ON THE EXISTENCE OF STEADY SUPERCRITICAL PLANE THERMAL DETONATIONS*

A. SHARON† and S. G. BANKOFF

Chemical Engineering Department, Northwestern Univ., Evanston, Illinois, U.S.A.

Abstract—The conditions for existence of strongly supercritical steady detonations, proposed by Board and Hall, are considered. Fragmentation by local boiling is excluded, and only hydrodynamic mechanisms, such as boundary-layer stripping and/or Taylor instability can be operative. Truly steady supercritical detonations are achieved only when the fragmentation zone is terminated by an equilibrium Chapman–Jouguet plane (zero velocity and temperature difference between fuel and coolant). Strong sideways constraints are also necessary.

NOMENCLATURE

$\mathbf{A}$, matrix of coefficients, equation (32);

Bo, Bond number, $(\rho_f g\, r_d^2/\sigma) = \dfrac{3}{8} C_D We$;

$\mathbf{b}$, source term vector;

C_p, specific heat;

C, speed of sound;

$\mathbf{C}$, matrix of coefficients, equation (32);

C_D, drag coefficient;

D, fuel debris volume fraction in the fluid;

d_o, initial drop diameter;

E, fraction of mass stripped from single drop;

F, drag force per unit volume exerted on drops;

g, drop acceleration;

h, heat transfer coefficient;

i, specific enthalpy;

i_{fg}, latent heat of evaporation;

i_{sf}, heat of fusion;

Δ_i, specific enthalpy difference;

k, thermal conductivity;

$K_{f,\,\Gamma,\,\varphi}$, parameters, equations (40), (41) and (42);

L, equilibrium reaction zone length, based on Stokes drag;

L_{ef}, effective reaction zone length;

Nu, Nusselt number, $(2h\, r_d/k_f)$;

n, number of fuel drops per unit volume immediately behind shock;

M, Mach number relative to shock front;

m_o, initial drop mass;

m_s, mass stripped from single drop;

P, pressure;

r_d, drop radius;

T, temperature;

T_b, dimensionless break-up time,

$$\frac{U_r t_b}{2 r_{d_0}}\left(\frac{\rho_f}{\rho_d}\right)^{1\cdot 2};$$

t, time after drop leaves shock front;

t_b, break-up time;

U, velocity relative to the shock;

U_1, shock velocity relative to stationary frame;

U_r, relative velocity between coolant–debris mixture and fuel drops;

$\bar{v}$, specific volume;

We, Weber number, $(\rho_f r_d U_r^2/\sigma)$;

$\mathbf{X}$, vector of flow variables, equation (32);

x, quality;

z, distance from the shock front;

z_r, relative displacement of the drop.

Greek symbols

α, void fraction;

Γ_f, fluid mass source term due to debris formation equation (16);

κ_f, state parameter, equation (38);

ε_v, volume fraction of coolant as vapor;

μ, viscosity;

v, kinematic viscosity;

ρ, density;

σ, interfacial tension;

τ, dummy time variable;

φ, direct contact heat flux per unit volume;

ξ, stripping parameter, $E/(1-E)$.

Subscripts

b, break-up;

c, liquid coolant;

d, fuel drop;

db, fuel debris particles;

eq, equilibrium;

f, homogeneous fluid mixture of coolant (liquid and/or vapor) and debris;

m,	melting;
o,	initial conditions immediately behind shock front;
s,	separated flow;
v,	coolant vapor;
w,	wall;
1,	undisturbed region ahead of shock;
2,	immediately behind shock front;
3,	Chapman–Jouguet plane at rear of steady fragmentation zone.

1. INTRODUCTION

VAPOR explosions, which result from rapid local mixing of a hot liquid (fuel) and a cold vaporizable liquid (coolant) on a time scale of 0.1–1.0 ms, are characterized by pressure shock waves with significant damage potential. In 1974 Board, Hall and Hall [1] suggested that there was a strong analogy between steady-state thermal and chemical detonation waves, since both are preceded by a pressure wave, behind which lies a subsonic (relative to the shock) reaction zone. In combustion shocks the reaction zone is terminated by a sonic velocity plane which serves to protect the shock from time-dependent rarefaction waves proceeding from the far-field boundary conditions. If the phase velocities are equal, both ahead of the shock and at the sonic velocity plane (homogeneous flow), the jump balances for the chemical and thermal detonations have the same form, and the well established theory of chemical detonation can be invoked. In particular, the tangency (Chapman–Jouguet or C–J) condition to the equilibrium Hugoniot curve in the P–V plane of the reaction path line from the initial point represents a local sonic velocity condition, which can be shown to result in both a stable and minimum shock velocity. In both types of detonations the energy release in the reaction zone between the shock front and the C–J plane serves to sustain the shock in the face of dissipation due to internal reflections, friction, nonlinear (dispersive) effects and sideways expansion. In the case of thermal detonations the energy release results from fragmentation of the hot fuel droplets and subsequent rapid temperature equilibrium of the fuel fragments with the surrounding coolant. A major problem, therefore, consists of obtaining a realistic estimate of the mean fragmentation (or mixing) rate of the fuel particles (which may be liquid or liquid with a surface crust before the passage of the shock), as a function of local conditions within the reaction zone.

