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CONTRIBUTIONS CONCERNING QUASI-STEADY PROPAGATION OF THERMAL DETONATIONS THROUGH DISPERSIONS OF HOT LIQUID FUEL IN COOLER VOLATILE LIQUID COOLANTS*

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Abstract—The two-phase flow model of 1-dim. propagation of thermal detonation is reformulated to permit isolation of both new and existing conclusions which are independent of fragmentation kinetics data. The two-phase flow model is found to be necessary for making quantitive predictions of detonation strength in hydrodynamic fragmentation. A wide spectrum of kinetics-independent permissible Chapman–Jouguet states is found possible for any specific intitial condition in calculations for the UO_2–sodium system, with sensitivity of these (C–J) states found to initial sodium (coolant) vapor blanket volume fraction. Arguments are presented which suggest our use of an equilibrium sonic velocity for C–J wave termination. The abrupt decrease of sonic velocity due to the presence of vapor or gas is found to be sufficiently severe as to render vaporization unlikely either in the steady detonation zone or at the C-J plane, and further identifies a lower threshold for thermodynamically permissible C–J propagations which occurs at coolant saturation.

NOMENCLATURE

C,	sonic velocity;
C_f,	frozen sonic velocity of 'fluid', equation (30);
$\bar{C}_f$,	equilibrium sonic velocity of 'fluid' composite, equations (19.6) and (20.7);
D,	volume fraction of fragmented fuel in 'fluid';
E,	local fraction of original fuel which has fragmented;
F,	volumetric drag force by 'fluid' on unfragmented fuel droplets ($-Z$ direction);
i,	specific enthalpy;
j,	total mass flux, equation (6.1);
P,	pressure;
P'_s,	$= dP_s/dT$, slope of vapor pressure curve for coolant;
s,	specific entropy;
T,	temperature [generic in equations (18) and (19)] 'fluid' value $T \equiv T_f$ in equations (19.2), (19.6) and (30);
u,	velocity (mass average when unscripted);
u_1,	shock velocity, equation (10.3);
x,	mass fraction of fragmented fuel in 'fluid' (x_{dB}), equation (2);
y,	mass fraction of coolant as vapor;
z,	distance downstream from shock front.

Greek symbols

α,	local volume fraction of unfragmented fuel (α_d);
β,	coefficient of thermal expansion; β_f, equation (19.5);
ω,	local mass fraction of unfragmented fuel (ω_d);
ρ,	mass density, equation (1) (total when unsubscripted);
ε,	local volume fraction of coolant as vapor, equation (3);
ζ,	$= \omega^{-1} - 1$, preceding equation (9.1);
Γ_f,	mass rate of fragmentation, equations (10.1) and (10.4);
ϕ,	volumetric heat transfer rate from droplets to fluid, equation (12.1);
Φ,	equation (22.2);
κ,	equation (19.7);
κ_ε,	equation (20.5).

Subscripts

d,	fuel droplets (except in drag coefficient);
f,	'fluid' composite (fuel fragments and coolant);
dB,	debris (fuel fragments);
c,	coolant (liquid, vapor or both);
l,	liquid coolant;
v,	vapor coolant;
vl,	vapor value minus liquid value;
r,	relative (velocity);
s,	saturation (vapor–liquid equilibrium);
1,	upstream side of shock front;
0,	downstream side of shock front.

1. INTRODUCTION

IN A RECENT article [1], Sharon and Bankoff have presented an extensive summary of their work on modelling of 1-dim. shock wave propagation through a coarse mixture of hot liquid (fuel) droplets sur-

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rounded by a colder but vaporizable liquid (coolant). In their detonation propagation concept, a shock wave might become self-sustaining as a result of mechanical energy release during the fragmentation and associated rapid heat transfer from fuel to coolant just behind the shock front, much like a chemical detonation is sustained by the release of energy in chemical reaction behind a shock front.

A major portion of the intuitive basis for this 'thermal detonation' concept of propagation and its analogy to chemical detonation was pioneered by Board *et al.* [2]. Although it is difficult to overvalue the physical basis which these authors have contributed to modelling the phenomena, their published intuitive approach suffers from extensive dependence upon analogy to Chapman–Jouguet (C–J) theory for combustion detonation involving only one chemical reaction. In this respect, the approach can lead to quantitatively erroneous conclusions. To explain this briefly, we submit that in prescribing the simplest, well defined quantitative model for the 1-dim. thermal detonation it appears necessary to invoke analogy to chemical detonation involving a minimum of two independent reactions, for in the relaxation zone just behind the shock there are at least two independent kinetic rate processes occurring. There are [1] fragmentation of fuel droplets with heat exchange from fragments to coolant, and [2], velocity equilibration of unfragmented fuel droplets and coolant by interphase drag forces. Progress of these two rate processes is interdependent for most physical mechanisms advanced, e.g. both sets of kinetics are dependent upon relative phase velocity in the hydrodynamic fragmentation models [1].

The significance of this distinction can be anticipated on comparing one- and two-reaction chemical detonation in a single phase medium. For the one reaction case classical Chapman–Jouguet wave analysis (including, if desired, its graphical solution technique based upon tangency of the Rayleigh line, representing progress viewed on a pressure–volume phase plane, to the equilibrium Rankine–Hugoniot curve) can characterize the strength of the propagation. Thus, conservation conditions, together with a sonic condition, enable jump balances and thermodynamics to uniquely fix conditions at the Chapman–Jouguet plane without use of kinetics. In contrast, for the two-reaction (or multiple reaction) case, the conservation conditions with a sonic condition are insufficient to characterize a unique propagation or its strength. Thus, regardless of what choice of sonic or choking condition is used, there will exist an entire spectrum of conceivable C–J detonation–termination points which satisfy the conservation and sonic conditions. Selecting the uniquely correct C–J point from this spectrum requires at least a 'phase plane' integration of the relative reaction kinetics which serve to resolve the competition among the reactions. Evidently a Chapman–Jouguet estimate of propagation strength for a two or multiple-reaction system, based upon a one reaction approximation, will be quantitatively inappropriate when the spectrum of admissible C–J points (based upon a similar sonic condition and jump balance conservation conditions) is a wide range of possible propagation strengths for the kinetics to select among. In calculations here, we present strong evidence that such is indeed the case for the analagous thermal detonation.

As additional support for the necessity of an explict multiple reaction analogy for hydrodynamic fragmentation, note that in the original developments [2] of the one-reaction analogy, calculations of the detonation magnitudes are based upon homogeneous flow, and do not employ explicit accounting of the relative velocities between fuel and coolant in the detonation zone even though the intuitive fragmentation physics centers on the role of this relative velocity. An explicit accounting of the relative velocity implies use of two-phase (or multiphase) flow kinematics. Thus, multiphase flow models are synonymous with the multiple reaction analogy, and appear essential to quantitative predictions of detonation strengths.

For these reasons we regard the formulations of multiphase flow models by Sharon and Bankoff [1] and by Scott and Berthoud [3] to be of major significance to quantitative predictions of thermal detonation strengths. The purpose of the present paper is to offer the complementary views, additional insights, conclusions, and emphasis afforded by a modified formulation of these developments. Since [1] is especially detailed, we emphasize comparison to it. These authors employ an effective two-phase flow simplification which defines the two-phase flow kinematics at any point of the detonation zone in terms of a first phase consisting of unfragmented fuel (droplets) having one phase velocity and thermal state, and a second 'fluid phase' which is a composite of finely fragmented fuel debris and coolant. The coolant is itself allowed to be a two-phase vapor–liquid mixture, while the fuel debris is considered thermally and mechanically equilibrated with coolant so that the 'fluid phase' has a single-phase velocity and thermal state, i.e. is in separated, homogeneous flow. This model obviously assumes the time scales for thermal and velocity equilibration of fragmented fuel and coolant to be much shorter than those for fragmentation or similar equilibration of unfragmented fuel droplets and coolant. The model allows the simplest of well defined multiphase flow treatments; hence we confine present discussions to it, and refrain from altering the above assumptions.

We attempt here to isolate that information which in this model can be obtained from a Chapman–Jouguet wave analysis for the effective two-reaction system without detailed knowledge of constitutive relations for the kinetics of fragmentation and fuel–coolant equilibration, i.e. can be obtained from jump balance conservation conditions, thermodynamic relations and sonic termination. An advantage of separating this information is that it is applicable as a framework for discussion independent of uncertainties concerning interpretation of kinetics data, and of purely kinetic parameters such as initial fuel-droplet size.

