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THE PROPAGATION OF LARGE SCALE THERMAL EXPLOSIONS

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Abstract—We suggest that, on present theoretical and experimental evidence, all large scale propagating thermal explosions have a detonation-like structure. We examine the effects on such a thermal detonation of sideways flow, interphase slip and thermal expansion of the coolant; the balance of these effects at the place in the reaction zone where the flow goes sonic controls the propagation, and hence efficiency of the explosion.

We show that:

(a) thermal explosions (like chemical explosions) will only propagate if the sideways constraint is high;

(b) in a detonation in which vapour is generated within the reaction-region (a 'vapour detonation') the efficiency can be low. We apply a model of this to metal/water explosions, and show that it predicts the general characteristics of these events.

NOMENCLATURE

A,	the area of contact between fuel and coolant;
C',	specific heat;
c,	velocity of sound;
d,	size of particles before fragmentation;
D,	detonation velocity;
F,	volume of the fuel;
h,	specific enthalpy;
j,	mass flux ($\mathbf{j} = \rho\mathbf{v}$);
k,	Boltzmann constant,
K,	conductivity;
l,	length of reaction zone;
L,	latent heat of evaporation;
M,	mass transported between fluids in unit volume;
M',	$\frac{M}{\alpha_i \rho_i}$, mass transport/unit mass of phase i;
m,	vapour mass/unit mass of mixture;
Q,	heat flux;
R,	gas constant;
r,	radius of curvature of surface orthogonal to the flow;
S,	specific entropy;
T,	temperature;
t,	time;
t',	vapour blanket thickness;
u,	x component of velocity $\mathbf{v}$ (i.e. parallel to direction of propagation);
v,	$\lvert\mathbf{v}\rvert$, velocity in frame of front;
V,	specific volume;
w,	y component of velocity $\mathbf{v}$;
Y,	thickness of reaction layer (Fig. A1) in y direction.

Greek symbols

α_i,	volume fraction of fluid i;
α',	thermal diffusivity;
β,	expansion coefficient;
γ,	ratio of specific heats;
δ,	boundary layer thickness;
η,	dynamic viscosity;
θ,	divergence parameter $\left(\frac{j}{j_i}\right)$ for 2-D flow; (see Appendix C);
λ,	$\left.\frac{\partial P}{\partial M'}\right)_{\rho,S}$;
μ,	entropy transported by interfluid mass transfer;
ρ,	density;
σ,	$\left.\frac{\partial P}{\partial S}\right)_{\rho,M'}$;
τ,	Lagrangian time co-ordinate (measured from the crossing of the shock front);
τ',	momentum transported by interfluid mass transfer;
Φ,	heat flux/unit area;
ψ,	momentum integral $\frac{1}{u_f - u_i}\int_i^f \theta \, du$; (see Appendix C);
χ,	numerator of pressure gradient expression (equation 1).

Subscripts

c,	the state at which vapour generation begins;
f,	the state at the C–J plane;
h,	fuel phase;
i,	the initial state ahead of the shock;
l,	coolant liquid phase;
s,	the state just behind the shock;

v, coolant vapour phase;
1, fluid 1, usually the coolant and its vapour;
2, fluid 2, usually the fuel.

Derivatives

$\frac{\mathrm{D}A}{\mathrm{D}t}, \frac{\partial A}{\partial \tau}, \dot{A}$ all denote $\mathbf{v}.\,\mathrm{grad}\,A + \frac{\partial A}{\partial t}$, the convective derivative of A.

1. INTRODUCTION

IN CERTAIN circumstances the mixing of a hot liquid and a cooler vaporisable one leads to an explosive rate of vapour production. Such occurrences could arise if molten metal is poured into water [1], when liquid-natural-gas is spilt at sea [2], and also, under extreme fault conditions, in liquid-cooled reactors if fuel-melting [3] occurs.

In such 'thermal explosions' we believe that a disturbance propagates through a coarse intermixture of the two liquids causing fine fragmentation and rapid energy transfer [4]; this energy transfer in turn causes expansion of the volatile phase, which sustains the propagation.

In two earlier papers [4, 5] we presented observations of propagating thermal explosions, and developed a simple model for the form these could take in a highly constrained geometry. In such a 'thermal detonation' the energy transfer is initiated by a shock front in a manner analogous to a chemical detonation. This concept of a propagating, self-sustained shock has been confirmed by our recent experimental work [6].

We now generalise our simple model and consider the effects on the propagation of sideways flow, slip and the expansion of the mixture (produced by heat transfer). We consider how the propagation is controlled by the balance of these effects at the plane where the flow becomes sonic (i.e. at the Chapman–Jouguet or C–J plane), and show that in this generalised model detonations can be significantly less efficient than predicted in [5]; (we found there that, when thermal equilibrium is achieved at the C–J plane, pressures and energy yields in excess of those calculated by Hicks and Menzies [7] could result).

By applying these considerations to a model of heat-transfer in a 'vapour-detonation' we show how temperature disequilibrium in the liquid coolant limits efficiency to a degree calculable from experimental data on transient heat transfer. We show also how sideways constraint must be high if detonation-like propagation is to be possible.

In deriving these new results, we make extensive use of published work on chemical-reactive flow and so begin by considering the analogy between chemical-reactive and thermal-reactive flows in detail.

2. CHEMICAL AND THERMAL REACTIVE FLOWS COMPARED

It seems likely that many of the important properties of large-scale thermal explosions can be modelled in the hydrodynamics of two-fluid two-dimensional reactive flow (see Appendix A). This field has been extensively studied in connection with chemical engineering and combustion problems.

Although we may expect parallels between the types of flow which could occur in the two areas, there are important differences between the way chemical-combustion reaction rates and thermal-explosion heat transfer rates vary with temperature and pressure. This will influence the relative importance of the two steady-state modes (detonation and deflagration) in the two cases.

2.1 *The deflagration mode*

In deflagration waves the propagation speed is subsonic; such chemical explosions can be considered temperature-controlled (more correctly, controlled by the migration of excited species ahead of the flame front). There appear to be several reasons why thermal explosions should not sustain stable deflagrating waves. Firstly, the equivalent subsonic initiating mechanism appears to be the temperature rise in the surrounding coolant caused by the diffusion of heat away from the energy release zone. Such a rise would however increase the stability of film boiling; moreover the fall in pressure which occurs through a deflagration wave, would enhance this stability and impede energy transfer. Secondly, thermal reactions are triggered by quite small pressure and velocity changes [4]; by contrast, most chemical reactions do not proceed at a significant rate below temperatures of 2000 K and to achieve these, even in shocks, pressure changes of tens of bars are required. We thus expect that the transition from deflagration to detonation, which is often observed in the chemical case, would happen much more easily for thermal explosions. For instance reinforcement of the precursor shock (e.g. by reflection) may lead to direct initiation of a new reaction zone close to the shock. Alternatively it seems likely that the reaction zone, being controlled only by the pressure and velocity fields could move forward and join with the precursor shock – such a coalescence is a detonation [8]. We thus suggest that the deflagration mode has no stable analogue in thermal explosions.