In thermal detonations, however, the mixture at the end of the reaction zone may consist of two, three (if vapor is present), or effectively four (if the fuel fragments are not in temperature- and velocity-equilibrium with the surrounding coolant) phases. In this mixture the sonic velocity is no longer uniquely defined, and in fact a continuous spectrum of characteristic velocities exists, depending upon the frequency of the disturbance and the distribution of the phases. Furthermore, except at infinity, it is not possible to have true velocity equilibrium, which will be shown below to be a requirement for the stable juncture of a steady-state reaction zone with a time-dependent supersonic expansion zone. A similar conclusion was reached independently by Scott and Berthoud [2]. Finally, it is quite possible to have an effective cut-off of fuel fragmentation, and hence of energy transfer, before complete dispersal is achieved, which would correspond to incomplete reaction at the Chapman–Jouguet plane. It is thus seen that the analogy is rather limited, and a careful examination of the necessary conditions for the existence of a steady-state plane thermal detonation is required.

This can be performed on two levels. The simplest approach assumes velocity and thermal equilibrium between the dispersed fuel and coolant at the (C–J) sonic velocity plane. In this case the mass, momentum and energy jump balances between a plane ahead of the shock and the C–J plane have the same form as in a combustion detonation. Two restrictions are implied: (1) thermal equilibrium implies essentially complete fragmentation of the fuel drops to fine debris (say $< 100\,\mu m$); (2) the disturbance wavelength must be large compared to the mean debris diameter for the homogeneous-mixture sonic velocity (and hence tangency condition) to be applicable. The conditions at the C–J plane are then determined solely by the upstream conditions, plus the tangency condition, and are independent of the kinetics of the fragmentation process. Pressures were thus predicted of $\sim 10^4$ bars for a UO_2/Na mixture, and $\sim 10^3$ bar for a Sn/H_2O mixture. Such pressures are, of course completely unacceptable from a reactor safety point of view, so that a more detailed examination becomes imperative. If it cannot be assumed that velocity equilibrium exists between the phases at the end of the effective fragmentation zone, the jump balance equations no longer have a unique solution, and the tangency condition in the (zero relative velocity) P–V plane is not applicable. Instead it is necessary to have recourse to the differential equations governing the behavior in the fragmentation zone. This has been done by Hall and Board [3], and independently by Scott and Berthoud [2] and the present authors [4, 5], with generally similar results. However, the details vary, depending upon the assumptions concerning the constitutive equations for fragmentation and mixing.

In the present paper we consider hydrodynamic instability as the fragmentation mechanism. This mechanism is basically independent of boiling characteristics and hence can result in pressures higher than the critical pressure. Fragmentation mechanisms based on boiling can result only in pressures less than the coolant critical pressure. In accordance with the observation of Henry et al. [6] on pressure thresholds for triggering thermal explosions, the boiling fragmentation mechanism is probably cut off long before the full pressure is realized. In finite region this would

imply unsteady behavior, in which a relatively weak pressure wave passes through the mixture, collapsing the vapor blankets, followed by unsteady heat transfer and expansion.

Hydrodynamic fragmentation is induced by the relative velocity between the fuel drops and the coolant. This relative velocity can be fully realized if the shock front is steep and there is a large density ratio between the constituents. Some studies on the propagation of shock waves in a two-phase region [7] show rapid attenuation and dispersion of the shock front, despite complete bubble collapse.

It should also be noted that coarse initial mixing with negligible energy transfer can probably only be achieved if film boiling is the mode of heat transfer between the fuel and the coolant. It is possible to obtain this initial condition with water and common metals, such as tin and aluminum. For UO_2/Na mixtures the interface temperature upon contact is lower than the minimum film boiling temperature, and stable film boiling can occur only if the sodium temperature is close to saturation (providing the pressure remains relatively constant). Even small amounts of subcooling will make the film boiling unstable, and hence it is doubtful whether the initial requirement can be satisfied.