As a matter of emphasis, note that from the viewpoint of the two phase model, a quasi-equilibrium condition applies, similar to a "first level simplest approach" (cf. [1], para. 3 of Introduction), but without assuming complete fragmentation or equilibration of unfragmented fuel and coolant. Thus, for hydrodynamic fragmentation, a zero relative velocity between fuel drops and coolant by itself implies zero fragmentation rate at the C–J sonic plane. The degree of fragmentation, and hence all other conditions at the C–J plane, are in this case no longer uniquely determined by upstream conditions plus a 'tangency' or sonic conditon, and now are dependent upon fragmentation kinetics. However, a spectrum, i.e. one parameter family, of potential C–J conditions is defined for each prescription of upstream conditions, cf. Fig. 1. In particular, pressures previously predicted and alluded to, ([1] par. 3 of Introduction) based upon complete fragmentation, are not unique even as "order of magnitude estimates" and appear unjustifiably selected as extremes among many possibilities. We see that from the viewpoint of the two-phase, two-reaction model, the assumption of complete hydrodynamic fragmentation at the C–J plane is itself arbitrary and much less appropriate than that of velocity equilibrium there. Therefore, realistic prediction of detonation strengths here require simultaneous prediction of incomplete fragmentation extents based upon fragmentation kinetics. (It is also desirable to separate this "phase-plane" prediction from that of rate-dependent detonation zone lengths.)

In this paper, we introduce the modifications which allow us to adapt the effective two-phase model presented in [1] to a form which permits the separation of information mentioned two paragraphs above. Calculations are reported for the kinetics-independent part, and the equations necessary for use of kinetics relations are recast into forms which entail integration of only one or two differential equations. Results of integrating these kinetics-dependent equations are deferred to a subsequent paper.

2. MODEL FORMULATION

For simplicity, brevity and continuity we adhere to notational conventions of [1], and emphasize the changes, additions and simplifications used here. Subscripts 1, 0, 3 will refer to: 1, the upstream state; 0, just behind the shock; and 3, at the sonic plane.

2.1. *Kinematical definitions*

If ω, $\alpha(\omega \equiv \omega_d$, $1-\omega=\omega_f$, $\alpha \equiv \alpha_d$, $1-\alpha=\alpha_f)$ denotes local mass and volume fraction of unfragmented fuel, these are related by $\rho\omega=\rho_d\alpha$, $\rho(1-\omega)=\rho_f(1-\alpha)$ so that total mixture density assumes the general working relations

$$\rho \equiv \rho_d\alpha+\rho_f(1-\alpha)=\left(\frac{\omega}{\rho_d}+\frac{1-\omega}{\rho_f}\right)^{-1}. \quad (1)$$

If x, $D(x \equiv x_{dB})$ denote local mass and volume fractions of fragmented fuel in the equilibrated fluid phase, their relationship is $\rho_f x=\rho_{dB}D$, $\rho_f(1-x)=\rho_c(1-D)$ and the fluid density is intrinsically

$$\rho_f=\rho_{dB}D+\rho_c(1-D)=\left(\frac{x}{\rho_{dB}}+\frac{(1-x)}{\rho_c}\right)^{-1} \cdot \quad (2)$$

Similarly if the coolant is comprised of both vapor and liquid, and ε, $y(\varepsilon=\varepsilon_v)$ denote local volume and mass fraction of coolant in the vapor phase, $\rho_c y=\rho_v\varepsilon$, $\rho_c(1-y)=\rho_l(1-\varepsilon)$, and the intrinsic coolant density is

$$\rho_c=\rho_v\varepsilon+\rho_l(1-\varepsilon)=\left(\frac{y}{\rho_v}+\frac{1-y}{\rho_l}\right)^{-1} \cdot \quad (3)$$

The local specific value of a composite property such as enthalpy, i, is then

$$i=i_d\omega+i_f(1-\omega), \quad (4)$$

with intrinsic specific enthalpies for fluid and coolant:

$$i_f=xi_{dB}+(1-x)i_c,$$
$$i_c=yi_v+(1-y)i_l. \quad (5)$$

The total (1-dim.) mass flux j is defined by

$$j \equiv \rho u=\rho\omega u_d+\rho(1-\omega)u_f \quad (6.1)$$

with the average velocity u, and relative velocity u_r:

$$u=\omega u_d+(1-\omega)u_f; \quad u_r=u_d-u_f. \quad (6.2)$$

These in turn determine the velocities u_f, u_d of composite fluid (coolant plus fragmented fuel debris) and unfragmented fuel droplets,

$$u_f=u-\omega u_r; \quad u_d=u+(1-\omega)u_r. \quad (6.3)$$

Since $1-E$ represents fraction of original fuel which has not been fragmented, E may be defined in steady flow by

$$\rho\omega u_d=\omega_1 j(1-E), \quad (7.1)$$

or using (6.1) and (6.3),

$$\rho\omega(1-\omega)u_r=j(\omega_1-\omega-E\omega_1), \quad (7.2)$$

wherein constancy of j has been used. Under these conditions the total flux of fuel (droplets and fragmented debris) is

$$\rho\omega u_d+x\rho(1-\omega)u_f=\omega_1 j. \quad (7.3)$$

When combined with (7.1) and separately with (6.1) and (6.3) this yields respectively

$$\rho(1-\omega)u_f=\omega_1 jE/x, \quad (8.1)$$

$$\rho\omega(1-\omega)u_r=j(\omega_1-\omega-x+x\omega)/(1-x). \quad (8.2)$$

Comparing (8.2) with (7.2) establishes relations between E and x, and hence the complete forms $(\zeta_1=\omega_1^{-1}-1)$:

$$x=\frac{E}{E+\zeta_1}=\frac{D}{D+(1-D)\rho_c/\rho_{dB}}, \quad (9.1)$$

$$D = \frac{x}{x+(1-x)\rho_{\mathrm{dB}}/\rho_{\mathrm{c}}} = \frac{E}{E+\zeta_1\rho_{\mathrm{dB}}/\rho_{\mathrm{c}}}, \qquad (9.2)$$

$$E = \frac{\zeta_1 x}{1-x} = \zeta_1\frac{\rho_{\mathrm{dB}}}{\rho_{\mathrm{c}}}\frac{D}{1-D}. \qquad (9.3)$$

Relations (9) together with velocity relations (7)–(8) express all kinematic variables in terms of an independent conversion variable such as E, and a dependent variable (chosen as either ω or α), plus thermodynamic intensive properties and quantities. These relations are consistent with [1], and though redundant are found most useful in the developments.

2.2. *Equations of change and conservation*

With the exception of differences to be noted, we start with equations for separated, two-phase, steady flow in one dimension, equivalent to those employed by Sharon and Bankoff [1]. Thus, the mass balances on fuel and coolant are respectively,

$$\frac{\mathrm{d}}{\mathrm{d}z}\rho\omega u_{\mathrm{d}} = -\frac{\mathrm{d}}{\mathrm{d}z}\rho(1-\omega)u_{\mathrm{f}} = -\frac{\mathrm{d}}{\mathrm{d}z}\rho(1-\omega)xu_{\mathrm{f}} = -\Gamma_{\mathrm{f}}, \qquad (10.1)$$

$$\frac{\mathrm{d}}{\mathrm{d}z}\rho(1-\omega)(1-x)u_{\mathrm{f}} = 0. \qquad (10.2)$$

The first equality (10.1) is equivalent to total mass conservation ($\mathrm{d}j/\mathrm{d}z = 0$), or

$$j \equiv \rho u = \mathrm{constant} = \rho_1 u_1 \qquad (10.3)$$

where u_1 is shock velocity relative to motionless conditions upstream of shock (we assume zero relative motion between fuel and coolant there). Combining the first and third terms of (10.1) and relating to upstream values also provides equation (7.3). Equation (7.1) in (10.1) then yields the first reduced kinetics form:

$$\omega_1 j\frac{\mathrm{d}E}{\mathrm{d}z} = \Gamma_{\mathrm{f}}. \qquad (10.4)$$

The individual equivalent-phase equations of momentum change are stated as

$$\rho\omega u_{\mathrm{d}}\frac{\mathrm{d}u_{\mathrm{d}}}{\mathrm{d}z} = -\alpha\frac{\mathrm{d}P}{\mathrm{d}z} - F \qquad (11.1)$$

$$\rho(1-\omega)u_{\mathrm{f}}\frac{\mathrm{d}u_{\mathrm{f}}}{\mathrm{d}z} = -(1-\alpha)\frac{\mathrm{d}P}{\mathrm{d}z} + F + u_{\mathrm{r}}\Gamma_{\mathrm{f}}. \qquad (11.2)$$

These combine to the total momentum conservation form:

$$\mathrm{d}[P+\rho\omega u_{\mathrm{d}}^2 + \rho(1-\omega)u_{\mathrm{f}}^2]/\mathrm{d}z = 0,$$

which upon use of the upstream value $P_1 + j^2/\rho_1$, equations (6.3) and (10.3), provides the momentum jump condition:

$$P_1 - P = j^2\left(\frac{1}{\rho} - \frac{1}{\rho_1}\right) + \rho\omega(1-\omega)u_{\mathrm{r}}^2. \qquad (11.3)$$

This form, generalizes the 'Rayleigh line' relationship between pressure and local specific volume, $v = 1/\rho$. It shows that non-zero relative velocity between fuel drops and coolant eliminates the classical straight-line character of progress through the detonation zone, as represented on a P–v phase plane. Of course u_{r} may be eliminated from (11.3) using (7.2).

