 crust by collapsing bubbles, resulting in pre-dispersal without shock wave formation.

A key step in the initiation and propagation of a vapor explosion has been identified to be the destabilization of film boiling, either liquid-liquid, or solid-liquid (in the event of a solidifying fuel). Our current experimental program is aimed particularly at studying this step.

2. Collapse of Liquid-Liquid Leidenfrost Boiling Due to Pressure Rise (M. Maeshima)

Critical Weber numbers for liquid-liquid contact in free-falling drop experiments were measured by Waldram^{9,10} and by Ochiai⁶, but theoretical analysis is difficult due to rapid and deep drop penetration into the hot liquid surface. A creeping-flow analysis has been provided by Segev⁷ for a saturated volatile drop approaching a hot plane surface, but the minimum approach distance was calculated to be $10^3 - 10^4 \text{ \AA}$, well above the interaction distance for London forces. To obtain a geometry more amenable to theoretical analysis, the collapse

of the vapor film supporting a pentane drop on a hot silicone oil (Dow-Corning 710) due to an increase in ambient pressure is being studied.

The boiling vessel consists of a 4-in. length of 2-in. diameter Pyrex pipe, heated from below by a hot plate. A 2-3 mm pentane drop is deposited on the hot oil surface through a water-cooled hypodermic needle in a vacuum atmosphere. After quasi-steady-state has been established, the vacuum is broken by a solenoid valve. Pressure rise times were quite slow, (~ 0.5 sec.), so that it is a good assumption that the pressure in the gas space was always spatially uniform. Two possible outcomes existed, as shown in Fig. 1 for a 2.26 mm drop: The drop might coalesce with the oil, forming a floating lens, or it might remain in film boiling. In the range of oil temperatures $50-75^{\circ}\text{C}$, the line of demarcation between the two regions depends only upon ΔP , the pressure step. For $T_h \sim 75-110^{\circ}\text{C}$, the critical ΔP increases nearly linearly with oil temperature. The reasons for this regime change are not clear, but it appears that at the lower temperatures the film boiling regime is metastable, requiring a threshold mechanical disturbance to produce wetting. Above 75°C , which corresponds to stable film boiling, the pressure rise (and hence subcooling) necessary for destabilization depends upon the hot oil temperature.

Fig. 2 shows the effect of droplet diameter on the critical ΔP for various oil temperatures. For 2-4 mm drops, the stability of film boiling increases with increasing surface curvature, while for 4-8 mm drops the stability is essentially independent of drop diameter. At all diameters the stability increases with increasing oil temperature. Presumably, the larger drops, which exhibit a flattened shape, destabilize by capillary wave motion, while the smaller drops lie within the cutoff range, and hence quickly damp out surface waves.

A critical Weber number can be defined as $We'_c = \frac{d\Delta P}{\sigma}$, which is the ratio of the external pressure rise to the capillary pressure, by analogy to the usual Weber number $We_c = \frac{\rho v^2 d}{\sigma}$. In these experiments, however, $We'_c \sim 10^3$, which is two orders of magnitude larger than the critical Weber number for droplet breakup and entrainment, and ~ 10 times larger than We_c for free-falling pentane drops onto silicone oil. One concludes that Weber number effects are indeed negligible here, and destabilization occurs primarily because of the elevation in boiling point.

Analytical studies in support of this work are being made.

3. Film Boiling From Liquid Metal Surfaces (Sharon)

Two types of scoping experiments were performed to examine film boiling of water and organic liquids in inert (nitrogen or argon) atmospheres. A steady-state film boiling study of 50% lead-50% tin alloy in Freon-22 resulted in rapid dispersal of the metal, with some discoloration due to chemical reactions. Free-fall dropping experiments of pentane, Freon-22 and water onto Woods' metal in a nitrogen atmosphere similarly showed the powerful effect of surface oxidation, even after wiping the metal surface clean with a straight edge. A distinct dulling of the surface could be observed within ten seconds after wiping, and the threshold height for wetting depended distinctly on the degree of surface oxidation.