In this paper an equilibrium model for the detonation wave is described. Based on this model the C–J conditions are derived and the behavior of the flow variables in the reaction zone is investigated. A second paper will deal with the application of this model to possible fuel–coolant interactions.

2. DESCRIPTION OF THE VARIOUS INTERACTION ZONES

Let us consider an idealized pressure shock wave, with zero rise time, passing through a fuel–coolant mixture initially at rest in the laboratory frame. The

vapor collapses immediately behind the shock and a relative velocity is induced between the fuel drops and the coolant, thus causing fuel stripping.

Due to drag and momentum exchange caused by mass transfer, the velocities of the unfragmented drops (d) and the fluid around it (f) approach each other in the relaxation zone until an equilibrium velocity is reached (Fig. 1).

The initial unreacted mixture (1) consists of fuel drops and coolant liquid and vapor (not necessarily in temperature equilibrium). Immediately behind the shock, region 2, only unfragmented fuel drops and liquid coolant exist ($\varepsilon_{v_2} = 0$), moving at velocities U_d and U_f, respectively (Fig. 2).

In the general case, the mixture at the velocity–equilibrium plane (3) consists of four components: unfragmented fuel drops (d), fuel debris (db), liquid coolant (c) and coolant vapor (v). The last three are the constituents of the fluid (f) surrounding the drops (Fig. 3).

Owing to the small debris particle size, it is reasonable to assume a uniform fluid temperature, $T_{f_3}^*$. Hence, vapor will exist ($\varepsilon_v > 0$) only if P_3 is less than the coolant critical pressure and T_{f_3} equals or exceeds the saturation coolant temperature $T_{sat}(P_3)$. If T_{f_3} is less than the fuel melting temperature, T_m, then the debris will freeze.

Let E be the fraction of mass stripped; $E = m_s/m_o$, where m_s is the mass stripped from a single drop and m_o is the initial mass of the drop.

The debris volume fraction in the debris–coolant "fluid" is then [4]

$$D = \xi \frac{\rho_d \ \alpha_{d_3}}{\rho_{db} \ \alpha_{f_3}} \tag{1}$$

where

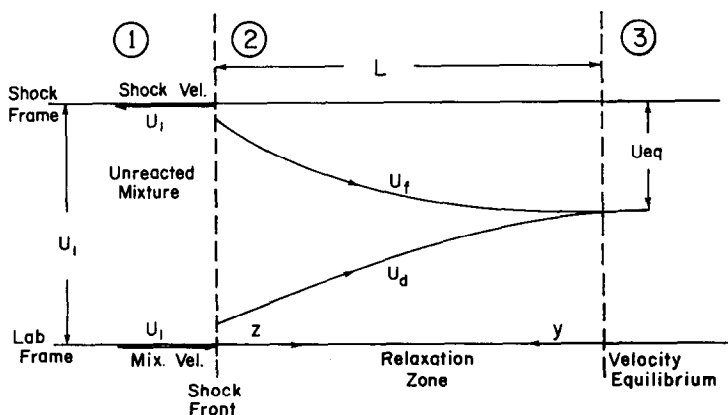$$\xi = \frac{E}{1-E} = \frac{m_s}{m_o - m_s}. \tag{2}$$

FIG. 1. Description of the various interaction zones.

3. BALANCE EQUATIONS

A given set of initial conditions will define the unreacted mixture properties, namely P_1, T_d, T_f, T_{c_1}, α_{d_1}, ϵ_{c_1} which are the pressure, temperature and volume fraction of the different components.

Four balance equations, connecting the initial conditions with conditions at any other plane, must be satisfied:

(A) fuel material balance,
(B) coolant material balance,
(C) overall momentum balance,
(D) overall energy balance.

Eight quantities specify conditions at a given plane: P, T_d, T_f, α_d, ϵ_c, E, U_f and U_d; together with the shock velocity, U_1, this gives 9 unknowns to be determined. T_d should change very little in the relaxation zone in view of the short time scales involved and the limited contact area. Moreover, P, T and ϵ_c are interconnected since if $\epsilon_c > 0$ then $T = T_{sat}(P)$ for $(P < P_{cr})$, and if $\epsilon_c = 0$ then $P > P_{cr}$ or $T < T_{sat}(P)$ for $(P < P_{cr})$. Hence, we have 4 equations and 7 unknowns (or 6 equations with 9 unknowns). Immediately behind the shock front, region 2, the stripping process has just started, i.e. $E = 0^*$; thus two additional conditions must be further determined. If "frozen" momentum transfer can be assumed (possibly for weak shocks), all the unknown quantities can be expressed in terms of a desired parameter. Most commonly this parameter is taken as the pressure, shock velocity (Mach number) or the Bond (or Weber) number.