2.2 *The detonation mode*

Our suggestion that only detonations have thermal explosion analogues implies that all large scale thermal explosions propagate supersonically through the medium ahead of them. This conclusion is supported by the velocities observed experimentally ($\sim 10^4$ cm/s, [4, 9]); these are of the order of sound velocities in two-phase media; recent observations in freon/water and tin/water systems confirm the presence of this supersonic front [6]. We consider the structure of the wave in detail.

The leading edge of such a front is a shock, in which the dominating mechanism controlling the width is probably the pressure induced collapse of the vapour phase—because of heat conduction away from the liquid–vapour interface, this is inherently an irreversible process. (We note in passing that the vapour phase need not be a stable vapour film—nucleate-boiling bubbles would behave similarly.) The collapse stage will be completed before any significant heat transfer from fuel to coolant can occur, and so it should be permissible to analyse the explosion in a manner similar to the chemical case, as a discrete initiating shock in the unreacted material, followed by an energy release zone. (The effects of energy release occurring within the shock-region have been considered by Fishlock [10]).

In the reaction zone behind the shock, the flow (in the frame of the front) is subsonic. The effect of the heat transfer into the coolant is, as we discuss further below, to cause expansion and allow a drop in pressure, which thus increases the Mach number of the flow. If the flow eventually reaches sonic velocity the choking point (C–J point) thus formed isolates the shock and heat transfer zones from the subsequent expansion of the products, and enables the wave to travel at a steady velocity. Now in both chemical and (probably) thermal explosions the reaction or heat transfer rates are considerably reduced when the materials are allowed to expand rapidly (in the former case because the temperature drops, in the latter because of vapour blanketing). In both cases therefore the rarefaction wave at the leading edge of the expansion zone probably terminates the energy transfer—only the presence of a sonic point prevents it extinguishing the whole reaction. If it can be shown that the energy transferred in the steady-state region is small, it is then likely that the overall efficiency is small. (This would break down however if the inertial constraint were so high that the final expansion could be adiabatic.) In a well-constrained chemical explosion it is usually true that the reaction is complete at the C–J plane and so the explosion makes full use of the available energy—this is not necessarily so however, expecially when sideways flow is allowed or the reactants are not in internal temperature equilibrium.

3. THE BALANCE CONDITION AT THE C–J PLANE

The work of Wood and Kirkwood [11, 12] and others showed that the necessary condition for the C–J plane to terminate the steady state region is that the gradients of the flow variables ($\mathrm{d}P/\mathrm{d}x$, $\mathrm{d}u/\mathrm{d}x$, etc.) are indeterminate there (so that there is no inconsistency with the adjoining time-varying expansion zone). In Appendix A we derive an expression for the pressure gradient for a two-fluid model with sideways flow. This is of the form (equations A8, A9)

$$\frac{\mathrm{d}P}{\mathrm{d}x}=\frac{\chi}{u^2-c^2}, \tag{1}$$

where χ contains terms giving the rate of change of pressure at constant volume; for indeterminacy, $\chi=0$ and $u=c$. The following terms contribute to χ:

(i) The heat flow into the more volatile fluid gives a positive term to χ; this leads to a negative pressure gradient which accelerates the subsonic flow behind the shock front;

(ii) The sideways flow out of the reaction zone; this gives a negative term to χ and so acts to prevent acceleration of the flow and to balance the effects of heat transfer;

(iii) The re-equilibration of the velocity between the phases also gives a negative term to χ (and so also opposes heat transfer). (The existence of slip however also complicates the meaning of 'c' in the denominator, see below.)

In well-constrained chemical reactions only the chemical-reaction term (analogous to (i)) is significant, and this term only vanishes when the reaction ceases. In thermal explosions, however, the heat transfer term is not the only significant one, nor need its contribution always be positive. We consider below the role of (i) and (ii), and more briefly (iii).

4. THE STRUCTURE OF THE ENERGY-TRANSFER REGION

4.1 *The effects of vapour blanketing—a 'vapour detonation' model*

In the explosion heat flows steadily from fuel to coolant, but its effectiveness in producing expansion may vary considerably, especially when vapour is present. When the coolant is single-phase or when the coolant has no temperature gradient within it, the expansion produced is usually positive. However, when vapour blankets form in an initially sub-cooled liquid, the expansion rate can become zero or negative whilst heat transfer continues, if recondensation effects at the vapour-liquid interface become important. (Such effects have been observed for instance in the experiments of Board *et al.* [13].)

Clearly, when vapour forms, the fraction of the heat flux going into vapour production controls the expansion rate; this flux Q_v is provided by the excess of that (Q_h) out of the fuel over the flux (Q_l) conducted away into the subcooled portion of the coolant, so $Q_v = Q_h - Q_l$. The latent heat of formation L of the mass of vapour m is the main contribution to Q_v, and so $Q_v = L\dot{m}$. We show in Appendix B that the C–J condition is reached when vapour condensation balances the liquid-phase expansion and the flow becomes sonic at an effective speed of sound $(PV^2/\Delta V)^{1/2}$ where $\Delta V/V$ is the vapour fraction (equations B4, B5). Now Q_v can vanish (or become negative) if vapour-blanketing reduces Q_h sufficiently rapidly whilst the subcooling remains high, sustaining Q_l; if this condition occurs well before equilibrium the efficiency would be low. Board *et al.* [13] found that on rapidly heating metal foils, vapour films about ten microns thick grew in $\sim 100\,\mu$s and the expansion then stopped, despite continuing heat flux. We may use these results, which applied under both acoustic loading and constant pressure conditions, to construct a simple model of a typical metal/water explosion [4, 5]. It follows from the expression for the speed of sound (equation B8 and Fig. 2) that the vapour volume at the C–J plane ΔV_f is about half that ahead of the shock; the explosion, if it is to be stable, must adjust its propagation pressure to achieve this (see Appendix B and D). The volume ΔV_f is the product of interphase area A and the vapour blanket thickness t', so

$$At' = \Delta V_f = \tfrac{1}{2}\Delta V_i. \qquad (2)$$

For an initial equal volume mixture of tin/water and vapour, the C–J vapour volume ΔV_f would therefore be $\sim 0.1\,\mathrm{cc\,gm^{-1}}$. If we take $t' = 10\,\mu\mathrm{m}$, then the fragmented area A would be about $10^2\,\mathrm{cm^2\,gm^{-1}}$ ($30\,\mu$m fuel particle size), and the heat transferred in $100\,\mu$s would be about $10\,\mathrm{J\,gm^{-1}}$; (the available heat in the mixture is about $100\,\mathrm{J\,gm^{-1}}$ so the overall efficiency is ten percent). Such particle sizes require differential velocities of order $4 \times 10^3\,\mathrm{cm\,s^{-1}}$ if they are produced by boundary-layer stripping [14], which in turn implies pressures at the C–J plane of ~ 30 bars (since $c^2 = PV^2/\Delta V$). (The energy in the vapour ($PA V.\ L/RT$) is then $\sim 1/3$ that in the water which is not inconsistent with the value of 1/5 found by Board *et al.*) These results are in encouraging agreement with those found in typical metal/water explosions, and strongly suggest that several features of such interactions might be predicted by a non-equilibrium 'vapour-detonation' model. Such a model is however, sensitive to details of vaporisation rates and fragmentation dynamics (see Appendix B), but these data can be found experimentally. We hope to develop this analysis further for application to our recent series of tin/water experiments.

