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MODELING OF STEADY PLANE THERMAL DETONATIONS

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MODELING OF STEADY PLANE THERMAL DETONATIONS

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1. INTRODUCTION

Steady plane thermal detonations proceeding through coarse fuelcoolant mixtures have been predicted to exhibit pressures of ~ 10^4 bar for UO₂'Na and ~ 10^3 bar for Sn/H₂O¹. Although detailed experimental information for the crucial fragmentation step is still largely lacking, some important preliminary conclusions can nevertheless be drawn from a detailed examination of the jump balances and solution of the steady, separated-flow conservation equations in the fragmentation zone behind the shock. In this paper we present a few key results of some parametric calculations of steady plane thermal detonations, and in addition offer some broader comments.

2. CHAPMAN-JOUGUET CONDITIONS

It is instructive, first of all, to examine the jump mass momentum, and energy balances across the shock front:

$$\begin{bmatrix} \Sigma & \alpha & \rho_{\mathbf{u}} \\ \mathbf{i} & \mathbf{i} & \mathbf{i}^{\mathbf{u}} \\ \mathbf{i} & \mathbf{i} \end{bmatrix} = 0 \tag{1}$$

$$\begin{bmatrix} \Sigma \alpha_{i} \left(P_{i} + \rho_{i} u_{i}^{2} \right) \end{bmatrix} = 0$$
⁽²⁾

$$\begin{bmatrix} \sum_{i} \alpha_{i} \rho_{i} u_{i} & (h_{i} + \frac{1}{2} u_{i}^{2}) \end{bmatrix} = 0$$
(3)

where the subscript i takes on the values cv, cl, and f, referring to coolant vapor, coolant liquid and fuel, respectively, and the square jump brackets refer to values of a point 1 before and a point 2 behind the shock. If velocity and pressure equality exists between the phases (homogeneous flow) at both points 1 and 2, Eqs. (1) and (2) reduce to those for classical single phase detonation theory^{1,2,3}. Providing the mixture at point 2 has a welldefined and unique specific volume, temperature equilibrium is not necessary. In particular, a plane (called the Chapman-Jouguet or C-J plane) of local sonic velocity relative to the shock front must exist at the end of the fragmentation and velocity-equilibrium zone in order to prevent weakening of the shock by rarefaction waves from the far field. If the fragmentation process takes place by removing small debris particles, either by boundary layer stripping or by surface boiling mechanisms, the degree of fragmentation, E, at the C-J plane can be treated as a parameter. If now it is assumed that

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heat transfer from the unfragmented portions of the fuel drops can be neglected, and that the debris particles equilibrate in temperature and velocity instantaneously with the surrounding coolant, families of partial-fragmentation Hugoniot curves can be constructed, as in Fig. 1. The pronounced knee on the curves for E < 1 marks the point at which vapor disappears as the pressure increases. From this simple model one sees immediately that the tangent from this particular initial point to the reaction adiabat for E < 1 will always intersect it close to the 1 ee, and hence at subcritical pressures. Indeed, a number of experimental studies of tin-water propagating interactions⁴⁻⁸ have failed to yield supercritical pressures behind the shock front.

For UO /Na the same effect exists, although less pronounced. For initially equal volumes of molten UO, liquid sodium and sodium vapor, Fig. 2 shows that only subcritical pressures can be achieved if E = 0.5 at the sonic velocity plane, but supercritical pressures are possible if E = 0.7. The points on the partial-fragmentation Hugoniots where the Mach number $M_3 = 1$, determined from the separated-flow multiphase sonic velocity criterion^{11,12,13}, differ somewhat from the tangency condition points (homogeneous flow assumption), as might be expected.