At the velocity equilibrium plane (3), the velocity of the two phases are equal $(U_d = U_f = U_{eq})$, and again two additional conditions have to be specified. On the other hand, if complete fragmentation is specified at the end of the fragmentation zone, and supercritical pressures exist $(\epsilon_c = 0)$, only 4 unknowns remain $(P, T_f, U_f$ and $U_1)$, which are determined solely by the four jump balances (Section 7).

4. EQUATIONS OF RELAXATION ZONE

To follow the drop break-up behind the shock the differential mass momentum and energy equations are integrated behind the shock in a manner similar to Kriebel [8] and Rudinger [9] for dusty gases. In this case, however, mass is transferred between the drops and the surrounding fluid, and the drop volumetric fraction is not negligible.

The dynamic equations were taken as for a separated 1-dimensional two-phase flow with irreversible mass transfer (exchange factor $\eta = 1$) [10]. The two phases consist of the unfragmented drops and the surrounding fluid, which is a homogeneous mixture of
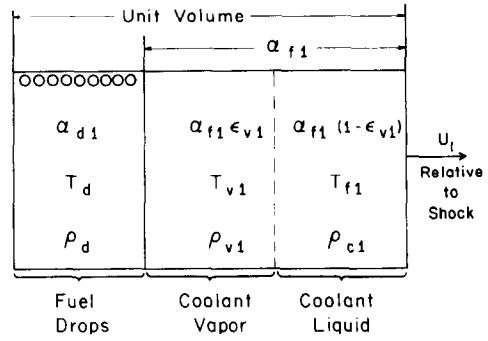
Fig. 2. Schematic description of a unit volume of unreacted mixture.
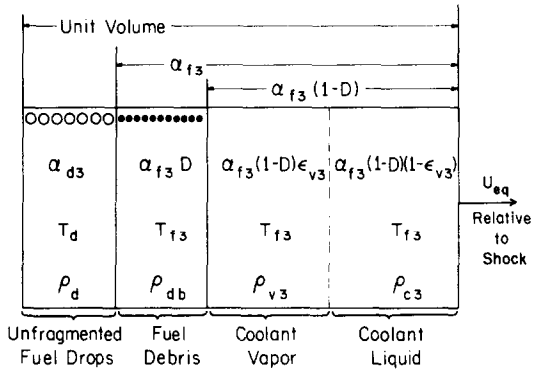

Fig. 3. Schematic description of a unit volume of mixture in the velocity equilibrium region.

coolant liquid and vapor and fuel debris. It is assumed that the debris reaches thermal and velocity equilibrium with the fluid immediately, whence

$$\frac{d}{dz}(\rho_d \alpha_d U_d) = -\Gamma_f, \tag{3}$$

$$\frac{d}{dz}(\rho_f \alpha_f U_f) = \Gamma_f, \tag{4}$$

$$\rho_d U_d \frac{dU_d}{dz} = -\frac{dP}{dz} - \frac{F}{\alpha_d}, \tag{5}$$

$$\rho_f U_f \frac{dU_f}{dz} = -\frac{dP}{dz} + \frac{F}{\alpha_f} + \frac{U_r \Gamma_f}{\alpha_f}, \tag{6}$$

$$\alpha_d \rho_d U_d \frac{d}{dz}(i_d + \tfrac{1}{2} U_d^2) = -\varphi - U_r F, \tag{7}$$

$$\alpha_f \rho_f U_f \frac{d}{dz}(i_f + \tfrac{1}{2} U_f^2)$$

$$= \Gamma_f[\Delta i_d + \tfrac{1}{2}(U_d^2 - U_f^2)] + U_r F + \varphi. \tag{8}$$

The drag force on the fuel drops, assumed to be spheres of uniform radius, at any instant is

$$F = \frac{3}{8} C_D \rho_f \frac{\alpha_d U_r^2}{r_d} \qquad (9)$$

while the drop radius is

$$r_d = \left[\frac{3m_o(1-E)}{4\pi \rho_d} \right]^{1/3} \qquad (10)$$

where m_o is the initial mass, and E, the fraction fragmented, can be considered to be progress parameter.