The energy equation for the fuel droplet phase takes the form

$$\alpha u_{\mathrm{d}}\left(\rho_{\mathrm{d}}\frac{\mathrm{d}i_{\mathrm{d}}}{\mathrm{d}z} - \frac{\mathrm{d}P}{\mathrm{d}z}\right) = -\phi \qquad (12.1)$$

with ϕ the volumetric heat transfer rate from droplets to fluid. In adopting this equation form we have assumed that all viscous dissipation of mechanical energy occurs in the coolant fluid phase, with only a negligible amount occurring in the unfragmented fuel droplets. An equivalent form,

$$\rho\omega u_{\mathrm{d}}\frac{\mathrm{d}}{\mathrm{d}z}\left(i_{\mathrm{d}} + \frac{1}{2}u_{\mathrm{d}}^2\right) = -u_{\mathrm{d}}F - \phi, \qquad (12.2)$$

is seen to differ in the velocity factor $F(u_{\mathrm{d}}$ vs $u_{\mathrm{r}})$ from that used in [1]. The corresponding fluid equation is

$$(1-\alpha)u_{\mathrm{f}}\rho_{\mathrm{f}}\frac{\mathrm{d}i_{\mathrm{f}}}{\mathrm{d}z} - \frac{\mathrm{d}P}{\mathrm{d}z} = \phi + u_{\mathrm{r}}F + (i_{\mathrm{d}} - i_{\mathrm{f}} + u_{\mathrm{r}}^2/2)\Gamma_{\mathrm{f}}. \qquad (12.3)$$

We shall employ the combination of these equations which states total energy conservation, viz.

$$\frac{\mathrm{d}}{\mathrm{d}z}\left[\rho\omega u_{\mathrm{d}}\left(i_{\mathrm{d}} + \frac{1}{2}u_{\mathrm{d}}^2\right) + \rho(1-\omega)u_{\mathrm{f}}\left(i_{\mathrm{f}} + \frac{1}{2}u_{\mathrm{f}}^2\right)\right] = 0. \qquad (13.1)$$

This may be written, using (6.3), (6.1), (10.3), and the upstream condition $u_{\mathrm{r}1} = 0$, as

$$2j[\omega_1 i_{\mathrm{d}1} - \omega i_{\mathrm{d}} + (1-\omega_1)i_{\mathrm{f}1} - (1-\omega)i_{\mathrm{f}}] + 2\rho\omega(1-\omega)u_{\mathrm{r}}(i_{\mathrm{f}} - i_{\mathrm{d}}) = j^3(\rho^{-2} - \rho_1^{-2}) + 3j\omega(1-\omega)u_{\mathrm{r}}^2 + \rho\omega(1-\omega)(1-2\omega)u_{\mathrm{r}}^3. \qquad (13.2)$$

We now replace u_{r} by j using (7.2) and i_{f} by i_{c} and i_{dB} using (5) and (9.1), to obtain the energy jump balance $(i_{\mathrm{f}1} = i_{\mathrm{c}1})$

$$(1-\omega_1)(i_{\mathrm{c}1} - i_{\mathrm{c}}) + \omega_1[E(i_{\mathrm{d}1} - i_{\mathrm{dB}}) + (1-E)(i_{\mathrm{d}1} - i_{\mathrm{d}})] = \frac{j^2}{2}\left[\left(\frac{1}{\rho^2} - \frac{1}{\rho_1^2}\right) + \frac{(1-2\omega)(\omega_1 - E\omega_1 - \omega)^3}{\rho^2\omega^2(1-\omega)^2} + \frac{3(\omega_1 - E\omega_1 - \omega)^2}{\rho^2\omega(1-\omega)}\right]. \qquad (13.3)$$

A general Rankine–Hugoniot relation for arbitrary E

may be identified by eliminating j^2 from (13.3) using (11.3) and (7.2).

Generally, in addition to (13.3), it is necessary to trace thermodynamic properties of unfragmented fuel with the kinetic equation (12.1). However, if we neglect the small heat transfer ($\phi = 0$), this equation reduces to the isentropic droplet condition $\rho_d \mathrm{d}i_d - \mathrm{d}P = 0$, so that to the extent the droplets are incompressible, (12.1) may be replaced by the insertion of

$$i_d - i_{d1} = (P - P_1)/\rho_d \qquad (14)$$

into (13.3). With this the requisite kinetic equation forms for tracing progress through the detonation zone are simply (10.4) and (11.1) for E and ω, with (13.3) and (11.3) determining thermodynamic conditions locally.

If one may treat the actual thickness of the shock zone as very thin, there will be very little momentum exchange between fuel droplets and coolant during the period of shock passage and collapse of vapor blankets. Under this condition the individual phase momentum-jump conditions (cf. also equation (66) of [1]) may be expressed as total momentum conservation ($\rho_1 u_1 = j_0 = j$) plus

$$\alpha_1 P_1 - \alpha_0 P_0 = \omega_1^2 j^2 (1/\rho_0\omega_0 - 1/\rho_1\omega_1)$$

$$= \left(\frac{\omega_1^2 j^2}{\rho_d}\right)(1/\alpha_0 - 1/\alpha_1). \qquad (15.1)$$

The final form here applies if we may treat fuel droplets as incompressible. [We have used (7.1) here with $E = 0$.] The shock compression ratio P_0/P_1 follows from (15.1) and total momentum jump [(11.3) with $E = 0$ in (7.2)].

The elimination of j^2 between that result and (15.1), may then be rearranged to the general working form,

$$\left(1 - \frac{P_1}{P_0}\right)\omega_1^2\left(1 - \frac{\rho_{d0}\alpha_0}{\rho_{d1}\alpha_1}\right) = \left(\alpha_0 - \alpha_1\frac{P_1}{P_0}\right)\eta \qquad (15.2)$$

with

$$\eta = (\omega_0 - \omega_1)^2/(1 - \omega_0) + (\omega_0 - \rho_{d0}\alpha_0/\rho_{d1}\alpha_1). \qquad (15.3)$$

Equation (15.2) is useful for fixing conditions just behind the shock front. In a similar manner, a second working relation obtains with $E = 0$ by eliminating j^2 between (13.3) and (11.3). The result is

$$i_{c1} - i_{c0} = \frac{P_1 - P_0}{\rho_1(1 - \omega_1)}(\Psi - \alpha_1) \qquad (15.4)$$

with definitions

$$\Psi \equiv (1 - a^2 + (1 - 2\omega_0)\delta^2/(\omega_1 - \omega_0) + 3\delta)/a(1 - a + \delta),$$

$$a = \rho_0/\rho_1 \equiv \alpha_0\omega_1/\alpha_1\omega_0,$$

$$\delta = (\omega_1 - \omega_0)^2/\omega_0(1 - \omega_0). \qquad (15.5)$$

To obtain (15.4), the simplification of (14), i.e. $\phi = 0$ and incompressible fuel, has been adopted.

We now develop important equations for the variations of fuel volume fraction, α, and pressure P which are required for kinetics integrations as well as in sonic termination considerations. Differentiation of the momentum conservation condition (11.3) eventually yields

$$(\rho_f u_f^2 - \rho_d u_d^2)\frac{\mathrm{d}\alpha}{\mathrm{d}z} = -\frac{\mathrm{d}P}{\mathrm{d}z} + \alpha u_d^2 \frac{\mathrm{d}\rho_d}{\mathrm{d}z}$$

$$+ (1 - \alpha)u_f^2 \frac{\mathrm{d}\rho_f}{\mathrm{d}z} + 2u_r\Gamma_f. \qquad (16.1)$$

A less symmetrical relation which follows from (11.1) is:

$$\rho_d u_d^2 \frac{\mathrm{d}\alpha}{\mathrm{d}z} = \alpha\frac{\mathrm{d}P}{\mathrm{d}z} - u_d^2\frac{\mathrm{d}\rho_d}{\mathrm{d}z} + F - u_d\Gamma_f. \qquad (16.2)$$

Application of either requires an explicit decoupled expression for pressure gradient. A general starting form for obtaining this has been provided by Sharon and Bankoff [1], viz.

$$\left(\frac{\alpha}{\rho_d u_d^2} + \frac{(1 - \alpha)}{\rho_f u_f^2}\right)\frac{\mathrm{d}P}{\mathrm{d}z} = \frac{\alpha}{\rho_d}\frac{\mathrm{d}\rho_d}{\mathrm{d}z} + \frac{(1 - \alpha)}{\rho_f}\frac{\mathrm{d}\rho_f}{\mathrm{d}z}$$

$$- F\left(\frac{1}{\rho_d u_d^2} - \frac{1}{\rho_f u_f^2}\right) - \Gamma_f\left(\frac{1}{\rho_f u_f} - \frac{1}{\rho_d u_d} - \frac{u_r}{\rho_f u_f^2}\right). \qquad (17)$$