To overcome this difficulty, another experiment has been devised in which the liquid metal will be squeezed through a porous stainless plate from which film boiling of an organic liquid (95% ethyl alcohol) has been established. The pressure in the boiling chamber, which is 1.5-in. diameter by 8-in. high, can be varied from -25 in. Hg to 100 psia by means of quick-opening solenoid valves, with a rise time of ~ 50 ms. A miniaturized conductivity probe, located ~ 0.02 cm from the boiling surface, monitors the extent of liquid-liquid or liquid-solid contact.

The output from a flush-mounted pressure transducer, together with the resistance signal, are recorded on a memory oscilloscope. One can readily distinguish between nucleate, transition and film boiling with this resistance signal.

To establish a basis for comparison between vapor film collapse at solid and at liquid surfaces, pressure rise tests are currently being conducted on a solid stainless-steel heating surface at temperatures of 150-300°C. Two outstanding facts have been established:

1. The initial collapse is very fast (~ 1 ms) once instability sets in, and occurs when the pressure has risen only one atm. or less.
2. Apparent contact is made even when the solid surface is above the liquid critical temperature, with vigorous transition-boiling-like heat transfer occurring for ~ 10 ms. before reverting to film boiling.

When the present series is completed, the solid heater will be replaced by a porous stainless plate mounted above an externally-heated stainless steel bellows. The liquid metal (tin or lead-tin) will be melted within the bellows, and then squeezed as a thin layer below the boiling liquid, just prior to opening the pressurization valve. It is hoped in this way to avoid significant surface contamination of the liquid metal.

4. Shock-Tube Apparatus for Film-Boiling Destabilization (Inoue)

To study vapor film collapse in an initially two-phase liquid upon arrival of a sharp pressure wave, a shock tube apparatus has been designed and is being constructed. It contains two separate diaphragms: one for initial pressurization up to 500 psi, and the second for rapid depressurization after a suitable time delay. This will allow the imposition of pressure waves of different amplitudes and widths. A horizontal 3 mm. nickel tube with 0.05 mm. wall thickness, heated by direct current, will constitute the first heating surface. The surface

temperature will be calculated from resistivity taps, based upon the center portion of the tube. Two pressure transducers are currently planned. One will measure the pressure above the boiling liquid. The second will measure the collapse pressure on the tube, and subsequent local pressurization due to boiling, transmitted through a small hole in the tube wall by an internal column of silicone oil. Two viewing ports are also provided for high-speed photography. It is hoped to deduce a considerable amount of information concerning the criteria for liquid-solid contact, the impact pressure and impact mode, the peak pressure due to local vaporization, and the transient heat transfer rate upon vapor film collapse.

Later work will include condensation shock propagation studies in a steam-water bubbly mixture, followed by pressure, temperature and disintegration measurements on a liquid-metal drop in a single-phase and two-phase medium.

5. Theoretical Studies: Propagation of Low-Pressure Shocks through a Fuel-Coolant Mixture (Sharon)

The breakup mechanism envisaged in the Board-Hall theory depends on the relative velocity of the heavy fuel drops and the lighter coolant induced by the shock. We have previously shown that neither Taylor instability nor boundary-layer stripping (Helmholtz instability) seems to be rapid enough to support a high-pressure (Chapman-Jouguet) wave in a dense mixture. Nevertheless, distinct detonation waves have been observed in a column of tin drops falling through water¹², although in no case was the critical pressure reached. Furthermore, Jacobs¹³ has calculated that complete droplet breakup occurs due to boundary layer stripping for a sodium- UO_2 mixture being expelled from the reactor core, using a modification of the MURTI code¹⁴. The details are not clear to us at this point, since a Lagrangian set of homogeneous-flow equations is employed to describe this highly-separated flow, and clarification is being sought. It seems that the production of new surface area is governed by

a semi-empirical expression due to Ranger and Nichols, based on measurements of breakup of water drops in an air shock. These predictions are of sufficient importance to warrant further examination by us.