The requirements for a stable C-J plane ¹¹⁻¹⁵ have been analyzed. They demand that the expression for the pressure gradient, deduced from the separated-flow differential equations of the fragmentation zone, be indeterminate, corresponding to the simultaneous vanishing of the numerator and denominator. Physically this is necessary in order to match the time-independent fragmentation region to the time-dependent supersonic expansion zone. With the assumption that the fuel debris particles form a homogeneous fluid mixture with the coolant, the pressure gradient is given by¹³

$$\frac{dP}{dz} = \frac{\frac{3}{8} c_{\rm D} \rho_{\rm f} \frac{\alpha_{\rm d}}{r_{\rm d}} - u_{\rm r}^2 \left(\frac{1}{\rho_{\rm f} U_{\rm f}} - \frac{1}{\rho_{\rm d} U_{\rm d}}\right) - \Gamma_{\rm f} \left(\frac{2}{\rho_{\rm f} U_{\rm f}} - \frac{U_{\rm d}}{\rho_{\rm f} U_{\rm f}^2} + \frac{1}{\rho_{\rm d} U_{\rm d}}\right)}{\frac{\alpha_{\rm f}}{\rho_{\rm f} U_{\rm f}^2} \left(1 - \frac{U_{\rm f}^2}{c_{\rm f}^2}\right) + \frac{\alpha_{\rm d}}{\rho_{\rm d} U_{\rm d}^2} \left(1 - \frac{U_{\rm d}^2}{c_{\rm f}^2}\right)}$$
(4)

where the mass source function, $\Gamma_{_{\rm F}}$, is given by

$$\Gamma = \frac{d^2 d^2 d}{1 - E} \frac{dE}{dz}$$
(5)

At supercritical pressures, boiling mechanisms for fragmentation cannot be operative, and velocity equilibrium (U = 0) implies that Γ is also zero. The vanishing of the denominator of Eq. (4) is the well-known requirement for the attainment of choked flow in a separated-flow system^{11,12}. This may be termed a normal, or equilibrium, C-J plane, corresponding to zero entropy production. Small disturbances would be expected to damp out, due to irreversibilities, resulting in a stable condition. Strictly speaking, entropy production due to heat transfer does not cease until temperature equilibrium is achieved. Since there is a finite relative velocity cutoff for fragmentation at supercritical pressures, the requirement of zero entropy production implies that the C-J plane is located at a great distance behind the shock front. In practice, however, the fragmentation is essentially cut off in a relatively short effective zone length¹³, as shown in Fig. 3. The conclusion that one can draw is that steady supercritical thermal detonations cannot exist, although in practice slowly-varying detonations are not ruled out. It is also possible that the numerator of Eq. (4) can be made to vanish at an isolated point, or points, with slip at supercritical pressures. However, in the absence of vapor there seems to be no obvious restoring force driving the perturbed system back to the singular C-J plane. On the other hand, at subcritical pressures a small increase in pressure tends to collapse the vapor layers, resulting in increased heat transfer and hence more vapor production. A stable C-J plane with U \neq 0 is then possible.

Further progress requires that an estimate be made of the reaction zone length for assumed initial conditions and drag coefficient as a function of dimensionless break-up time, T. The curves shown in Fig. 4 were obtained¹³ by assuming the pressure and the degree of fragmentation at the C-J plane, calculating the C-J plane conditions from the component jump mass balances and the total momentum jump balance, and integrating the four mass and momentum differential equations backwards from a point where $U_{\rm r}/U_1 = 0.005$

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to the shock front, taken to be given by E = 0. The Reinecke-Waldman¹⁰ expression for the rate of fragmentation was used. This expression was obtained empirically from air-water data in the boundary-layer stripping range, but a slope function appropriate to Taylor instability does not change the results materially, providing the same time scale, T, for fragmentation is used. It is seen that the zone length is unrealistically long for these examples if T > 1.5, which is indicated by gas-liquid experiments^{16,17}, as well as some mercury-water experiments^{18,19}. However, other liquid-liquid experiments over a wide range of Bond numbers^{20,21} give T ~ 0.4, which implies reaction zone lengths of 5-10 cm., which seems physically acceptable. This discrepancy cannot at present be considered to be fully resolved.