{An elegant derivation of (17) is presented in [1] by combining the individual phase momentum balances (our 11.1, 11.2), cf. their equation (47).} It may also be obtained by combination of (16.1) and (16.2). Further decoupling now awaits relations for fluid and droplet density variations. The fuel droplet density change in (17) follows generally from the thermodynamic identity

$$\mathrm{d}\rho/\rho = \mathrm{d}P/\rho C^2 - (\beta/C_p)T\mathrm{d}s \qquad (18)$$

with use of the energy equation (12.1). Here C, β, C_p are respectively the (single-phase) sonic velocity, coefficient of thermal expansion, and constant pressure heat capacity; and, of course, in (12.1) use

$$T\mathrm{d}s \equiv \mathrm{d}i - \mathrm{d}P/\rho \equiv C_p\mathrm{d}T - T\beta\mathrm{d}P/\rho. \qquad (19)$$

The fluid density variations needed in (16) and (17) are more complicated since equations of type (18) apply to pure phase components. Our composite fluid–thermodynamic results for this are not strict agreement with equation (49) of [1], and, in addition, show very significant differences between cases of (i) subcooled or supercritical (single phase) coolant, and (ii) coolant in equilibrium flashing, i.e. lower sonic (choke) velocities in case (ii). Consequently we sketch some derivation detail. Our starting point may be obtained from equations (2) and (9):

$$\frac{\mathrm{d}\rho_f}{\rho_f} = \rho_f\left(\frac{1}{\rho_c} - \frac{1}{\rho_{dB}}\right)\mathrm{d}x + D\frac{\mathrm{d}\rho_{dB}}{\rho_{dB}} + (1 - D)\frac{\mathrm{d}\rho_c}{\rho_c}. \qquad (19.1)$$

The pure phase density variations, $\mathrm{d}\rho_{dB}$, $\mathrm{d}\rho_c$, are eliminated in case (i) using equations of type (18) and the latter part of (19). The result contains a temperature variation, dT, which is in turn eliminated by applying an equation similar to (5) for entropy, and again eliminating pure component entropy variations with (19). We ultimately obtain

$$C_{\mathrm{Pf}}\mathrm{d}T = T\mathrm{d}s_{\mathrm{f}} - (i_{\mathrm{dB}}-i_{\mathrm{c}})\mathrm{d}x + T\beta_{\mathrm{f}}\mathrm{d}P/\rho_{\mathrm{f}}, \tag{19.2}$$

$$\frac{\mathrm{d}\rho_{\mathrm{f}}}{\rho_{\mathrm{f}}} = \frac{\mathrm{d}P}{\rho_{\mathrm{f}}\bar{C}_{\mathrm{f}}^2} - \frac{\beta_{\mathrm{f}}}{Cp_{\mathrm{f}}}T\mathrm{d}s_{\mathrm{f}} + \kappa\mathrm{dx}, \tag{19.3}$$

with

$$C_{\mathrm{Pf}} = x\,C_{\mathrm{PdB}} + (1-x)\,C_{\mathrm{Pc}}, \tag{19.4}$$

$$\beta_{\mathrm{f}} = D\beta_{\mathrm{dB}} + (1-D)\beta_{\mathrm{c}}, \tag{19.5}$$

$$\frac{1}{\rho_{\mathrm{f}}\bar{C}_{\mathrm{f}}^2} = \frac{D}{\rho_{\mathrm{dB}}C_{\mathrm{dB}}^2} + \frac{(1-D)}{\rho_{\mathrm{c}}C_{\mathrm{c}}^2} + T\left[\frac{D\beta_{\mathrm{dB}}^2}{\rho_{\mathrm{dB}}C_{\mathrm{PdB}}} + \frac{(1-D)\beta_{\mathrm{c}}^2}{\rho_{\mathrm{c}}C_{\mathrm{Pc}}} - \frac{\beta_{\mathrm{f}}^2}{\rho_{\mathrm{f}}C_{\mathrm{Pf}}}\right], \tag{19.6}$$

$$\kappa = \left[\rho_{\mathrm{f}}\left(\frac{1}{\rho_{\mathrm{c}}} - \frac{1}{\rho_{\mathrm{dB}}}\right) + \frac{\beta_{\mathrm{f}}}{C_{\mathrm{Pf}}}(i_{\mathrm{db}}-i_{\mathrm{c}})\right]. \tag{19.7}$$

Equation (19.6) defines an equilibrium 'sonic' velocity of the composite fluid which incorporates corrections to the 'homogeneous flow sonic velocity' for coolant and debris due to relative thermal expansion of these components at constant entropy s_{f} and debris mass fraction, x. These corrections shall be included in subsequent calculations. They are, however, generally less significant than the corresponding corrections for case (ii).

In case (ii), or equilibrium coolant flashing, the coolant density variation in (19.1) is decomposed using (3), so that (19.1) becomes

$$\frac{\mathrm{d}\rho_{\mathrm{f}}}{\rho_{\mathrm{f}}} = \rho_{\mathrm{f}}\left(\frac{1}{\rho_{\mathrm{c}}} - \frac{1}{\rho_{\mathrm{dB}}}\right)\mathrm{d}x + D\frac{\mathrm{d}\rho_{\mathrm{dB}}}{\rho_{\mathrm{dB}}} + \frac{(1-D)}{\rho_{\mathrm{c}}}(\rho_{\mathrm{vl}}\mathrm{d}\varepsilon + \varepsilon\mathrm{d}\rho_{\mathrm{v}} + (1-\varepsilon)\mathrm{d}\rho_{\mathrm{l}}). \tag{20.1}$$

A similar decomposition of coolant and fluid entropy using equations similar to (5) yields a relation for dε,

$$\frac{(1-D)\rho_{\mathrm{v}}\rho_{\mathrm{l}}s_{\mathrm{vl}}}{\rho_{\mathrm{c}}\rho_{\mathrm{f}}}\left[\mathrm{d}\varepsilon + \varepsilon(1-\varepsilon)\left(\frac{\mathrm{d}\rho_{\mathrm{v}}}{\rho_{\mathrm{v}}} - \frac{\mathrm{d}\rho_{\mathrm{l}}}{\rho_{\mathrm{l}}}\right)\right] = \mathrm{d}s_{\mathrm{f}} - (s_{\mathrm{dB}}-s_{\mathrm{c}})\mathrm{d}x - x\,\mathrm{d}s_{\mathrm{dB}} - (1-x)(y\,\mathrm{d}s_{\mathrm{v}} + (1-y)\,\mathrm{d}s_{\mathrm{l}}), \tag{20.2}$$

which replaces (19.2). If the coolant vapor and liquid are approximately in equilibrium, the fluid temperature variations follow the coolant vapor pressure curve, $dT = \mathrm{d}P/P_{\mathrm{s}}'(T)$. Thus, the entropies, and densities of fuel debris, coolant liquid, and coolant vapor, all obey the generic thermodynamic relations,

$$\rho\,\mathrm{d}s = \left(\frac{\rho C_{\mathrm{P}}}{TP_{\mathrm{s}}'} - \beta\right)\mathrm{d}P \tag{20.3}$$

$$\frac{\mathrm{d}\rho}{\rho} = \left(\frac{1}{\rho C^2} + \frac{T\beta^2}{\rho C_{\mathrm{P}}} - \frac{\beta}{P_{\mathrm{s}}'}\right)\mathrm{d}P. \tag{20.4}$$

We eliminate dε from (20.1) using (20.2), insert the above density and entropy variations for each of the pure phases, apply the Clausius Clapeyron equation form, $\rho_{\mathrm{v}}\rho_{\mathrm{l}}s_{\mathrm{vl}} = -\rho_{\mathrm{vl}}P_{\mathrm{s}}'$, and the equilibrium condition $i_{\mathrm{dB}} - i_{\mathrm{c}} = T(s_{\mathrm{dB}} - s_{\mathrm{c}})$. This produces the replacement of (19.3) applicable to flashing conditions,

$$\frac{\mathrm{d}\rho_{\mathrm{f}}}{\rho_{\mathrm{f}}} = \frac{\mathrm{d}P}{\rho_{\mathrm{f}}\bar{C}_{\mathrm{f}}^2} - \frac{\rho_{\mathrm{f}}}{P_{\mathrm{s}}'}\mathrm{d}s_{\mathrm{f}} + \kappa_{\varepsilon}\,\mathrm{d}x. \tag{20.5}$$