To determine an upper bound for the breakup in the fragmentation zone behind a thermal detonation wave, it is sufficient to consider a steady-state wave. Our experimental results indicate that vapor film collapse is achieved at overpressures of the order of 1-3 atm., so that one expects vapor to be absent behind a shock of $10^2 - 10^3$ atm. The jump shock relations can be summarized by the six equations:

$$[\alpha_i \rho_i u_i] = 0 \quad i = d, f \quad (1,2)$$

$$[\alpha_i (P_i + \rho_i u_i^2)] = 0 \quad (3,4)$$

$$[\alpha_i \rho_i u_i (h_i + \frac{1}{2} u_i^2)] = 0 \quad (5,6)$$

where the subscripts d and f refer to drops and surrounding fluid, α is the volumetric fraction; P is the pressure; ρ is the density; u is the velocity relative to the shock; h is the enthalpy; and the (square) jump brackets refer to values ahead of and behind the shock. For the pressure ranges involved here, liquid compressibility can be neglected relative to vapor collapse in determining the density change of the coolant, and hence the relative velocity induced by the shock. Likewise, thermal expansion effects turn out to be negligible, so that Eqs. (5,6) need not be carried in the calculation. For isolated drops Harper, et al.⁴ predict rapid breakup by Taylor instability at constant relative velocity, or constant Bond numbers, $Bo > 10^5$. The corresponding Weber number is much larger than the minimum for inertial breakup ($We \sim 20$), since

$$We = \frac{\rho_f u_r^2 d}{\sigma} = \frac{3}{8} C_D Bo \quad (7)$$

where C_D is the drag coefficient ($C_D \gtrsim 2$, and may be much larger for a disintegrating drop); $u_r = u_f - u_d$ is the relative velocity; d is the fuel drop diameter; and σ is the surface tension. For a given pressure jump Eqs. (1-4) then serve to determine the four unknowns: the two velocities behind the shock (and hence the Weber number), the volumetric fraction of coolant behind the shock and the shock velocity.

To follow the drop breakup behind the shock we integrate the differential mass and momentum equations behind the shock, in the manner of Kriebel¹⁴ and Rudinger¹⁵ for a dusty gas. In their case, however, no mass transfer occurred between the solid particles and the surrounding free stream, while here the droplet breakup can induce large momentum and heat transfer. Further, since a dense dispersion is treated, it is assumed that the small particles stripped from the fuel drops mix instantaneously with the surrounding coolant, coming into temperature and velocity equilibrium with no time lag. Following Wallis¹⁶ the mass and momentum equations for the drops and surrounding fluid become:

$$\frac{d}{dz} (\rho_d \alpha_d u_d) = - \Gamma_f \quad (8)$$

$$\frac{d}{dz} (\rho_f \alpha_f u_f) = \Gamma_f \quad (9)$$

$$\rho_d u_d \frac{du_d}{dz} = - \frac{dp}{dz} - \frac{3}{8} C_D \rho_f \frac{(u_d - u_f)^2}{R_d} \quad (10)$$

$$\rho_f u_f \frac{du_f}{dz} = - \frac{dp}{dz} + \frac{3}{8} \frac{\rho_f (u_d - u_f)^2}{R_d} \frac{\alpha_d}{\alpha_f} - (u_d - u_f) u_d \frac{dm_s}{dz} \quad (11)$$

where the radius of the drop changes according to:

$$\frac{dR_d}{dz} = \frac{1}{\rho_d 4\pi R_d^2} \frac{dm_s}{dz} \quad (12)$$

and the mass source function for the fluid is

$$\Gamma_f = u_d \frac{dm_s}{dz} \frac{\alpha_d}{\frac{4\pi R_d^3}{3}} \quad (13)$$

One can look upon the mass transfer from the drops to the surrounding flux as a Reynolds flux¹⁶, with the exchange factor $\eta = 1$. To determine the rate of mass stripping, the Ranger-Nichols equation⁵ is employed (as in the Jacobs calculation¹²):

$$\frac{dm_s}{dt} = u_d \frac{dm_s}{dz} = (12\pi^3)^{1/2} \left(\frac{\rho_f}{\rho_d}\right)^{1/3} \left(\frac{v_d}{v_f}\right)^{1/6} \rho_d v_d^{1/2} u_r^{1/2} R^{3/2} \quad (14)$$