It is clearly of importance to know whether such vapour blanketing behaviour is possible in systems where the coolant has high conductivity, most importantly the sodium/UO_2 system. This differs from the majority of metal/water systems in that the contact temperatures are sub-critical and so wetted layers of coolant will probably be left on the fuel surface when vapour is nucleated. The evaporation of these layers enhances heat transport out of the fuel into the vapour, and on their disappearance some measure of condensation appears very likely. This behaviour, if coherent within the medium, could be sufficient to compensate for the continuing expansion of the liquid coolant and allow the formation of a sonic plane. Detailed heat transfer data may be required to resolve this important question.

4.2 *The effects of two-dimensional single-fluid flow*

We can express the equations of 2-D flow in a form analogous to those of 1-D flow, for flow on the axis of symmetry ($y = 0$) (see Appendix A, Fig. A1). These equations (C9, C10) are given in Appendix C as relations between state s just behind the shock and state f at the C–J plane. (The initial state i and state s are of course related by the normal 1-D shock relationship.)

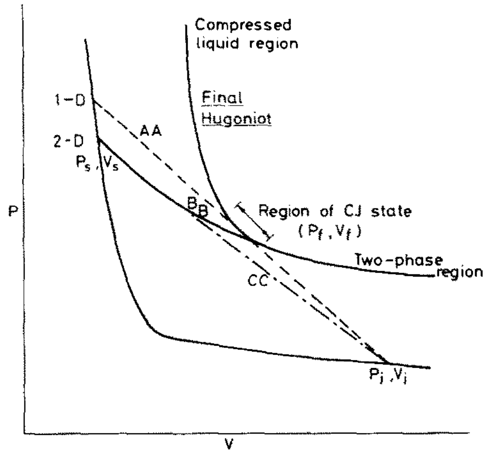

FIG. 1. Detonation Hugoniot and path of the reaction in sub-critical 2-D flow.

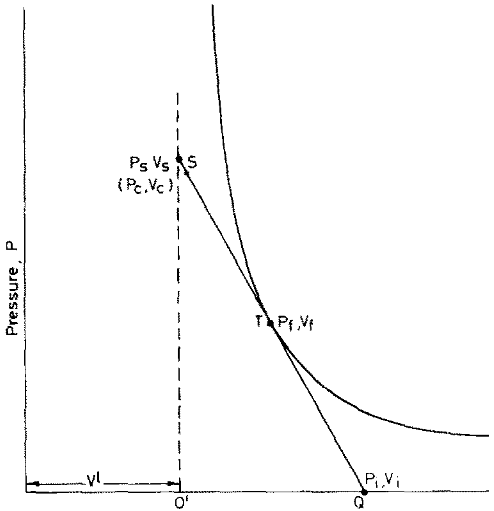

FIG. 2. Path on (P, V) diagram of unit mass in a vapour detonation (Fig. B1) with respect to a curve of constant vapour mass m, (a displaced hyperbola); thus $O'T = TQ$.

The first of these equations can be approximated for thermal explosions, where the (P, V) terms are small compared with the enthalpy terms, by

$$h_f - h_s \sim h_f - h_i \sim 0, \qquad (3)$$

and so is unchanged by the sideways flow.

When internal disequilibrium effects are not important, and the coolant temperatures are below critical, the curves (Hugoniots) defined by (3) fall into two distinct regions in the P, V plane; one region is a line nearly parallel to the V axis, and represents the highly compressible behaviour of the mixture when vapour is present—the other region is a line nearly parallel to the P axis, representing the very incompressible behaviour when all the vapour is condensed; at the junction between these two regions the speed of sound changes very rapidly. In the absence of sideways flow, the usual graphical method for finding the C–J state [5] shows this to be in this transition region (Fig. 1, line AA, tangent to the Hugoniot) for a wide range of initial conditions (P_i, V_i).

With sideways flow the path of the reaction on the (P, V) diagram is no longer a straight line (line BB); it follows from Euler's equation (C27) that

$$-\frac{\mathrm{d}P}{\mathrm{d}V} = j^2 + \frac{V}{2}\frac{\mathrm{d}j^2}{\mathrm{d}V}, \tag{4}$$

where $j = \rho u$ is the local flux. This slope of the reaction path (BB) is always less than j_i^2 (the flux through the shock, line CC), and decreases steadily with increasing V.

Now for nearly $1-\mathrm{D}$ flow, we expect that the reaction will nearly go to completion (only near the end of the reaction will heat transfer drop to a level at which its effects are comparable with those of the small amounts of sideways flow (Fig. 1)). Moreover the reaction will still terminate in the transition region of the Hugoniot since the velocity of sound changes rapidly there. We conclude therefore, from Fig. 1, that the principle effect of small amounts of sideways flow is to leave the C–J state nearly unchanged but to reduce the peak pressure P_s just behind the shock.

Increasing the amount of sideways flow decreases the pressure difference $(P_s - P_f)$ across the wave (and also makes the detonation less efficient). Since it is this difference which reaccelerates the flow it must be positive if the wave is to be sustained—if this is not so the detonation must certainly fail (cf chemical case). Now from equation (C10)

$$\frac{P_s - P_f}{\psi(\theta V_f - V_s)} = j_i^2 > 0,$$

and so detonation propagation can only occur if $(\theta V_f - V_s) > 0$; since $\theta \equiv \exp(-l/r)$, then

$$\frac{l}{r} < \ln\left(\frac{V_f}{V_s}\right). \tag{5}$$

(Here r is the radius of curvature of the surface orthogonal to the flow and l is the distance from shock to C–J plane—their ratio is thus a measure of the sideways constraint.)

For the case of the vapour blanketed model given in Appendix B we may develop this result further. Substitution of (4) into (B3) shows the flow to be sonic when

$$j_f^2 = \frac{P_f}{\Delta V_f} = \theta^2 j_i^2 \sim \frac{P_s \theta^2}{\Delta V_i}, \text{ so } \frac{\theta^2 \Delta V_f}{\Delta V_i} \simeq \frac{P_f}{P_s} < 1 \tag{6}$$

(We have again assumed liquid phase expansion is negligible compared with the vapour volume ΔV and that $P_s \gg P_i$.)