The density of the fluid mixture, ρ_f, is

$$\rho_f = \rho_{db}D + [\rho_c(1-\varepsilon_v) + \rho_v \varepsilon_v](1-D) \qquad (11)$$

while φ, the direct contact heat transfer rate per unit volume, is

$$\varphi = \frac{3h(T_d - T_f)\alpha_d}{r_d}. \qquad (12)$$

This term is generally negligible, but can be taken into account by taking the Nusselt number, Nu, to be

$$Nu = \frac{2hr_d}{k_f} \sim 4. \qquad (13)$$

Here h is the average heat transfer coefficient and k_f is the average fluid thermal conductivity.

$$k_f \sim x_{c_f} k_c + (1 - x_{c_f}) k_d \qquad (14)$$

where

$$x_{c_f} = \rho_c(1 - \varepsilon_v)(1 - D)/\rho_f. \qquad (15)$$

The mass source function for the fluid is

$$\Gamma_f = u_d n \frac{dm_s}{dz} = \frac{U_d \alpha_d \rho_d}{1 - E} \frac{dE}{dz} \qquad (16)$$

and the stripping rate, dE/dz, must be given independently. If vapor exists in the reaction zone, $T_f = T_{sat}(P)$ and the vapor volumetric fraction will be determined from equation (8).

5. STRIPPING EQUATIONS

Harper, Grube and Chang [11] identified two mechanisms for liquid drop break-up behind a shock wave passing through a gas–liquid mixture:

(A) Taylor instability mechanism for Bond numbers greater than 10^5,

(B) boundary layer stripping for $\sim 10 < Bo < 10^5$.

The Bond number is defined as:

$$Bo = \frac{\rho_d g r_d^2}{\sigma} = \frac{3}{8} C_D We = \frac{3}{8} C_D \frac{\rho_f r_d U_r^2}{\sigma} \qquad (17)$$

where g is the drop acceleration. Although the theory is derived for a fluid of negligible density surrounding the drop, the derivation can be applied approximately to a single drop immersed in a lighter liquid, with the substitution $Bo = (\rho_d - \rho_f) g r_d^2 / \sigma_{fd}$.

Taylor instability is the faster mode, with break-up time, t_b, given by Simpkins and Bales [12] based on their air–water data as:

$$T_b = \frac{t_b U_r}{2r_d} \left(\frac{\rho_f}{\rho_d} \right)^{1/2} \sim 22 \, Bo^{-1/4} \qquad (18)$$

where the reference quantities are evaluated immediately behind the shock. Two studies have been conducted to date on shock-induced drop fragmentation in liquid–liquid systems, both in an isothermal mercury drop–water configuration. Baines et al. [13] subjected mercury drops, initially on the bottom of a horizontal tube, to suddenly applied water flows of 4–17 m/s (Weber numbers of 100–2000). Complete fragmentation was observed, predominantly by boundary-layer stripping, with $T_b = 3$–5, in agreement with the air–water observations.

On the other hand, Patel and Theofanous [14, 15] subjected mercury drops to much stronger shocks ($P_{max} \sim 300$ bars; $We_{max} \sim 2.10^4$) and observed a quite different mode of break-up, which they attributed to Taylor instability, with dimensionless break-up times an order of magnitude smaller ($T_b \sim 0.4$). The reasons for this discrepancy are not at present clear. We consider at this time the case when boundary-layer stripping is the predominant mode. Taylor instability will be considered in a second paper.

Other studies of droplet fragmentation in air shocks [16–19] are in general agreement with $T_b = 3$–5. However, for a single water drop subjected to an air shock, as in these experiments, the relative velocity changes very little during the fragmentation process, since the air velocity is unchanged by the break-up, and the drop velocity is always small compared to the air velocity. Hence the relative displacement at break-up, $z_{rb} \approx U_{ro} t_b$, where U_{ro} is the relative velocity immediately behind the shock. One can therefore write equation (30) in the form

$$T_b = \frac{z_{rb}}{2r_d} \left(\frac{\rho_f}{\rho_d} \right)^{1/2}. \qquad (19)$$

In dispersed liquid–liquid systems, however, the relative velocity falls rapidly behind the shock. Since t_b is a Lagrangian time variable following a single drop to its destruction, the relative displacement between the drop and the surrounding fluid mixture at the end of the fragmentation zone is given by

$$z_{rb} = \int_0^{t_b} U_r(\tau) \, d\tau. \qquad (20)$$

We shall use equation (19), rather than the initial relative velocity, in extending the air–water results to dispersed liquid–liquid systems, since this approximates the integrated effect of the relative velocity, even after the local Bond number falls below the theoretical cut-off value of $\sim 10^5$. This modification is therefore probably conservative, but the need for additional liquid–liquid data in densely dispersed systems is clearly evident.