Two examples were chosen, corresponding to those discussed by Board, et al³. The first was a tin-water mixture, in the proportions 1 cc steam and 1 cc water at 100°C and 1 cc tin drops at 1000°C, initially at atmospheric pressure. The second is a UO_2 -Na mixture, in proportions corresponding to 10 g UO_2 , 1 g Na, plus 1 cc vapor initially at atmospheric pressure. The initial relative velocity, shock velocity and pressure immediately behind the shock were calculated by Eqs. (1) - (4), followed by a numerical integration of Eqs. (8) - (11) through the fragmentation zone. Two initial shock strengths were chosen in each case, corresponding to $We = 10^5$ and 10^6 . These Weber numbers are, in fact, larger than the range of interest for breakup by boundary-layer stripping, since for $Bo > 10^5$ Taylor instability dominates. Hence the calculation, summarized in Table 1, is conservative. It is seen that a negligible fraction of the drop mass is stripped away in the time available before velocity equilibration. The pressure rise across the shock is due to the vapor blanket collapse, which results in slowing-down of the coolant relative to the shock as it passes through the front. This calculation would indicate that a small disturbance cannot escalate into a shock wave by the boundary-layer stripping mechanism created by Ranger and Nichols.

A model has been formulated for propagation of a low-pressure ($P_{\max} < P_{cr}$) shock, by a mechanism which depends upon vapor production after liquid-liquid contact is made. Results will be given in the next progress report.

References

1. S. G. Bankoff and J. H. Jo, "On the Existence of Steady-State Fuel Coolant Thermal Detonation Waves", S. G. Bankoff and J. H. Jo, Paper SNI 6/30, Proc. Third Spec. Mtg on SFI in Fast Reactors, Tokyo (1976).
2. S. G. Bankoff and J. H. Jo, "Mechanisms of Vapor Explosions", ANS/ENS Int. Meeting on Fast Reactor Safety and Related Physics, Chicago (1976).
3. S. J. Board, R. W. Hall and R. S. Hall, "Detonation of Fuel Coolant Explosions", Nature, 254, 319, (March 1974).
4. E. Y. Harper, et al., "On the Breakup of Accelerating Liquid Drops", J. Fluid Mech., 55, 629 (1972).
5. A. A. Ranger and J. A. Nichols, "Aerodynamic Shattering of Liquid Drops", AIAA J., 7, 285 (1969).
6. M. Ochiai and S. G. Bankoff, "Local Propagation Theory for Vapor Explosions", Paper SNI 6/3, Proc. 3rd Spec. Mtg. for SFI, Tokyo (1976).
7. M. Ochiai and S. G. Bankoff, "Liquid-Liquid Contact in Vapor Explosions", ANS/ENS Int. Mtg. on FRS, Chicago (1976).
8. A. Segev and S. G. Bankoff, "The Minimum Air Film Thickness between a Free-Falling Volatile Drop and a Hot Liquid Surface", NU-2512-3 (1975).
9. K. L. Waldram, "Interaction of Low Boiling Point Liquid Drops on a Hot Surface", M.S. Thesis, Northwestern University, Evanston, IL (1973).
10. K. L. Waldram, H. K. Fauske and S. G. Bankoff, "Impaction of Volatile Liquid Droplets onto a Hot Liquid Surface", AIChE-ASME National Heat Transfer Conf., San Francisco, CA (1975).
11. H. Jacobs, "Computational Analysis of Fuel-Sodium Interactions with an Improved Method", ANS/ENS Int. Mtg. on FRS, Chicago (1976).
12. H. Jacobs, KFK 2260, Karlsruhe (1976).
13. G. Rudinger, Phys. Fluids, 1, 658 (1964).
14. A. R. Kriebel, ASME J. Basic Eng., 86, 655 (1964).
15. G. A. Wallis, "One-Dimensional Two-Phase Flow", McGraw-Hill, NY (1969).