Here,

$$\kappa_{\varepsilon} = \rho_{\mathrm{f}}\left(\frac{1}{\rho_{\mathrm{c}}} - \frac{1}{\rho_{\mathrm{dB}}}\right) + (i_{\mathrm{dB}} - i_{\mathrm{c}})/TP_{\mathrm{s}}', \tag{20.6}$$

$$\frac{1}{\rho_{\mathrm{f}}\bar{C}_{\mathrm{f}}^2} = \frac{D}{\rho_{\mathrm{dB}}C_{\mathrm{dB}}^2} + (1-D)\left(\frac{\varepsilon}{\rho_{\mathrm{v}}C_{\mathrm{v}}^2} + \frac{(1-\varepsilon)}{\rho_{\mathrm{l}}C_{\mathrm{l}}^2}\right) + T\left[\frac{D\beta_{\mathrm{dB}}^2}{\rho_{\mathrm{dB}}C_{\mathrm{PdB}}} + (1-D)\left(\frac{\varepsilon\beta_{\mathrm{v}}^2}{\rho_{\mathrm{v}}C_{\rho\mathrm{v}}} + \frac{(1-\varepsilon)\beta_{\mathrm{l}}^2}{\rho_{\mathrm{l}}C_{\mathrm{Pl}}}\right) - \frac{2\beta_{\mathrm{f}}}{TP_{\mathrm{s}}'} + \frac{\rho_{\mathrm{f}}C_{\mathrm{Pf}}}{(TP_{\mathrm{s}}')^2}\right] \tag{20.7}$$

with (19.4) and (19.5) applicable here also provided one uses

$$C_{\mathrm{Pc}} = yC_{\mathrm{pv}} + (1-y)C_{\mathrm{Pl}};\quad \beta_{\mathrm{c}} = \varepsilon\beta_{\mathrm{v}} + (1-\varepsilon)\beta_{\mathrm{l}}. \tag{20.8}$$

Equation (20.7) defines an effective sonic velocity $\bar{C}_{\mathrm{f}}$ for the composite fluid under flashing conditions. The correction terms to the 'homogeneous flow sonic velocity' arise both from thermal expansion and from vaporization expansion. Because these terms involving P_{s}' can dominate the entire expression, drastic reductions (discontinuities) occur in $\bar{C}_{\mathrm{f}}$ when the coolant vapor–liquid phase boundary is approached from the sub-cooled liquid side, thereby effectively suppressing C–J propagations.

The requisite density variations required in (17) and (16) are now obtained from either (19.3) for single-phase coolant, or (20.5) for equilibrium flashing of coolant. In the first case, (i), we apply the fluid energy equation (12.3) with (19), along with (9.1) and (10.4) to obtain

$$\frac{\mathrm{d}\rho_{\mathrm{f}}}{\mathrm{d}z} = \frac{1}{\bar{C}_{\mathrm{f}}^2}\frac{\mathrm{d}P}{\mathrm{d}z} + \frac{\kappa(1-x)}{u_{\mathrm{f}}(1-\alpha)}\Gamma_{\mathrm{f}} - \frac{\beta_{\mathrm{f}}}{C_{\mathrm{Pf}}u_{\mathrm{f}}(1-\alpha)}[\phi + u_{\mathrm{r}}F + (i_{\mathrm{d}} - i_{\mathrm{f}} + u_{\mathrm{r}}^2/2)\Gamma_{\mathrm{f}}]. \tag{21.1}$$

Similarly from (12.1)

$$\frac{\mathrm{d}\rho_\mathrm{d}}{\mathrm{d}z} = \frac{1}{C_\mathrm{d}^2}\frac{\mathrm{d}P}{\mathrm{d}z} + \frac{\beta_\mathrm{d}}{C_{\mathrm{Pd}}u_\mathrm{d}\alpha}\phi. \tag{21.2}$$

From these the pressure gradient of equation (17) assumes the general form of Sharon and Bankoff [1], [their equation (52)], viz.

$$\Phi\frac{\mathrm{d}P}{\mathrm{d}z} = K_\mathrm{F}F + K_\Gamma\Gamma_\mathrm{f} + K_\phi\phi \equiv K, \tag{22.1}$$

and here with

$$\Phi = \frac{\alpha}{\rho_\mathrm{d}}\left(\frac{1}{u_\mathrm{d}^2} - \frac{1}{C_\mathrm{d}^2}\right) + \frac{(1-\alpha)}{\rho_\mathrm{f}}\left(\frac{1}{u_\mathrm{f}^2} - \frac{1}{\bar{C}_\mathrm{f}^2}\right), \tag{22.2}$$

$$K_\phi = \frac{\beta_\mathrm{d}}{\rho_\mathrm{d}C_{\mathrm{Pd}}u_\mathrm{d}} - \frac{\beta_\mathrm{f}}{\rho_\mathrm{f}C_{\mathrm{Pf}}u_\mathrm{f}}, \tag{22.3}$$

$$K_\mathrm{F} = \frac{1}{\rho_\mathrm{f}u_\mathrm{f}^2} - \frac{1}{\rho_\mathrm{d}u_\mathrm{d}^2} - \frac{\beta_\mathrm{f}u_\mathrm{r}}{\rho_\mathrm{f}C_{\mathrm{Pf}}u_\mathrm{f}}, \tag{22.4}$$

$$K_\Gamma = \frac{1}{\rho_\mathrm{d}u_\mathrm{d}} + \frac{u_\mathrm{r}}{\rho_\mathrm{f}u_\mathrm{f}^2} - \frac{1}{\rho_\mathrm{f}u_\mathrm{f}} + \frac{\kappa(1-x)}{\rho_\mathrm{f}u_\mathrm{f}} - \frac{\beta_\mathrm{f}}{\rho_\mathrm{f}C_{\mathrm{Pf}}u_\mathrm{f}}(i_\mathrm{d} - i_\mathrm{f} + u_\mathrm{r}^2/2). \tag{22.5}$$

We shall not state the corresponding results for flashing [case (ii)] but simply note that equations (22.1) and (22.2) hold as general forms, but (20.7) replaces (19.6) as definition of $\bar{C}_\mathrm{f}$ in that case. {The definition (19.6) also distinguishes our (22.2) from Φ of [1] equation (52). Differences in our K_f and K_Γ stem from our adopted forms for the energy equation, (12.1), (12.3).} Equation (22.1), plus the result of substituting it into (21.1), may be applied to (16.2) to obtain

$$\rho_\mathrm{d}u_\mathrm{d}^2\frac{\mathrm{d}\alpha}{\mathrm{d}z} = G_\mathrm{F}F + G_\Gamma\Gamma_\mathrm{f} + G_\phi\phi \equiv G \tag{23.1}$$

with $M = u/c$ denoting Mach number in

$$G_\phi = \alpha(1 - M_\mathrm{d}^2)K_\phi/\Phi \quad - \beta_\mathrm{d}u_\mathrm{d}/C_\mathrm{pd}, \tag{23.2}$$

$$G_\mathrm{F} = \alpha(1 - M_\mathrm{d}^2)K_\mathrm{F}/\Phi \quad + 1 \tag{23.3}$$

$$G_\Gamma = \alpha(1 - M_\mathrm{d}^2)K_\Gamma/\Phi \quad - u_\mathrm{d}. \tag{23.4}$$

Equation (23.1) provides a reduced kinetic equation for direct integration utilizing the conservation conditions and (10.4). Numerical results based upon such integrations will be presented in a subsequent paper. An equation for the fluid temperature also follows from (19.2), which ultimately becomes

$$\rho_\mathrm{f}\alpha_\mathrm{f}u_\mathrm{f}C_\mathrm{Pf}\frac{\mathrm{d}T}{\mathrm{d}z} = \tau_\mathrm{F}F + \tau_\Gamma\Gamma_\mathrm{f} + \tau_\phi\phi \tag{24.1}$$

with

$$\tau_\Gamma = \alpha_\mathrm{f}u_\mathrm{f}T\beta_\mathrm{f}(K_\Gamma/\Phi) + i_\mathrm{d} - i_\mathrm{dB} + u_\mathrm{r}^2/2, \tag{24.2}$$

$$\tau_\mathrm{F} = \alpha_\mathrm{f}u_\mathrm{f}T\beta_\mathrm{f}(K_\mathrm{F}/\Phi) + u_\mathrm{r}, \tag{24.3}$$

$$\tau_\phi = \alpha_\mathrm{f}u_\mathrm{f}T\beta_\mathrm{f}(K_\phi/\Phi) + 1. \tag{24.4}$$

Though redundant, in numerical procedures this equation may be used as a replacement for the total energy balance (13.3), which then serves as an accuracy or consistency check.