Now from (5)

$$\frac{\theta V_f}{V_s} = \theta\left(1 + \frac{\Delta V_f}{V_s}\right) > 1;$$

it follows that

$$\frac{l}{r} < \frac{\Delta V_i}{V_s}, \tag{7}$$

the propagation criterion $(P_s > P_f)$ is simply related to the initial vapour fraction.

Equations (5) and (7) show that the degree of constraint (l/r) required for detonation is high when the expansion $(V_s - V_f)$ driving the explosion forward is low. Now $V/\Delta V$ is typically of order a few, and the radius of curvature r is of the same order [12] as the thickness of the reaction layer, (Y_i, Fig. A1) so that this layer must be several reaction lengths thick if propagation is to proceed by detonation. Such a detonation criterion seems consistent with experiment. Explosions in relatively unconstrained geometries (such as when the materials are in a shallow layer ~ a few cm), have often failed to propagate steadily but have apparently progressed between sites of low stability under influence of the triggering pressure wave [4].

4.3 *Some comments on the importance of slip*

The role of slip in producing fine fragmentation was emphasised in [5]. Although our original estimate of the breakup efficiency provided by these mechanisms has been criticized by several authors [15, 16], recent experiments at BNL (summarised in [3]) seem to confirm our original suggestions.

We concern ourselves now with the effect of slip on the C–J condition.

A consideration of the relative magnitudes of heat and momentum transfer suggests that, for any individual particle, the momentum would equilibrate before heat was transferred; the drag force is of order $\rho_1(u_1 - u_2)^2 \pi r_2^2 C_D$, giving a characteristic decay time

$$\frac{r_2 \rho_2}{(u_1 - u_2)\rho_1},$$

whilst the thermal diffusion time is

$$\sim \frac{r_2^2}{\alpha_2'}.$$

For say UO_2 fragments of radius (r_2) 100 µm in a differential velocity $(u_1 - u_2)$ of $10^4\,\mathrm{cm\,s^{-1}}$, these times are about 10^{-5} s and 10^{-3} s respectively. We must also consider the time over which fragmentation takes place. For boundary-layer stripping this time is approximately

$$\frac{3d}{u_1 - u_2}\sqrt{\frac{\rho_2}{\rho_1}},$$

where d is the unfragmented fuel-particle size (say 0.2 cm, for the typical sodium/UO_2 flow considered above); for this case the time is $\sim 10^{-4}$ s, which is also somewhat shorter than the thermal equilibration time. (Note that this would not be so if the initial particle size were rather larger, or if the fragmentation were finer than assumed.) In this case there is no slip at the C–J plane, and the integral equations appropriate for homogeneous flow apply. An interesting problem remains however [17] because of the dispersive nature of the speed of sound in two-fluid media [18].

Indeterminacy in the gradients of the flow variables can be shown (*ibid.*) to be achieved when the flow is choked at the high-frequency speed of sound.

However it can also be shown, (following Wood and Salzburg [19]) that in a flow in which slip decays quickly the flow is sufficiently choked to decouple steady-state and expansion zones when it achieves the lower speed of sound given by the slope of the usual (non-slip) Hugoniot—indeed this is the highest speed the flow can reach in the steady-state region. Although this result means that in such cases the simple single-fluid analysis is justified, it suggests that in general the problem when slip is significant is a complex one, which is not truly time-stationary (because the flow is not choked at all frequencies).

Numerical calculations which allow the stability of the solution to be tested by including time variation, may be the only satisfactory way of dealing with this case, [and are indeed in hand at various centres, e.g. by Scott (Grenoble), Jacobs [20] and Bankoff and Sharon, (North-Western University)].

5. CONCLUSIONS

We suggest that all steadily propagating thermal explosions have structures analogous to chemical detonations; that is, they have a steadily propagating zone headed by a shock, and terminated by a sonic (C–J) plane.

The wide variation of efficiency can be explained by considering the balance condition at the C–J plane in 2-dimensional two-fluid flow, in which the phases are not necessarily in internal thermodynamic equilibrium. We have examined the nature of these flows in a few simple cases and these suggest:

(a) Non-equilibrium effects due to the production of vapour from a low conductivity coolant could result in stable detonating explosions of quite low efficiencies.

A model of such non-equilibrium behaviour has been developed, which shows that the vapour volume at the sonic plane is about half the initial vapour volume. Using this model and data from transient boiling experiments gives results (e.g. efficiences ~10%) consistent with metal/water explosion data.

Whether such non-equilibrium effects are significant in high conductivity systems (e.g. Sodium/UO_2) needs further investigation.

(b) The effects of sideways flow may be straightforwardly accounted for. Small amounts of sideways flow reduce the pressures immediately behind the shock without changing too much the final C–J condition.

A large flow divergence however would cause detonation failure—this would probably arise when the depth of the reacting layer was less than several times the length of the reaction region (i.e. the length between shock and C–J plane).

(c) Slip may not be of importance (at the C–J plane) in sodium/UO_2 flows if the fuel after fragmentation is coarser than ~30 μm. However, the analysis of flows in which slip is important at the C–J plane is complicated by the rather complex choking condition, and is probably best done numerically—it seems preferable that such calculations allow for time varying flows however, to check the stability of the final solution.

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APPENDIX A

THE C–J CONDITION IN 2-FLUID 2-DIMENSIONAL REACTIVE FLOW

We consider a layer of fuel/coolant mixture lying on a solid bottom and an explosion front moving steadily through the slab; this geometry is similar to that of the Winfrith THERMIR experiments [9]. We consider a two-dimensional section with the x-axis in the direction of propagation, and the y-axis out of the mixture. We will assume that the pressure front as well as being supersonic with respect to the mixture itself is also supersonic in the fluid above (Fig. A1) so that the pressure ahead of the shock is unchanging. (Gas and vapour bubbles rising from the mixture region will probably ensure this in practice.)

The general thermal explosion problem is multiphase; coolant vapour and liquid, and fragmented and unfragmented fuel are usually at different temperatures and velocities. The approximation scheme used to reduce the problem to two fluids only depends on the relative magnitude of the interphase equilibration times (see 3(iii)). Mass transfer, due to fuel fragments reaching velocity and temperature equilibrium with the coolant, is usefully included in calculations of conditions at the C–J plane if fragmentation time is long compared with those for thermal and velocity equilibration of the fragments (as in the models of Scott (private communication) and Bankoff and Sharon (North-Western University)).

We here identify two fluids, phase 1 being the volatile one. We allow for mass-transfer between the fluids, but bracket such terms [thus] for clarity. The conservation equations for such a system have been given by say Ishii [21].