Based on air–water data, the stripping rate can be calculated by two different correlations:

(A) *Ranger and Nichols* [16] (R–N) equation

$$\frac{dm_s}{dt} = m_o U_d \frac{dE}{dz} = (12\pi^3)^{1/2} \left(\frac{\rho_f}{\rho_d}\right)^{1/3}$$

$$\times \left(\frac{v_d}{v_f}\right)^{1/6} \rho_d v_d^{1/2} U_r r_d^{3/2} \quad (21)$$

where v denotes kinematic viscosity. This correlation usually underestimates the stripping rate.

(B) *Reinecke and Waldman* [17] *(R–W) equation*

$$E = \frac{1}{2}\left[1 - \cos\left(\frac{\pi t}{t_b}\right)\right]. \quad (22)$$

We now define a dimensionless time taking into account variations in relative velocity by

$$T = \frac{z_r}{2r_{d_o}} \left(\frac{\rho_f}{\rho_d}\right)^{1/2}. \quad (23)$$

Since the relative velocity decreases monotonically with time, it follows that

$$\frac{t}{t_b} \leq \frac{z_r}{z_{rb}} = \frac{T}{T_b}. \quad (24)$$

Substituting this inequality into equation (22) one gets an upper bound to the stripping:

$$E \leq \frac{1}{2}\left[1 - \cos\left(\frac{\pi T}{T_b}\right)\right] = \frac{1}{2}$$

$$\times \left\{1 - \cos\left[\frac{\pi z_r}{2r_{d_o} T_b}\left(\frac{\rho_f}{\rho_d}\right)^{1/2}\right]\right\}. \quad (25)$$

The relative displacement, z_r, can be found from:

$$\frac{dz_r}{dz} = \frac{U_r}{U_d}. \quad (26)$$

Hence, the stripping rate can be overestimated by:

$$\frac{dE}{dz} = \frac{\pi}{4r_{d_0} T_b \rho_d^{1/2}} \sin\left[\frac{\pi z_r}{2r_{d_o} T_b}\left(\frac{\rho_f}{\rho_d}\right)^{1/2}\right]$$

$$\times \left(\rho_f^{1/2} \frac{U_r}{U_d} + \frac{z_r}{2\rho_f^{1/2}} \frac{d\rho_f}{dz}\right). \quad (27)$$

If one assumes that z_{rb} is a constant, rather than T_b, then the second term in the round brackets disappears. From now on we shall assume that this term is zero, since otherwise continuing fragmentation is predicted at zero relative velocity.

Finally, in order to interpret single-drop fragmentation data, it is necessary to take into account the difference in the relative velocity behavior behind the shock front for a dense dispersion of drops in surrounding fluid. For a dense dispersion, the relative velocity decreases rapidly behind the shock, with a time constant that depends upon the effective drag coefficient. Denoting T_{bo} as the dimensionless break-up time based on the initial relative velocity, for these data a rough estimate might be

$$T_b \sim \frac{2}{3} T_{bo}. \quad (28)$$

We turn now to a consideration of the Chapman–Jouguet conditions for a steady plane thermal detonation.

6. EXTENDED CHAPMAN–JOUGUET CONDITIONS FOR A THERMAL DETONATION WAVE

6.1. *Preliminary consideration*

Chapman–Jouguet conditions for single-phase combustion detonations have been extensively treated [20–22], although little is known about the stability of the detonation with competing chemical reactions, some of which do not proceed to equilibrium at the end of the steady-state reaction zone. The extension to multiphase thermal detonations is considerably more complex, and has only recently been attacked by Hall and Board [3], and independently by Sharon and Bankoff [5] and by Scott and Berthoud [2]. The treatment given below follows our earlier development, but presents several generalizations.