2.3. *Equations for conditions at Chapman–Jouguet plane*

We shall adhere, here, to the principle that in hydrodynamic fragmentation, termination of the quasi-steady detonation zone corresponds to a quasi-equilibrium condition that relative velocity approaches zero, hence from (7.2)

$$u_\mathrm{r} = 0 \text{ or } \omega = \omega_1(1 - E). \tag{25}$$

Under this circumstance j^2 is eliminated between the energy and momentum-jump balances (11.3), (13.3). If we also apply the relationship obtained from (9.1), (1), and (2) along with (25), viz.

$$\rho^{-1} = \omega_1(1-E)/\rho_\mathrm{d} + \omega_1 E/\rho_\mathrm{dB} + (1-\omega_1)/\rho_\mathrm{c}, \tag{26}$$

we obtain

$$\omega_1 E\left[2(i_\mathrm{d} - i_\mathrm{dB}) + (P - P_1)\left(\frac{1}{\rho_\mathrm{dB}} - \frac{1}{\rho_\mathrm{d}}\right)\right] = 2[\omega_1(i_\mathrm{d} - i_\mathrm{d1}) + (1-\omega_1)(i_\mathrm{c} - i_\mathrm{c1})] - (P - P_1)\left(\frac{1}{\rho_1} + \frac{\omega_1}{\rho_\mathrm{d}} + \frac{1-\omega_1}{\rho_\mathrm{c}}\right) \tag{27.1}$$

This explicit solution for E amounts to a general Rankine–Hugoniot relationship among thermodynamic variables (for fuel droplets plus fluid) and E. If we neglect the small heat transfer rate ($\phi = 0$) and take nearly incompressible fuel droplets ($\rho_\mathrm{d} = \rho_\mathrm{dl}$) equation (14) reduces (27.1) to the simpler form,

$$E\left[2(i_\mathrm{dl} - i_\mathrm{dB}) + (P - P_1)\left(\frac{1}{\rho_\mathrm{dB}} + \frac{1}{\rho_\mathrm{d}}\right)\right] = -\zeta_1\left[2(i_\mathrm{cl} - i_\mathrm{c}) + (P - P_1)\left(\frac{1}{\rho_\mathrm{c}} + \frac{1}{\rho_\mathrm{cl}}\right)\right]. \tag{27.2}$$

This Rankine–Hugoniot relation relates E to pressure P and temperature T of the fluid only, or in the case of equilibrium flashing, to $P = P_\mathrm{s}(T)$ and vapor fraction $\varepsilon(\zeta_1 = \omega_1^{-1} - 1)$. There remain two degrees of freedom, only one of which may be removed by a sonic termination condition.

In view of the variety of possible sonic velocities which can be defined for the multiphase system, it is possible to rationalize more than one detonation–termination condition. However, Sharon and Bankoff [1] have argued that Chapman–Jouguet termination should occur at a singularity in the kinetic equations, i.e. $\Phi = 0$ in (22.1), (23.1) or (24.1). Although rigorous stability arguments remain to be advanced, other conditions such as tangency to a constant E Rankine–Hugoniot appear less justified.

Introducing (25) into (22.2), or equivalently $u_d = u_f = u \equiv j/\rho$ in the choke conditions $\Phi = 0$, we obtain the C–J condition

$$\frac{(P_1 - P)}{\rho\left(1 - \frac{\rho}{\rho_1}\right)} = \left(\frac{\alpha}{\rho_d} + \frac{(1-\alpha)}{\rho_f}\right) \bigg/ \left(\frac{\alpha}{\rho_d C_d^2} + \frac{(1-\alpha)}{\rho_f \bar{C}_f^2}\right) = \frac{j^2}{\rho^2} \tag{28}$$

in which we have inserted the momentum-jump condition (11.3). To apply this we, of course, may use (26) along with relations for α, $(1-\alpha)$, and ρ_f obtained from using (25) in (9), and (2), cf. also (19.6). For completeness, we supply also the tangency condition for the constant E Rankine–Hugoniot curve in reduced explicit form:

$$\left(\frac{dP}{d\rho}\right)_E = \left(1 - \frac{(P-P_1)\beta_f}{2\rho_f C_{Pf}}\right) \bigg/ \rho(1-\alpha)\left(\frac{1}{\rho_f \bar{C}_f^2} + \frac{\beta_f}{2C_{Pf}}\left[\frac{1}{\rho_f} - \frac{1}{\bar{\rho}_{f1}}\right]\right) \tag{29}$$

with $1/\bar{\rho}_{f1} \equiv x/\rho_{d1} + (1-x)/\rho_{c1}$. Equation (29) is derived using (27.2) and (26), may be compared with (28) for incompressible fuel droplets, i.e. for $1/C_d \approx 0$.

3. KINETICS INDEPENDENT CALCULATIONS FOR THE UO$_2$–SODIUM SYSTEM

3.1. *Chapman–Jouguet plane evaluation*

In this section, we utilize the primary equations (27.2) and (28) to calculate conditions at a variety of hypothetical Chapman–Jouguet planes. The variety is due to the observed fact that for each unique completely stated upstream (initial) condition, the C–J plane conditions are determined in the absence of kinetics integrations, to within one unspecified degree of freedom. Such a parameter may be chosen to be fractional fragmentation E or shock velocity j/ρ. Thus, any two C–J plane variables (e.g. P and T) may be plotted as a single-curve locus of permissible C–J points. Such a locus is altered by any changes in specifications of upstream initial conditions. Our calculations show that the primary sensitivity is to changes in volume fraction of coolant vapor in the vapor blankets surrounding fuel droplets upstream of shock, i.e. ε_1. Hence our results are assembled as a set of C–J point curves with ε_1 as parameter, keeping all other upstream conditions constant.

A procedure for performing such computations of the following form has been employed. A pressure is fixed. To define a point for this P, coolant temperature is determined by iteration on (28). For each temperature tried during iteration E is determined by (27.2), from which all other kinematical, thermodynamic, and conserved quantities are evaluated using above formulae. We use the approximation of incompressible fuel droplets. Sodium-coolant properties are based upon the correlations of Breton [4]. Since these do not apply above the critical temperature, calculations are aborted when coolant temperatures reach 2700 K. Figure 1 shows a sequence of C–J point curves thus obtained for the following upstream initial conditions: liquid coolant temperature $T_{c1} = 600$ K. (A chosen coolant vapor blanket temperature of 1200 K is unimportant), fuel droplet temperature $T_{d1} = 3500$ K, fuel to coolant mass ratio of 9.671 ($\omega_1 = 0.9063$), $P_1 = 0.1$ MPa.

Figure 1(a) represents the C–J point curve sequence on a $P - v$ ($v = 1/\rho_c$) diagram for sodium, showing also the liquid side saturation curve. For ε_1 above a small lower limit, the C–J curves all initiate at the saturation curve. This important fact originates in the discontinuous jump of sonic velocity $\bar{C}_f$ for the composite fluid from its subcooled liquid value (19.6) to the flashing value (20.7). The latter value is found to be so much lower that no solution to the C–J equations [(28) and (27.2)] is possible. This suggests that a propagation cannot exist with flashing occurring in the steady zone or at the C–J point. It also suggests that the coolant saturation curve defines a lower limit threshold boundary for C–J curves. If, with a specific upstream condition and ε_1, fragmentation kinetics is not able to sustain C–J conditions for subcooled liquid above this saturation curve threshold, steady propagation appears improbable, and triggered propagation is likely to fizzle. Since the threshold C–J point can be calculated without recourse to fragmentation kinetics information, we shall term it a thermodynamic threshold.

Additional characteristics of the points on the C–J curves in Fig. 1(a) are shown in Figs. 1(b–d) showing coolant temperature, pressure, and fractional fragmentation E vs propagation velocity. A striking observation is the wide range of possible C–J conditions which are admitted, with complete fragmentation ($E = 1$) an implausible, hypothetical extreme. Similar charts (not shown) and observations are found for other upstream initial conditions. Thus if the mass ratio is reduced to 4.00 ($\omega_1 = 0.8$), the primary differences appear as larger values of E. This difference is due mainly to the fact that there was proportionally less fuel available to be fragmented. The actual amounts of fuel fragmented are more comparable. Similarly, by raising the initial pressure, a significant alteration is an observed elevation of lower C–J thresholds, which places more stringet demands upon kinetic fragmentation ratès for sustaining minimum level propagation. A physical explanation for this requires further investigation.