Let α_1, α_2 be the volume fractions of each phase, so that

$$\alpha_1 + \alpha_2 = 1. \tag{A1}$$

For each phase the conservation of mass in unit volume gives

$$\operatorname{div}(\alpha\rho v) + \partial\frac{(\alpha\rho)}{\partial t} = 0 + [\dot{M}], \tag{A2}$$

where $\dot{M}$ is the interphase mass flux/unit control volume.

Each material has an equation of state of the form:

$$dP = c^2 d\rho + \sigma dS + [\lambda dM'],$$

where

$$\sigma = \left.\frac{\partial P}{\partial S}\right|_{\rho,M'}, \quad M' = \frac{M}{\alpha\rho}, \quad \lambda = \left.\frac{\partial P}{\partial M'}\right|_{\rho,S}, \tag{A3}$$

and S is the specific entropy of the phase.

The mass of each phase in unit volume $(\alpha\rho)$ is subject to a share of the pressure field proportional to its volume (α grad P), a force due to its share in changing the momentum of the transferred mass, $(\tau'\dot{M})$, and an interphase drag force (which is oppositely directed on the other phase), F:

$$\alpha\rho\frac{Dv}{Dt} + F + \alpha\,\mathrm{grad}(P) = 0 + [\tau'\dot{M}]. \tag{A4}$$

Here we take F and $\dot{M}$ as positive on phase 1.

Heat is conducted across the interfacial area A per unit volume at a rate $A\Phi$, and convected across by mass transfer at a rate $\mu\dot{M}$. Accordingly,

$$\alpha\rho T\frac{DS}{Dt} = (\Phi A + [\mu\dot{M}]) \tag{A5}$$

We specialise these equations to the x axis $(y = 0)$ of the steady-state region, so that $\partial/\partial t \equiv 0$, and $v_y(= w) = 0$.

Furthermore, we assume F, A, α, Φ do not depend on $\partial v/\partial x$ etc.

Moreover

$$\frac{D}{Dt} \to u\frac{\partial}{\partial x},$$

and by symmetry,

$$\frac{\partial P}{\partial y}, \frac{\partial \rho}{\partial y}, \frac{\partial \alpha}{\partial y} = 0 \left(\text{but } \frac{\partial w}{\partial y} \neq 0\right).$$

The equations of continuity for each phase (A2) are thus

$$\frac{\partial}{\partial x}(\alpha\rho u) + \alpha\rho\frac{\partial w}{\partial y} = 0 + [\dot{M}], \tag{A6}$$

and may be written (using A3, A5 to eliminate $\partial\rho/\partial x$) as

$$\alpha\rho\left(\frac{\partial u}{\partial x} + \frac{\partial w}{\partial y}\right) + \rho u\frac{\partial \alpha}{\partial x} + \frac{\alpha u}{c^2}\left(\frac{\partial P}{\partial x} - \frac{\sigma A\Phi}{\alpha\rho T u}\right) = 0 + \left[\left(\frac{\sigma}{c^2}\frac{\mu}{\rho T} + \frac{\lambda}{\rho c^2}\right)\dot{M}\right]. \tag{A7}$$

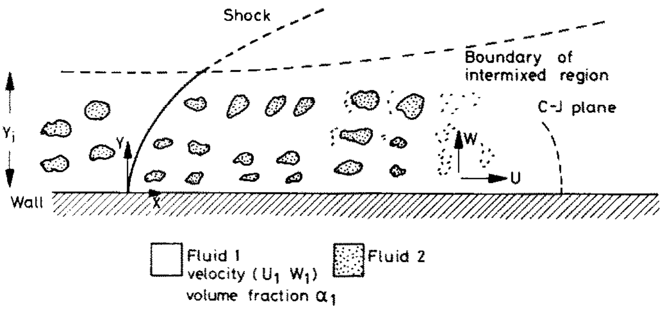

FIG. A1. Geometry of 2-fluid 2 – D detonation model.

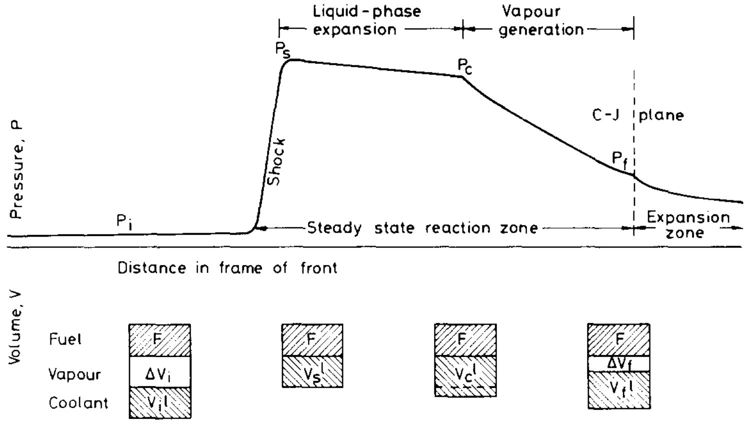

FIG. B1. Behaviour of unit mass on passage through front of 'vapour-detonation' model.

Substituting for

$$\frac{\partial u}{\partial x}=\frac{1}{\rho u}\left(\pm\frac{F}{\alpha}-\frac{\partial P}{\partial x}+\left[\frac{\tau'_x}{\alpha}\dot{M}\right]\right)$$

and noting

$$\frac{\partial \alpha_1}{\partial x}=-\frac{\partial \alpha_2}{\partial x}$$

we may arrive at the following expression for the pressure gradient:

$$\frac{\partial P}{\partial x}=\frac{A\Phi K_\Phi+FK_f-K_w+[K_m\dot{M}]}{\left(\frac{\alpha_1}{\rho_1 u_1^2}\left(\frac{u_1^2}{c_1^2}-1\right)+\frac{\alpha_2}{\rho_2 u_2^2}\left(\frac{u_2^2}{c_2^2}-1\right)\right)}. \tag{A8}$$

Here

$$K_\Phi=\left(\frac{\sigma_i}{T_i\rho_i^2c_i^2u_i}\right)_2^1$$

$$K_f=\left(\frac{1}{\rho_iu_i^2}\right)_2^1$$

$$K_w=\frac{\alpha_1}{u_1}\frac{\partial w_1}{\partial y}+\frac{\alpha_2}{u_2}\frac{\partial w_2}{\partial y} \tag{A9}$$

and

$$K_m=\left(\frac{1}{\rho_iu_i}\left(1-\frac{\tau'_i}{u_i}+\frac{\sigma_i\mu_i+(T_i/\rho_i)\lambda_i}{\rho_ic_i^2T_iu_i}\right)\right)_2^1.$$

$K_{\phi,f,m}$ are the differences of the bracketed quantities for phase 1 and 2 [i.e. $(A_i)_2^1=A_1-A_2$].