3. EFFECTS OF SOLIDIFICATION ON FUEL/COOLANT TAYLOR INSTABILITY

Cooper and Dienes²² have given a model for fragmentation due to Taylor instability, based upon a method of generalized coordinates due to Dienes²³, which in turn stems from earlier work by Fermi²⁴ and Miles and Dienes²⁵. The general theory makes no assumptions concerning the existence of a potential, and hence is applicable to dissipative media. When applied to plane periodic inviscid flow of an incompressible fluid (the inertia of the lighter fluid is ignored, to this approximation) potential flow can be assumed in a coordinate system in which acceleration is replaced by an effective gravity g(t). Because of the exponential growth, exp(n(k)t), of the Fourier component of the potential, $\frac{1}{2}(k,t)$, during the early phase of instability growth, the Fourier integral for the potential is rapidly dominated by the fastest-growing wavelength, determined by dn(k)'dk = 0 at k = k. The potential is thus approximated by

$$\frac{\dot{q}(x,y,t)}{k} = \frac{\dot{q}(t)}{k} \cos(kx) e^{-ky}$$
(6)

where it is understood hereafter that k is evaluated at k_0 . Here q(t) may be looked upon as a generalized coordinate, and the overdot signifies a time derivative. From this the explicit kinematic relation for the surface perturbation is obtained:

$$y(x,t) = k^{-1} \ln (1 + q(t) \cos kx); \ 0 \le q \le 1$$
(7)

which has the characteristic spike-and-bubble configuration of latetime Taylor instability as $q(t) \rightarrow 1$. The differential equation for q(t) is obtained from an energy balance over one wavelength, equating the rate of energy dissipation to the rate of change of kinetic and potential energy. The potential energy consists of "gravitational" and surface energy, and, if the denser material is frozen or freezing, elastic energy. When the deformation energy density exceeds the yield strength, there is energy dissipation in the plastic regime, where the integration over y is over the frozen region, as well as viscous dissipation. The thickness of the frozen region, d(t), is approximately given by the plane geometry result²³:

$$d(t) = 2\lambda^* \left(\frac{\alpha}{d}t\right)^{\frac{1}{2}}$$
 (8)

where α_{λ}^{\star} is the thermal diffusivity of the fuel drops, and λ^{\star} is the solution of a transcendental equation²⁶.

The mixing time scale, t_{mix} , is of the order of 10-100 milliseconds while the time scale for instability growth is two or three orders of magnitude smaller. Consequently, the time for crust growth $t_{fr} \sim t_{mix}$ and the crust thickness, d, can be considered constant during the instability growth¹³.

Cooper and Dienes 22 found that the equation describing the early instability growth is given by the following linearized second order ODE:

$$\dot{q} + 4k^{2} v_{d} \dot{q} + \left[-\tilde{g}k + \frac{4k^{2}}{\rho_{d}} (1 - e^{-2kd}) G H \left(\frac{Y_{o}}{2G} - q\right)\right] q$$

$$+ sgn(\dot{q}) \frac{4k^{2}}{\rho_{d}} (1 - e^{-kd}) H(q - \frac{Y_{o}}{2G}) = 0$$
(9)

where H(x) is the Heaviside step function, sgn(x) is the sign function, and 2.2

$$\widetilde{g} = g - \frac{\sigma^2 k^2}{\rho_d}$$
(10)

Here g is the acceleration given by:

$$g = \frac{3}{8} c_{\rm D} \frac{\rho_{\rm f}}{\rho_{\rm d}}^{\rm T} r^{\rm 2}$$
(11)

k is the wave number $(2\pi'\lambda)$, Y is the yield stress and G is the modulus of rigidity of the fuel (for UO Y = 10^9 dynes/cm² and G = $3.7 \cdot 10^{13}$ dynes/cm²).

The initial conditions are taken to be:

$$q(0) = 0; q(0) = \pi^{-1} k U_{ro} = 2\lambda^{-1} U_{ro}$$
 (12)

Eq. (9), with the initial conditions (12), was solved numerically¹³, assuming constant relative velocity (U = U), C = 2 and $\lambda = r_d = 0.5$ cm. By varying the crust thickness, d, as a parameter for a given initial relative velocity, the critical crust thickness above which the instability will not grow can be determined. A plot of the critical crust thickness vs. the (initial) relative velocity is shown in Fig. 5.