In general, the total number of conservation equations for mass, momentum and energy in the fragmentation zone behind the shock front will be $3n$, where n is the number of distinct phases or pseudo-phases. We define a pseudo-phase as a mixture of two or more phases on a scale sufficiently fine that local velocity and thermal equilibrium is preserved for all perturbation frequencies of interest relative to the characteristic time scales of the fragmentation zone. According to this definition, tin debris particles $100 \, \mu m$ in diameter mixing uniformly with water, or UO_2 particles $10 \, \mu m$ in diameter mixing with sodium, both in absence of vapor, would serve as examples of pseudo-phases. For the equations (3)–(8) given earlier, $n = 2$, and this will be the thrust of the following discussion. However, if the fragmented UO_2 debris is much larger, thermal equilibrium may require a longer time than velocity equilibrium between the fragmented fuel drops and the surrounding coolant mixture, as noted by Hall and Board [3]. In this case $n = 3$. If, in addition, vapor is present at the end of the fragmentation zone, $n = 4$. The complete set of equations for $n = 3$ or 4 has not been treated, in view of the lack of experimental information, and approximate methods, using six or even fewer equations, are at present necessary. Nevertheless, an important distinction can be drawn between the cases for $n \geq 2$. If the pressure at the C–J plane, which terminates the reaction zone, is below the coolant critical pressure, vapor can exist at that point, and $n > 2$. On the other hand, if the shock pressure is well above the critical pressure, vapor will not be present behind the shock, and $n < 4$, and for finely-dispersed debris, $n = 2$, throughout the fragmentation zone. Furthermore, if fragmentation is complete at the C–J plane, $n = 1$ and homogeneous flow is achieved, as postulated in [1].

In general, the steady-state 1-dimensional conservation equations can be written in vector-matrix form as

$$A \frac{dX}{dz} = b; \quad X = (X_i), \quad i = 1, \ldots N \quad (29)$$

where $\mathbf{X}$ is a vector of flow variables, $\mathbf{b}$ is a source-term vector, and $N \leq 3n$, since some of the flow variables may be redundant due to algebraic constitutive relationships.

In order for the C–J plane to join the time-independent reaction zone and time-dependent supersonic expansion zone, $d\mathbf{X}/dz$ must be indeterminate, which implies that

$$\det \mathbf{A} = 0, \tag{30}$$

$$\det \mathbf{B}_j = 0, \quad j = 1, \dots N \tag{31}$$

where $\mathbf{B}_j$ is obtained by replacing the jth column of $\mathbf{A}$ with $\mathbf{b}$. Equation (30) is the sonic velocity condition, while equation (31) is automatically satisfied if $\mathbf{b} = 0$ (all source terms vanish at the C–J plane, implying complete equilibrium).

More information can be obtained from the characteristic velocities of the unsteady conservation equations:

$$\mathbf{C}\frac{\partial \mathbf{X}}{\partial t} + \mathbf{A}\frac{\partial \mathbf{X}}{\partial z} = \mathbf{b}. \tag{32}$$

To protect the shock from rarefaction waves progressing from the far-field boundary conditions of the form $\delta\mathbf{b}\exp\left[i\left(\omega t + kz\right)\right]$, where $\lambda = \omega/k$ may be complex, it is sufficient that

$$\mathrm{Re}\,\lambda_1 \geq \mathrm{Re}\,\lambda_2 \geq \dots \geq \mathrm{Re}\,\lambda_{N-1} \geq \lambda_N = 0 \tag{33}$$

where characteristic velocities $\lambda_i, i = 1, \dots N$ are the roots of

$$\det\left(\lambda\mathbf{C} + \mathbf{A}\right) = 0. \tag{34}$$

In view of equation (33), this reduces to equation (30). Physically, this implies that the C–J mixture velocity is equal to the largest sonic velocity relative to the shock front, but in fact the flow becomes choked when the smallest sonic velocity relative to the shock is achieved. It is doubtful, therefore, whether a truly steady thermal detonation can be attained. On the other hand, Wood and Kirkwood [23] have suggested that the higher perturbation velocities, which correspond to higher frequencies, are rapidly attenuated due to friction. The possibility of quasi-steady (slowly-varying) thermal detonations is discussed in the next section.