The denominator of this expression is clearly a generalisation of the speed of sound. When $u_1=u_2$ it corresponds to the well-known 'stratified speed of sound' [22]. The four terms of the numerator are respectively the components of the pressure gradient due to heat transfer, interphase drag, flow divergence and effects of mass transfer.

The heat transfer term is positive (and thus gives a negative pressure gradient) in all subsonic flows of interest to us. The flow divergence term is of opposite sign, since $\partial w/\partial y$ is positive [23]. The drag term requires more careful consideration; if phase 1 be the lighter phase ($\rho_1<\rho_2$) then in the frame of the shock $u_1\leqslant u_2$ and so $F_1<0$. Accordingly we expect $\rho_1u_1^2<\rho_2u_2^2$ everywhere and the interphase drag thus always opposes heat transfer—this conclusion agrees both with calculation (by say Kreibel [24] on shock-waves in a dusty gas) and nozzle-flow experiments using bubbly liquids [25]. The mass transfer terms may be adequately represented as additional contributions to the heat transfer (1st and 3rd terms in K_m) and interphase drag (2nd term in K_m).

Finally, we note that for the single-phase, $1-\mathrm{D}$ flow approximation the equation A8 simplifies considerably to

$$\frac{\mathrm{d}P}{\mathrm{d}x}=\frac{A\Phi\left(\frac{\sigma_1}{T_1\rho_1}\right)u_1}{u^2-c^2}. \tag{A10}$$

APPENDIX B

A 'VAPOUR-DETONATION' MODEL, WITH THERMAL DISEQUILIBRIUM IN THE COOLANT

We consider the dynamics of a region containing unit mass of fuel and coolant, with interfacial area A after fragmentation.

This volume passes through the following sequence of events, (Fig. B1):

(a) *Initial state i.* The initial pressure is P_i; this is assumed much less than any other pressures considered.

The fuel volume is F, and will not change significantly.

The initial vapour volume is ΔV_i and the initial coolant volume V_i^l; its temperature is T_1, and the fuel temperature is T_c. The detonation velocity is D.

Clearly

$$V_i=V_i^l+F+\Delta V_i.$$

(b) Immediately behind the shock the material is in *state s*. We assume that all vapour has been condensed in the shock but the coolant has not been significantly compressed. The pressure is P_s and so

$$\frac{P_s-P_i}{\Delta V_i}=j^2=\frac{D^2}{V_i^2},\quad [5]. \tag{B1}$$

The interface temperature rises to T_c, the contact value, but the pressure exceeds the saturation pressure $P_c(T_c)$ and so a period of liquid-phase expansion begins. We assume that the growing thermal boundary layers in the coolant are too thin and far apart to interact with each other.

(c) In *state c* the pressure has fallen to P_c and vapour generation can start. The liquid has expanded to V_c^l and a time τ_c has elapsed since the material passed through the shock front. The deposited heat is

$$\frac{(T_c-T_i)}{2}KA\sqrt{\frac{\tau_c}{\pi\alpha'}}$$

where K is the conductivity, α' the diffusivity.

The expansion of the liquid phase is

$$V_c^l-V_s^l=\frac{\beta}{C'}\frac{(T_c-T_i)}{2}\sqrt{\frac{\tau_c}{\pi\alpha'}}. \tag{B2}$$

where β is the expansion coefficient, C' the coolant specific heat.

(d) Growth of the vapour blanket then ensues until the flow reaches sonic velocity at *state f*. We consider this stage in detail.

The heat flux leaving the fuel is Q_h; this flux can be divided into some fraction Q_v which goes into vapour generation (at a rate $\dot{m}$) and raising the temperature of the vapour, and remainder Q_l which is conducted away into the coolant;

$$Q_h - Q_l = Q_v = L\dot{m} + C'_v \dot{T} m, \tag{B3}$$

where L is the latent heat of vaporisation and C'_v the heat capacity of the vapour. (We have assumed that all the vapour is at the interface temperature T_i to evaluate the heat capacity term which is in any case small.)

Q_l causes liquid phase expansion at a rate

$$\dot{V}^l = \frac{\beta}{C'_l} Q_l. \quad \text{Now} \quad m = \frac{P\Delta V}{RT}, \; P = P(T)$$

and moreover

$$\frac{\mathrm{d}P}{\mathrm{d}V} = -j^2.$$

Thus we may express $\dot{P}$, $\dot{V} = \Delta\dot{V} + \dot{V}^l$ and hence $\dot{m}$ in terms of $\dot{T}$:

$$Q_h - Q_l\left(1 - \frac{\beta}{C'_l}\frac{PL}{RT}\right) = \frac{\dot{T}L}{RT}\left[\left(\frac{\mathrm{d}P}{\mathrm{d}T} - \frac{P}{T}\right)\Delta V - j^{-2} P \frac{\mathrm{d}P}{\mathrm{d}T}\right] + \dot{T}\frac{C'_v P\Delta V}{RT}. \tag{B4}$$

(The LHS now contains no D/Dt terms.)

Clearly $\dot{T}$ (and hence $\dot{P}$, $\dot{m}$) is indeterminate when both (i) the LHS vanishes and (ii)

$$j^2 = \frac{u^2}{V^2} = \frac{\dfrac{\mathrm{d}P}{\mathrm{d}T}\cdot P}{\Delta V\left(\dfrac{\mathrm{d}P}{\mathrm{d}T} + \dfrac{P}{T}\left(\dfrac{C'_v T}{L} - 1\right)\right)}, \tag{B5}$$

which identifies the choking condition. In the absence of significant liquid phase expansion condition (i) becomes $Q_v = 0$, a result analogous to $(A\Phi) = 0$ (see A10) when the vapour is the only working fluid. We consider (B5) further.

Now $P = Ae^{-}\dfrac{L}{RT}$ and so

$$\frac{\mathrm{d}P}{\mathrm{d}T} = \frac{L}{RT}\frac{P}{T} \gg \frac{P}{T}\left(1 - \frac{C'_v T}{L}\right). \tag{B6}$$

Accordingly

$$u_f^2 \simeq \frac{P_f V_f^2}{\Delta V_f}, \tag{B7}$$

and so

$$\frac{P_f - P_i}{V_f - V_i} \sim \frac{P_f}{\Delta V_f - \Delta V_i + V_f^l - V_i^l} = j^2 = -\frac{P_f}{\Delta V_f}. \tag{B8}$$

From these equations we see that, when the liquid phase expansion is small

$$2\Delta V_f \sim \Delta V_i, \quad \text{and} \quad P_c \sim 2P_f. \tag{B9}$$

This simple result can be illustrated on the (P, V) diagram by considering curves of (P, V) states having the same vapour mass m (Fig. 2); (Hugoniots lose their usefulness in non-equilibrium situations, since h is not uniquely related to (P, V)). These curves are of the form

$$V = V^l + \frac{mRT}{P(T)}. \tag{B10}$$

The initial state i lies on the $P \sim 0$ axis, whilst the shock state s (and state c) lies near $V \sim V^l$, (this being the form of (B10) when $m \sim 0$). The flux-line $\mathrm{d}P/\mathrm{d}V = -j^2$, is tangent to a curve of constant m at P_f, V_f, because $\mathrm{D}m/\mathrm{D}t = 0$ at the C–J (f) state. Now (B10) is nearly the equation of a displaced hyperbola (since $T \propto \ln(P)$ only), and (B9) follows from this geometry.