If we neglect the effect of viscosity, the stability of Eq. (9) can be analytically determined by considering the trajectories in the \dot{q} - qphase space²³. The stability criterion becomes:

$$\frac{16 k^{3} y^{2}}{q(0)^{2}} = \frac{k^{2} v^{2} r_{0}}{\pi^{2}} \geq \frac{16 k^{3} y^{2} (1 - e^{-kd})}{\rho_{d}^{2} \tilde{g}}$$
(13)

and the critical crust thickness, d_{cr}, is:

$$d_{cr} = \frac{1}{k} \ln \left(1 - \frac{p_{d} \overline{v}_{ro} \widetilde{g}^{\frac{1}{2}}}{4\pi Y_{o} k^{\frac{1}{2}}} \right)$$
(14)

As shown in Fig. 5 the numerical solution and Eq. (14) are in good agreement. $^{\rm 27}$

In all the cases investigated for UO $^{/}$ Na mixture, the initial relative velocity was in the range of 100 - $^{2}200$ m/s, so that the critical crust thickness is of the order of 10 μ m.

For $\hat{\sigma}_{r} = 600$ K, $\lambda^{*} = 0.93$, and hence for $d_{r} = 10 \ \mu m$, $t_{r} \sim 7 \cdot 10^{-5}$ sec. If one assumes a constant crust growth rate of 2 cm/sec^T(28), $t_{r} \sim 0.5$ ms. However this growth rate is associated with crystallization-kinetics-controlled advance of a solidification front into a highly supercooled liquid, which is not relevant to the present case. Hence, we conclude that if the mixing time scale for UO_/Na is larger than 0.1 ms, the crust will be thick enough to prevent the growth of interfacial waves and hence no hydrodynamic fragmentation can occur.

For carbide fuel (UC) the initial relative velocity can be of the order of 300 - 400 m/s ($\rho_{\star} \sim 12$ g/cm³). The critical crust thickness is estimated from Eq. (14) as d ~ 60 μ m (for UC Y = 1.5 \cdot 10⁹ dyne/cm²). The crust growth constant, cr λ *, is 0.67, hence from Eq. (8) t_{fr} ~ 4 \cdot 10⁻⁴s. Such rapid premixing on a coarse scale, for both UC₂ and UC fuels, seems to be very highly improbable in any large-scale event.

CONCLUDING REMARKS

Film boiling of subcooled sodium from molten UO, is unstable²⁹, but it has been suggested that the delay before collapse may be as long as 200 ms³⁰. If the delay is much shorter (favored by small fuel drops, high relative velocity, low sodium temperature), subcooled nucleate boiling will result in rapid fragmentation³¹. The collapsing bubbles at the freezing interface produce a inwardly-pointing jet³², which can exceed the yield strength of the growing UO₂ crust³³. On the other hand, if the vapor film is stable for ~ 200 ms, the nonlinear Taylor instability theory for elastic-plastic solids sketched here indicates that the crust thickness will prevent fast breakup by Taylor instability. In either case a supercritical detonation would be prevented.

Most of the effort on nuclear reactor vapor explosion has been aimed at UO 'Na interactions, for which it is not known whether a large-scale vapor²explosion can take place. For the reasons outlined above, the probability of a steady detonation at supercritical pressures appears to be very low. However, the consequences of vigorous interactions with longer rise times and lower pressures must be explored for each accident scenario.

CORRECTION

We wish to thank an earlier reviewer who pointed out to us (unfortunately ^{13,27} too late to prevent publication) that we had misinterpreted the description of the initial conditions in the UO₂/Na example of a supercritical propagating detonation given in Ref. 1. Based on the Hugoniot curves, the tangency point for the correct initial conditions was indeed in the supercritical pressure region, whereas it was not for the composition assumed by us. We apologize for the error.