Table 1

Mixing by Boundary Layer Stripping in a
Dense Fuel-Coolant Mixture

	<u>Tin - H₂O</u>		<u>UO₂ - Na</u>	
<u>Initial Conditions</u>				
Mixture Proportions:				
Mass fuel, g	6.518	(1 cc)	10	(1.22 cc)
Mass liquid coolant, g	0.960	(1 cc)	1	(1.176 cc)
Mass vapor, g	$5.86 \cdot 10^{-4}$	(1 cc)	$6.47 \cdot 10^{-4}$	(2.4 cc)
Temp. fuel, °C	1000		3300	
Temp. coolant, °C	100		430	
Pressure, atm	1.0		1.0	
Drop radius, cm	0.5		0.5	
Void fraction coolant	0.667		0.6222	
<u>Conditions Immediately Behind Shock Front</u>				
Weber No.	10 ⁵	10 ⁶	10 ⁵	10 ⁶
Pressure, P ₂ , atm	129	1190	107.6	1066
Vel. shock, u ₁ , cm/sec	$2.33 \cdot 10^4$	$7.0 \cdot 10^4$	$2.4 \cdot 10^4$	$7.6 \cdot 10^4$
Vel. drops, u _{d2} , cm/sec	$2.20 \cdot 10^4$	$6.69 \cdot 10^4$	$2.33 \cdot 10^4$	$7.38 \cdot 10^4$
Vel. coolant, u _{f2} , cm/sec	$1.18 \cdot 10^4$	$3.43 \cdot 10^4$	$8.10 \cdot 10^3$	$2.5 \cdot 10^4$
Relative velocity, u _{r2}	$1.02 \cdot 10^4$	$3.26 \cdot 10^4$	$1.53 \cdot 10^4$	$4.88 \cdot 10^4$
Void fraction coolant	0.653	0.652	0.613	0.613
<u>Equilibrium Conditions Behind Shock</u>				
Drag coefficient, C _D = 2				
Pressure, P _e	462	4300	806	8080
Mass fraction stripped, x _e	$3.3 \cdot 10^{-4}$	$1.8 \cdot 10^{-4}$	$6.5 \cdot 10^{-5}$	$4.2 \cdot 10^{-5}$
Time for equilb., t _e , sec	$1.3 \cdot 10^{-3}$	$3.5 \cdot 10^{-4}$	$6 \cdot 10^{-4}$	$2.7 \cdot 10^{-4}$
Mixture vel., u _e , cm/sec	$1.54 \cdot 10^4$	$4.8 \cdot 10^4$	$1.38 \cdot 10^4$	$4.35 \cdot 10^4$
Drag coefficient, C _D = 20				
Pressure, P _e	470	4400	813	8156
Mass fraction stripped, x _e	$4.5 \cdot 10^{-5}$	$3 \cdot 10^{-5}$	$1.3 \cdot 10^{-5}$	$7 \cdot 10^{-6}$
Time for equilb., t _e , sec	$2.2 \cdot 10^{-5}$	$7.1 \cdot 10^{-5}$	$2 \cdot 10^{-4}$	$6.6 \cdot 10^{-5}$
Mixture vel., u _e , cm/sec	$1.54 \cdot 10^4$	$4.8 \cdot 10^4$	$1.39 \cdot 10^4$	$4.4 \cdot 10^4$

*drop and coolant velocities are relative to shock front.

List of Figures

1. Typical experimental data for Leidenfrost boiling stability for a particular drop size ($d = 2.26$ mm), as a function of ΔP , the pressure rise, and T_h , the hot oil temperature.
2. Destabilization of Leidenfrost boiling on a hot liquid surface due to increase in pressure: Pentane drop on Dow-Corning 710 Silicone oil surface. $\Delta P = P_{\text{initial}} - P_{\text{final}}$. $P_{\text{final}} = 1$ atm. Drop diameter, d , estimated from photograph. Lines represent stability boundaries, above which coalescence (unstable film boiling) and below which rebound (stable film boiling) resulted. Parameter is the boiling point of n-pentane at the initial pressure.

Fig 1

Fig 2