We now consider further the conditions an explosion must satisfy if it is to propagate stably satisfying equation (B9). The vapour volume ΔV is the product of the interphase area A and the vapour blanket thickness t'. We assume that fragmentation is complete by the C–J plane; in this case we may use the data from transient heating of thin foils (e.g. [13]), for predicting the value $t' = t'_f$ at which Q_h and Q_l balance (typically 10μ at 10 bars). A full description of the process by which this balance occurs cannot presently be given, but it seems likely that if the coolant makes contact with the freshly generated surface area, it will start by nucleate boiling before reaching film boiling. The formation of micro-layers and the effects of nucleation delays ensure Q_h greatly exceeds Q_l in the nucleate boiling stage. However, when the coolant layer wetting the fuel or any superheated layer in the bulk liquid are evaporated, Q_h falls rapidly, instantaneously balancing with Q_l before falling below it. The flux Q_l into the liquid coolant is probably controlled by the degree of subcooling and so will be quite sensitive to pressure. We may approximate the overall behaviour by

$$t'_f \propto p_f^{-m}, \quad \text{where} \quad 1 > m > 0. \tag{B11}$$

(We do not expect t'_f to be influenced by the volume V_f because the thermal boundary layers around each particle are too thin to interact with each other.)

Turning now to the fragmented area A, we can consider two limiting cases. If the area generation is limited by energy considerations (T. P. Fishlock, Winfrith, private communication), so that $A\sigma \sim \rho(u_1 - u_2)^2$, we may expect the area to change quite rapidly with pressure ($\sim P^{+1}$ since $u_i - u_s \sim \sqrt{P_s \Delta V_i}$ and $u_1 - u_2 \lesssim u_i - u_s$ if one phase is heavy). Conversely, in fully developed boundary-layer stripping the thickness of the boundary layer, δ, and hence the size of the stripped particles is [14]:

$$\delta = \left(\frac{3\pi d\eta_2}{2\rho_2 u_s}\right)^{1/2}, \text{where } u_s = \left(\frac{\eta_1\rho_1}{\eta_2\rho_2}\right)^{1/3}(u_1 - u_2). \tag{B12}$$

This implies a very weak variation with pressure ($\sim P^{1/4}$).

A general variation for A would thus be

$$A \propto (P_s \Delta V_i)^n \text{ where } 0 < n < 1. \tag{B13}$$

Combining (9, 11 and 13), we find that

$$P_f \propto (\Delta V_i)^{(n-1)/(m-n)}. \tag{B14}$$

Now for stability (At'_f) must decrease with pressure, (see Appendix D), and so we have $m - n > 0$. Therefore this model predicts that the generated pressure P_f will fall with increasing initial void fraction ΔV_i.

APPENDIX C

SOME EQUATIONS OF TWO-DIMENSIONAL SINGLE-FLUID FLOW

The equations of steady 2 – D flow can be written

$$\frac{u\partial\rho}{\partial x} + \frac{\rho\partial u}{\partial x} + \frac{\rho\partial w}{\partial y} + \left[\frac{w\partial\rho}{\partial y}\right] = 0 \tag{C1}$$

$$-\frac{\partial P}{\partial x} = \left[\rho w\frac{\partial u}{\partial y}\right] + \rho u\frac{\partial u}{\partial x} \tag{C2}$$

$$\left[-\frac{\partial P}{\partial y} = \rho u\frac{\partial w}{\partial x} + \rho w\frac{\partial w}{\partial y}\right] \tag{C3}$$

$$u\frac{\partial}{\partial x}\left(h+\frac{v^2}{2}\right)+\left[w\frac{\partial}{\partial y}\left(h+\frac{v^2}{2}\right)\right]=0,$$
$$\text{where } v^2=u^2+w^2. \qquad \text{(C4)}$$

The terms bracketed [ ] disappear on the x-axis (which is an axis of symmetry, Fig. A1).

We consider further the flow close to the axis and we follow Cowperthwaite [23] in defining a quantity θ which is the inverse ratio of the area of a pencil of particle paths, centred about the x-axis at some point in the reaction zone, to its area just ahead of the shock.

Clearly $\theta^{-1}\rho v=j_i$ is constant, and θ is related to the divergence of the flow by

$$\theta=\exp\left(-\int\frac{\partial w}{\partial y}\frac{\mathrm{d}x}{u}\right)=\exp\left(-\int\frac{\mathrm{d}x}{r}\right). \qquad \text{(C5)}$$

Here we have used $\partial w/\partial y=+u/r$, where r is the radius of curvature of the surface orthogonal to the flow.

(Note that this differs from Cowperthwaite's result by a factor of 2 because we consider a slab geometry, whilst he considered a radially symmetric geometry.)

This substitution also allows him to rewrite the energy equation of the flow (C4) as

$$h_f-h_i=\frac{1}{2}\rho_i u_i(u_i-u_f)\left(\frac{\theta}{\rho_f}+\frac{1}{\rho_i}\right). \qquad \text{(C6)}$$

Now Euler's equation (C2) can be written:

$$\frac{\partial P}{\partial x}=-j\frac{\partial u}{\partial x}=-j_i\theta\frac{\partial u}{\partial x}, \qquad \text{(C7)}$$

and so $P_f-P_i=j_i(u_f-u_i)\,\psi$ say,

$$\text{where } \psi=\frac{1}{(u_f-u_i)}\int\theta\frac{\partial u}{\partial x}\,\mathrm{d}x; \qquad \text{(C8)}$$

this allows us formally to write

$$h_f-h_i=\frac{1}{2}\left(\frac{P_f-P_i}{\psi}\right)(\theta V_f+V_i), \qquad \text{(C9)}$$

and

$$\frac{P_f-P_i}{\psi}\bigg/(V_i-\theta V_f)=j_i^2 \text{ where } V=\frac{1}{\rho}. \qquad \text{(C10)}$$

(We note that both ψ and $\theta\to 1$ when $V\to\infty$ and so the equations reduce to the $1-\mathrm{D}$ expressions when the flow divergence is small.) We may approximate ψ, θ if we consider, instead of state i just ahead of the shock, the state s just behind it. States i and s are related by the normal $1-\mathrm{D}$ expressions because there is no flow divergence across the shock. We may then assume r, $\partial u/\partial x$ are constant between states s and f to approximate θ as $\exp(-l/r)$ and ψ as

$$\frac{r}{l}\left(1-\exp\left(-\frac{l}{r}\right)\right). \qquad \text{(C11)}$$

(Here $l=x_f-x_s$ is the length of the steady-state reaction zone.)