3.2. *Determination of shock-jump state conditions*

Treating the shock-jump as sufficiently sharp, we consider now the individual phase momentum conservation requirement (15.2). This additional relation

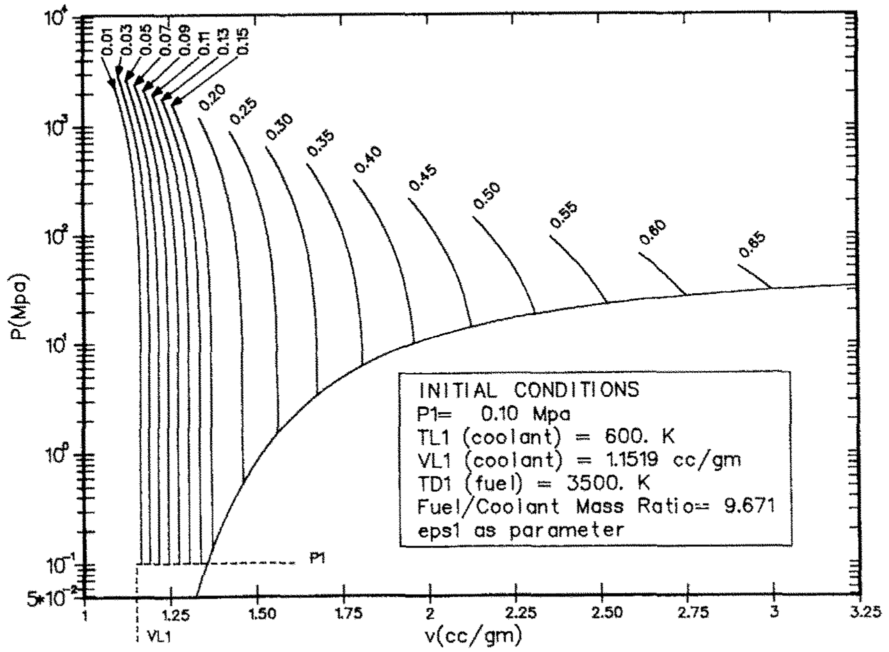

FIG. 1(a). Admissable C–J propagation states on a pressure–volume diagram for sodium for specified upstream (initial) states of a coarse mixture of sodium and UO_2. Each curve corresponds to a labelled value of sodium vapor volume fraction ε_1, and hence to a uniquely specified initial state. Each curve terminates at a near critical temperature of 2700 K. The lower curve represents liquid saturation.

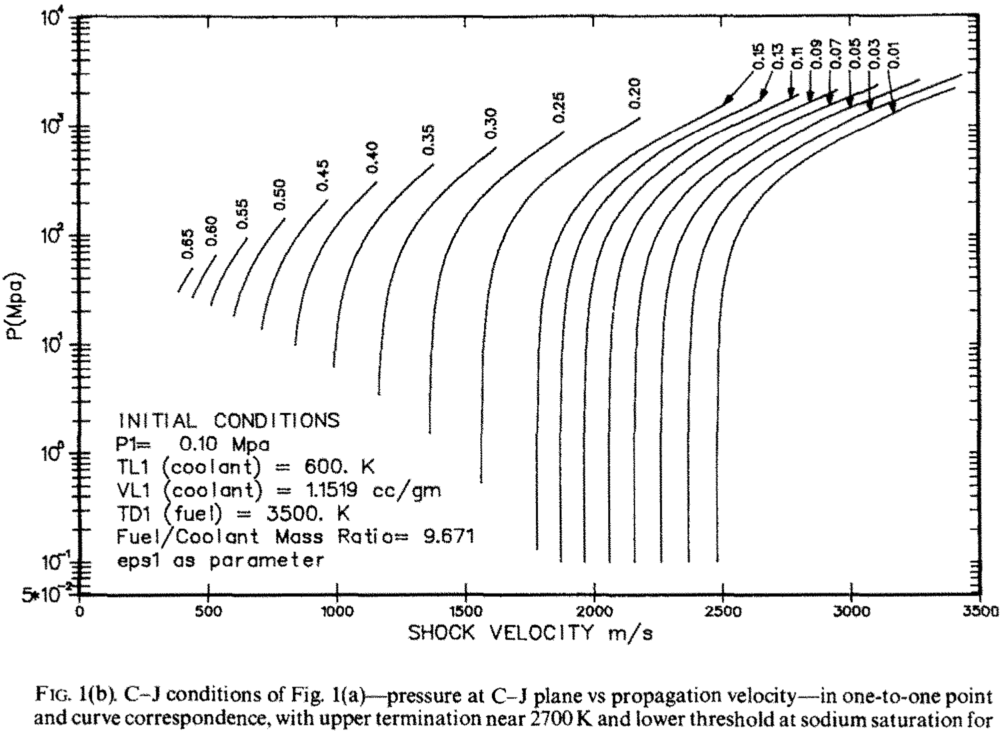

FIG. 1(b). C–J conditions of Fig. 1(a)—pressure at C–J plane vs propagation velocity—in one-to-one point and curve correspondence, with upper termination near 2700 K and lower threshold at sodium saturation for $\varepsilon_1 \geq 0.14$.

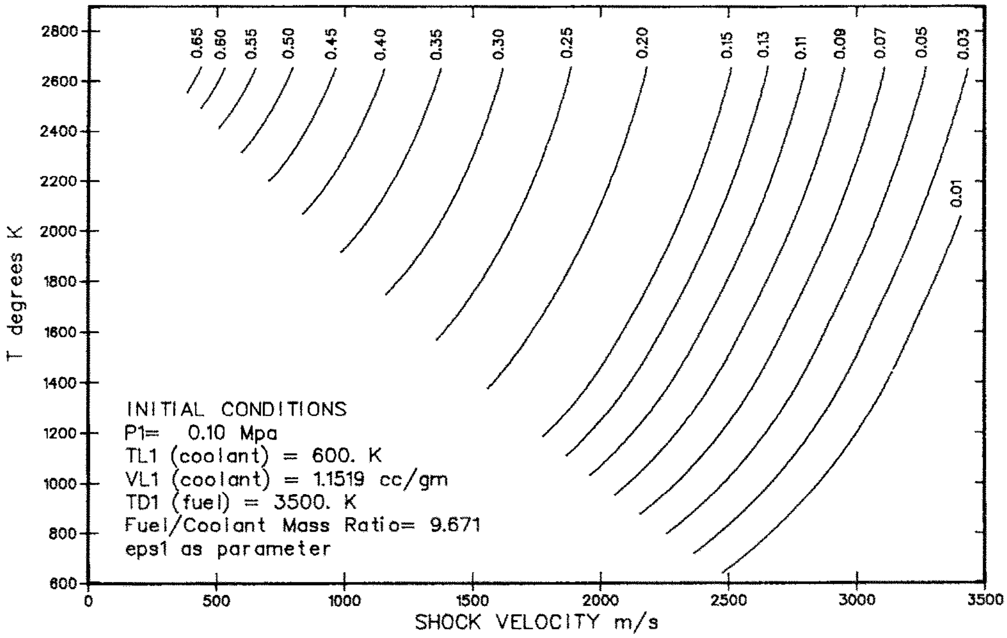

FIG. 1(c). C–J conditions of Fig. 1(a)—coolant (sodium) temperature vs propagation velocity—in one-to-one point and curve correspondence with Figs. 1(a, b), with upper termination near 2700 K and lower threshold at sodium saturation for $\varepsilon_1 \geq 0.14$.

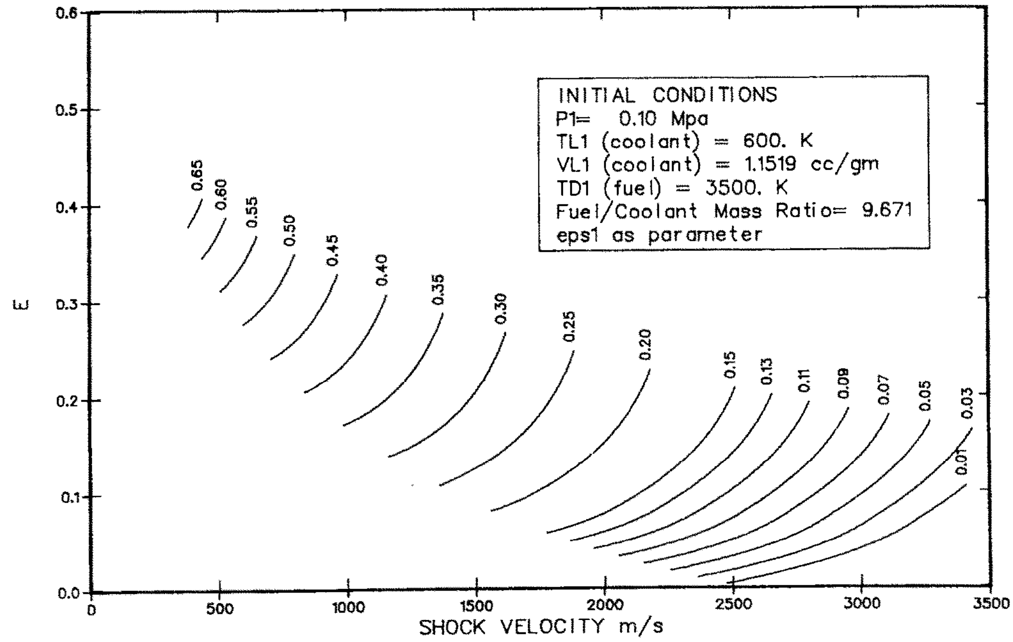

FIG. 1(d). C–J conditions of Fig. 1(a)—fraction of fuel (UO_2) fragmented, E, vs propagation velocity—in one-to-one point and curve correspondence with Figs. 1(a–c), with upper termination of curves near 2700 K and lower threshold at sodium saturation for $\varepsilon_1 \geq 0.14$.

permits determination of a state condition just behind the shock for any hypothetical C–J point calculated via Section 3.1. The following calculational procedure has been employed and automated successfully. A coolant temperature ($T_{f0} \equiv T_{c0}$) is fixed (initially only a few degrees above the upstream value T_{f1}). Conditions corresponding to this temperature are found by double iteration. In an inner iteration step, P_0 is presumed so that thermodynamic properties of coolant including $i_{f0} \equiv i_{c0}$, ρ_{c0} are identifiable. Then equation (15.2), with $\rho_{d0} = \rho_{d1}$, is iterated to corresponding values of α_0, or equivalently ω_0. This provides basis for calculating equation (15.4). The outer iteration consists of systematic repeating for new selections of P_0 until (15.4) is satisfied. Either j or shock velocity at this point, as well as u_{r0}, u_{d0}, u_{f0}, then follow from (15.1) or (11.3), with equation (7–9). This process is then repeated for new points at higher values of T_{c0}.