NOMENCLATURE

Во	-	Bond number
С	-	Speed of sound
C_	-	Specific heat
ď	-	Crust thickness
Е	-	Fraction of mass stripped
G	-	Modulus of rigidity
8	-	Acceleration
~ g	-	Modified acceleration
H	-	Heaviside step function
h	-	Heat transfer coefficient
ĥ	-	Specific enthalpy
ĥ _{fg}	-	Latent heat of evaporation
k	-	Thermal conductivity
k	-	Wave number $(2\pi/\lambda)$

L	-	Relaxation zone length
P	-	Pressure
P	-	Generalized coordinate
rd	-	Drop radius
T	-	Temperature $U t_{1} / P_{2} \sqrt{2}$
T.	-	Dimensionless breakup time = $\frac{r}{2r} \frac{b}{\rho}$
t	-	Time
ប	-	Velocity relative to the shock
Y _o	-	Yield stress
z	-	Distance behind shock front

Greek Symbols

α.	Volumetric fraction										
a [*]	Thermal diffusivity										
Г _f	Fluid source term										
ε	Vapor volume fraction in coolant										
Ŋ	Amplitude of interfacial wave										
λ	Wave length										
λ*	Crust growth constant										
14	Viscosity										
ν	Kinematic viscosity										
ρ	Density										
σ	Surface tension										

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Subscripts

ь	Breakup	Ċ.	Init	ial		•	
c	Liquid coolant	1	Ahea	ad of	shock		
d	Drop	2	Imme	diat	ely behind	i sh	lock
r	Relative (between f	uel 3	End	of f	ragmentati	lon	zone
	and coolant)	REFERENCES					

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LIST OF FIGURES

- Fig. 1 Partial-fragmentation Hugoniot curves for a tin-water mixture. Initial conditions: Vol. fraction fuel drops, a = 1/3 vol. fraction coolant vapor in coolant liquid/vapor mixture e = 0.5 (equal volume of coolant vapor and liquid). Mass fuel/mass coolant = 6.5. Parameter E is mass fraction of the fuel drops fragmented at the Chapman-Jouguet plane.
- Fig. 2 Partial-fragmentation Hugoniot curves for UO/Na mixture, initially with equal volumes fuel, coolant vapor and coolant liquid. Mass fuel/mass coolant = 10. Fuel temp. = 3550K; liquid coolant temp. 1200K. This example shows C-J pressures of θ order 10^2 MPa for E = 1, in agreement with Ref. 1, but subcritical pressures if only half of the drop mass is fragmented at the sonic-velocity plane. A different mixture with equal volumes of liquid coolant and fuel, but a vapor volumetric fraction of 0.5, permits only subcritical detonation pressures, and was erroneously identified in an earlier version^{13,2} as the mixture referred to Ref. 1.
- Fig. 3 Theoretical calculation of fragmentation zone behind plane shock in UO₂'Na mixture. $\alpha = 1/3$, $\varepsilon = 0.5$; dimensionless breakup time T₁ = 0.9; C₂ = d1₂. Note v1 that velocity equilibrium is never achieved, but that the relative velocity between fuel drops and coolant'fuel debris mixture is reduced to 5% of the relative velocity immediately behind the shock in an effective length, L_{ef}, of ~ 3 cm.
- Fig. 4 Reaction zone length vs. dimensionless breakup time for Sn/H_{2}^{0} and $UO_{2}^{'}Na$. E = 1.
- Fig. 5 The effect of the frozen crust on the relative velocity required for the instability to grow.



Fig. 1 Partial-fragmentation Hugoniot curves for a tin-water mixture. Initial conditions: Vol. fraction fuel drops, and 1/3 vol. fraction coolant vapor in coolant liquid/vapor mixture colant vapor in coolant liquid/vapor mixture cliquid). Mass fuel/mass coolant a 5.5. Parameter E is mass fraction of the fuel drops fragmented at the Chapman-Jouguet plane.



Fig. 2 Partial-fragmentation Hugoniot curves for a UO_/Na mixture, initially with equal volumes fuel, coolant vapor and coolant Higuid. Mass fuel/mass coolant = 10. Fuel temp. = 3550K; liquid coolant temp. 1200K. This example shows C-J pressures of θ order 10² MPa for E = 1, in agreement with Ref. 1, but subcritical pressures if only half of the drop mass is fragmented at the sonic-velocity plane. A different mixture with equal vols. of liq. coolant and fuel, but a vapor volumetric fraction of 0.5, permits only subcritical detonation press. 6 was erroneously identified in an earlier version as mixture referment to in Ref 1.



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Fig. 5 The effect of the frozen crust on the relative velocity required for the instability to grow.

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