APPENDIX D

THE QUESTION OF STABILITY OF A STEADY STATE DETONATION

We review first the reason why a C–J detonation with complete energy transfer is normally stable against small perturbations in its velocity of propagation.

In the C–J steady state the energy transfer behind the shock is just sufficient to re-accelerate the flow to sonic velocity at the end of the steady state region. If the mass flux (j) were increased slightly, (but slowly compared with the time for material to traverse the front) the shock pressure would rise and the Mach number of the flow behind the front would fall. The energy transfer would be insufficient to re-accelerate the flow to sonic velocity and at the end of energy transfer the flow would still be subsonic. Although such a wave could exist if there were a 'piston' of high pressure gas behind the wave to 'support' the detonation, there is in general a rarefaction wave immediately behind the steady state region; if the flow were subsonic this would progress forward and weaken the shock front. The rarefaction wave would thus reduce the velocity of propagation of the shock, decreasing it towards its original value—the flow is therefore stable. Conversely, decreasing j leads to the flow reaching sonic velocity with heat transfer still occurring. In steady state this would lead to a discontinuity in the flow, which would propagate back upstream and increase j back to its unperturbed value.

Now consider the case of partial energy transfer; if we increase the mass flux into the shock we reduce the Mach number of the flow, but change the expansion energy available for re-accelerating it (this change would in general be an increase, e.g. because of increased fragmentation). If this increase is sufficient to accelerate the flow to above sonic velocity, the flow is unstable because such a situation leads to further increase in j.

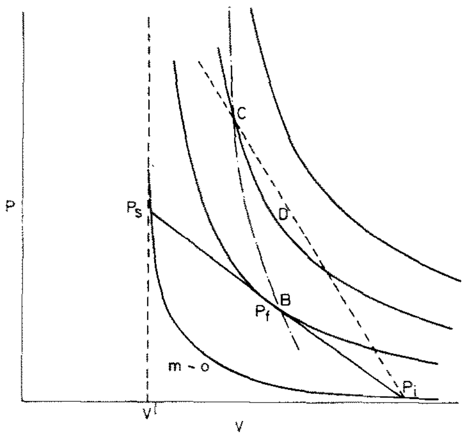

FIG. D1. Illustrating the stability criterion for a 'vapour-detonation' (— · — · joins states for which the vapour generation rate, $\dot{m}=0$).

We can analyse this situation graphically for the model of Appendix B say by considering the set of P–V curves for differing vapour masses (Fig. D1).

We can then mark on these the locus of those states which have the equilibrium vapour blanket thickness (line BC). In general one of these will be a C–J state (B). Now perturb the flow to some higher j (point C say). In the case shown, the vapour volume (which is a product of the fragment area and the new equilibrium blanket thickness) reaches its equilibrium value when the flow is still subsonic. The detonation will thus decay back to the unperturbed state B. We see that stability requires the equilibrium vapour volume (line BC, Fig. D1), to decrease with pressure more rapidly than the C–J volume (line BD).

For the model of appendix B the line BD is vertical (C–J vapour volume equals half of the initial vapour volume) and hence the condition for stability is that the equilibrium vapour volume should fall with pressure.

We note in passing that instability of the flow against slow perturbations in detonation velocity is not the only possible mode. Chemical detonations are, for instance, prone to the growth of acoustic waves within the reaction region [26] which modify the flow into a $3-\mathrm{D}$ structure; this modification however does not seem to affect the usefulness of the $1-\mathrm{D}$ analysis for describing the overall propagation.

PROPAGATION DES EXPLOSIONS THERMIQUES A LARGE ECHELLE

Résumé—On suggère, à partir de l'évidence théorique et expérimentale, que toutes les explosions thermiques à grande échelle ont une structure semblable à la détonation. On examine les effets d'une telle détonation thermique sur l'écoulement, le glissement de l'interface, l'expansion thermique du réfrigérant et on considère le bilan de ces effets dans la zone de réaction où l'écoulement devenant sonique contrôle la propagation et par suite l'efficacité de l'explosion.

On montre que:

(a) Les explosions thermiques (comme les explosions chimiques) se propagent seulement si la contrainte est élevée:

(b) Dans une détonation avec vapeur créée dans la région de réaction (une détonation avec vapeur), l'efficacité peut être faible. On applique un modèle de ces explosions métal/eau et l'on montre qu'il en prédit les caractéristiques générales.

DIE AUSBREITUNG GROSSRÄUMIGER THERMISCHER EXPLOSIONEN

Zusammenfassung—Wir sind der Meinung, daß nach dem gegenwärtigen Stand der theoretischen und experimentellen Erkenntnisse alle sich großräumig ausbreitenden thermischen Explosionen einen detonationsartigen Charakter haben. Wir untersuchen den Einfluß von Seitwärtsströmung, Schlupf zwischen den Phasen und der thermischen Expansion des Kühlmittels auf eine solche thermische Detonation; das Zusammenwirken dieser Effekte an der Stelle der Reaktionszone, wo Schallgeschwindigkeit herrscht, bestimmt die Ausbreitung und damit die Wirksamkeit der Explosion. Wir zeigen, daß:

(a) thermische Explosionen (wie chemische Explosionen) sich nur dann ausbreiten, wenn der seitliche Widerstand groß ist,

(b) die Wirksambeit von Detonationen, bei welchen in der Reaktionszone Dampf/erzeugt wird (Dampf-Detonationen), gering sein kann.

Wir wenden ein derartiges Modell auf Metall/Wasser-Explosionen an und zeigen, daß es das allgemeine Verhalten solcher Vorgänge beschreibt.

РАСПРОСТРАНЕНИЕ КРУПНОМАСШТАБНЫХ ТЕПЛОВЫХ ВЗРЫВОВ

Аннотация — На основании представленных в работе теоретических и экспериментальных данных сделано предположение о детонационной структуре всех крупномасштабных распространяющихся тепловых взрывов. В работе исследовалось влияние на такую тепловую детонацию боковых потерь, межфазного скольжения и термического расширения. Суммарное влияние этих эффектов в месте перехода потока в звуковой в реакционной зоне определяет распространение, а следовательно, и эффективность взрыва.

Показано, что (*а*) тепловые взрывы (подобно химическим) распространяются только в случае наличия очень незначительных боковых потерь; (*б*) при детонации с образованием пара в пределах реакционной области («паровая детонация») эффективность взрыва может быть незначительной. На примере применения модели этого процесса к случаю взрывов в системе металл-вода показано, что с помощью данной модели можно рассчитать общие характеристики указанных процессов.