A one-to-one correspondence between shock jump point conditions and C–J point conditions is made by comparing j or shock velocity. Thus, T_{c0} (and corresponding P_0) values which yield shock velocities below the thermodynamic C–J threshold (Section 3.1) are ruled out. Similarly, upper limits on C–J curves define upper limits on T_{c0}, P_0. From these calculations for the UO_2–sodium system, the following is observed on charts (not shown). Coolant temperatures rise only slightly through the shock front, and are well below their values at the corresponding C–J plane, in agreement with [1]. Pressures, P_0, may jump to values either above or below those at the C–J plane. Velocities of fuel droplets tend to drop only by 10% or less of shock propagation velocity, while velocities of coolant typically drop ~ 50% of propagation velocity. These values, of course, are due principally to the high density of UO_2 ($\rho_d = 8.4$ g/cc) relative to that of sodium.

4. CONCLUDING REMARKS

The above calculations have identified a saturation curve threshold for potential Chapman–Jouguet points, below which no such propagation solution is possible. The basis for this conclusion is the size of the large precipitous drop of effective sonic velocity $\bar{C}_f$, of the coolant–debris fluid when coolant itself becomes a vapor–liquid mixture. While this observation is based upon an equilibrium-flashing model, the sharp reductions of effective sonic velocities due to the presence of vapor is well known [5]. Thus, the assumption of equilibrium should not be of consequence to threshold existence. However, a non-equilibrium formation of vapor in subcooled liquid would effectively raise the threshold above the saturation curve, and therefore, under special circumstances, have the effect of suppressing thermal detonation propagation. We consider vapor formation highly unlikely in the steady zone of the C–J propagation wave.

In contrast to this, coolant vaporization is quite probable in the unsteady expansion wave beyond (behind) the Chapman–Jouguet plane. This has most interesting stability implications The 'protection' of the C–J plane from disturbances in this zone may be facilitated considerably by the much lower sonic velocities prevalent in the rarefaction wave due to vaporization.

Finally, we note that the use of local equilibrium between fragmented fuel debris and coolant has a stringent test in its prediction of the equilibrium sonic velocity $\bar{C}_f$ [equation (19.6)]. We anticipate that the introduction of a three-phase model in which heat transfer and velocity equilibration of fragmented debris occurs on a slower time scale, so as to be neither instantaneous nor synonymous with fragmentation, will give rise to the use of the alternative 'frozen' sonic velocity C_f, which is identical to that of Sharon and Bankoff [1]. For comparison, equation (19.6) may be written

$$\frac{1}{\rho_f T}\left(\frac{1}{\bar{C}_f^2} - \frac{1}{C_f^2}\right) = \frac{D\beta_{dB}^2}{\rho_{dB}C_{PdB}} + \frac{(1-D)\beta_c^2}{\rho_c C_{pc}} - \frac{\beta_f^2}{\rho_f C_{Pf}}$$

$$\equiv \left(\frac{\beta_{dB}}{\rho_{dB}C_{PdB}} - \frac{\beta_c}{\rho_c C_{Pc}}\right)^2 \Bigg/ \left(\frac{1}{D\rho_{dB}C_{PdB}} + \frac{1}{(1-D)\rho_c C_{Pc}}\right) \tag{30}$$

the first form defining C_f. The second form demonstrates that the general $\bar{C}_f < C_f$, so that the equilibrium condition limits the Chapman–Jouguet propagation velocities in comparison to the frozen condition. The significance of this may be greater than that of finite debris-equilibrium kinetics.

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ETUDE DE LA PROPAGATION QUASI-STATIONNAIRE DE DETONATIONS THERMIQUES A TRAVERS DES DISPERSIONS DE COMBUSTIBLE CHAUD LIQUIDE DANS DES LIQUIDES PLUS FROIDS ET VOLATILES

Résumé—La modèle d'écoulement diphasique pour la propagation undirectionnelle d'une détonation thermique est reformulé pour permettre la formulation de deux conclusions nouvelles qui sont indépendantes des données cinétiques de fragmentation. Un large spectre d'états possibles de Chapman–Jouguet est trouvé pour toute condition initiale spécifique dans les calculs pour le système UO_2–sodium, avec la sensibilité de ces états C–J. On présente des arguments qui sugèrent l'utilisation d'une vitesse sonique d'équilibre pour la terminaison d'onde C–J. La diminution abrupte de la vitesse sonique due à la présence de vapeur ou de gaz est trouvée être suffisamment forte pour rendre la vaporisation soit dans la zone de détonation permanente ou dans le plan C–J et on identifie une limite inférieure pour les propagations C–J thermodynamiquement possibles qui se produisent à la saturation du réfrigérant.

BEITRAG ZUR QUASI-STATIONÄREN AUSBREITUNG THERMISCHER DETONATIONEN IN DISPERSIONEN VON HEISSEM, FLÜSSIGEM BRENNSTOFF IN KÜHLEREN, FLÜCHTIGEN UND FLÜSSIGEN KÜHLMITTELN

Zusammenfassung—Das Zweiphasen-Strömungsmodell für eindimensionale Ausbreitung thermischer Detonationen wird so umformuliert, daß sowohl neue als auch bekannte von fragmentationskinetischen Daten unabhängige Folgerungen getrennt betrachtet werden können. Es zeigt sich, daß das Zweiphasen-Strömungsmodell notwendig ist, um quantitative Voraussagen über die Detonationsstärke bei hydrodynamischer Fragmentation machen zu können. Bei den Berechnungen für das System UO_2-Natrium stellt sich heraus, daß für jede spezifische Anfangsbedingung ein breiter Bereich kinetikunabhängiger erlaubter Chapman–Jouguet (CJ)-Zustände möglich ist. Diese ermittelten CJ-Zustände sind vom anfänglichen Volumenverhältnis von Natrium (Kühlmittel) zu Dampffilm abhängig. Es werden Argumente genannt, die die von uns benutzte Gleichgewichts-Schallgeschwindigkeit zur Bergrenzung der CJ-Wellen begründen. Die plötzliche Abnahme der Schallgeschwindigkeit aufgrund der Anwesenheit von Dampf oder Gas erweist sich als so einschneidend, daß die Verdampfung sowohl in der stationären Detonationszone als auch in der CJ-Ebene unwahrscheinlich wird. Ferner kennzeichnet sie einen unteren Schwellenwert für thermodynamisch zulässige CJ-Ausbreitungen, die bei Sättigung des Kühlmittels auftreten.

К ВОПРОСУ О КВАЗИСТАЦИОНАРНОМ РАСПРОСТРАНЕНИИ ТЕПЛОВОЙ ДЕТОНАЦИИ В СУСПЕНЗИЯХ ГОРЯЧЕГО ЖИДКОГО ТОПЛИВА, НАХОДЯЩИХСЯ В БОЛЕЕ ХОЛОДНЫХ ЛЕТУЧИХ ЖИДКИХ ТЕПЛОНОСИТЕЛЯХ

Аннотация — Представлена новая формулировка модели двухфазного течения при одномерном распространении термической детонации, позволяющая сделать новые и подтвердить существующие выводы о процессе, не прибегая к данным по кинетике диспергирования. Показано, что для количественных оценок интенсивности детонации при гидродинамическом дроблении необходимо использование модели двухфазного течения. В расчетах для системы UO_2–натрий установлена возможность существования широкого спектра кинетически независимых допустимых состояний Чепмена-Жюге (C–J) для любого конкретного начального условия, а также определено влияние на эти (C–J) состояния начальной объемной доли паров натрия (теплоносителя). Высказаны соображения, подтверждающие возможность использования равновесной звуковой скорости для области затухания волны C–J. Показано, что снижение скорости звука в присутствии пара или газа происходит настолько резко, что процесс испарения весьма маловероятен как в зоне стационарной детонации, так и в плоскости C–J. Кроме того, это снижение позволяет определить более низкое значение предельного порога термодинамически допустимых состояний C–J, что имеет место при насыщении теплоносителя.