6.2. Equilibrium vs non-equilibrium C–J planes

We see that equation (31) is satisfied if complete equilibrium exists at the C–J plane, implying that Γ_f, F, and φ, the interphase mass, momentum and heat transfer terms, vanish. As noted by Scott and Berthoud [2], equilibrium also implies that the entropy gradient vanishes. This state tends to be relatively stable, since small perturbations from equilibrium tend to be damped out by friction and/or heat transfer. We call these normal C–J solutions. A simplification is possible by noting that φ is generally small, and, in the

absence of vapor, has a negligible effect on the droplet and fluid mixture densities. Hence, to a good degree of approximation, it is sufficient that Γ_f and F vanish at the C–J plane. This is achieved when $U_r = 0$. This quasi-equilibrium condition will be called the zero-slip C–J condition, and applies strictly for supercritical pressures. Zero-slip is approached at constant C_D only asymptotically, so that there appears to be some arbitrariness concerning the degree of approximation to zero-slip at the C–J plane that is required with a given set of initial conditions and geometry for a near-stationary solution. This in turn determines the effective reaction zone length, and hence the vulnerability to sideward expansion. In fact, however, this arbitrariness is computational rather than physical. When the Reynolds number $Re = 2r_d\rho_f U_r/\mu_f < 1$, Stokes flow exists ($C_D = 24/Re$). One finds, however, that for $Re = 1$, and the radius of the remaining drops $r_d = 0.1$ cm in water, $U_r/U_{ro} \sim 5 \times 10^{-6}$. Hence one finds that the true equilibrium reaction zone is of the order of 10^2–10^4 m.

Such steady reaction zone lengths can only be achieved in geophysical applications, such as lava–water interactions, or in astrophysical detonations. From a practical point of view, it is therefore necessary to consider alternative definitions of the reaction zone length, such as the distance behind the shock where fragmentation effectively ceases. We call such detonations quasi-steady, on the assumption that the reaction zone will be slowly varying in time compared to the time for propagation of the shock through a characteristic length. The satisfaction of this condition can only be checked by recourse to the unsteady equations.

It is also possible for equations (31, 32) to be satisfied under non-equilibrium conditions [3] for particular combinations of the flow variables. For supercritical pressures, these isolated solutions will be called singular C–J planes. Stability to small perturbations cannot be established, and indeed there seems to be no obvious restoring force from a physical point of view.

A quite different picture is presented at subcritical pressures, where fragmentation may be considerably aided by violent boiling, as noted previously [24]. Hall and Board [3] have presented a vapor-detonation model, in which the coolant may be below the local saturation temperature, so that a portion of the heat transferred from the fuel increases the liquid enthalpy, and the remainder produces additional vapor. This is also a singular solution, but may be stable, since a small decrease in vapor blanket thickness around the fuel drops increases the heat transfer, which tends to restore the vapor film. In fact, quasi-steady thermal detonation waves have been observed in metal–water stratified mixtures, [25, 26] qualitatively agreeing with the model.

Our present concern, however, is with the equilibrium coolant–debris mixture model, which is particularly applicable in examining possible supercritical thermal detonations.

6.3. One-dimensional homogeneous coolant–debris mixture C–J condition

In view of equation (31) all components of dX/dz become indeterminate at the same plane, so that it is sufficient to consider only the pressure gradient.

Equations (3)–(6) are the continuity and momentum equations of the fuel droplets and the surrounding mixture. These equations can be re-arranged in the form:

$$\left(\frac{\alpha_d}{\rho_d U_d^2} + \frac{\alpha_f}{\rho_f U_f^2}\right)\frac{dP}{dz} = \left(\frac{U_d}{\rho_f U_f^2} - \frac{2}{\rho_f U_f} + \frac{1}{\rho_d U_d}\right)\Gamma_f$$
$$+ \left(\frac{1}{\rho_f U_f^2} - \frac{1}{\rho_d U_d^2}\right)F + \frac{\alpha_f}{\rho_f}\frac{d\rho_f}{dz} + \frac{\alpha_d}{\rho_d}\frac{d\rho_d}{dz}. \quad (34)$$

The droplet phase has the equation of state $\rho_d = \rho(P, S_d)$, so that

$$d\rho_d = C_d^{-2}\,dP - \frac{T_d\beta_d\rho_d}{C_{p_d}}\,dS_d \quad (35)$$

where β_d is the thermal expansion coefficient of the fuel. By assumption, the fluid phase is a homogeneous mixture of coolant and fuel debris, and its equation of state is $\rho_f = \rho_f(P, S_f, x_{db})$, where x_{db} is the debris quality (weight fraction) in the fluid. Since dx_{db} depends only on the mass transfer, dE, for constant pressure and entropy the fluid equation of state is of the form

$$d\rho_d = C_f^{-2}\,dP - \frac{T_f\beta_f\rho_f}{C_{p_f}}\,dS_f + \kappa_f\,dE \quad (36)$$

where κ_f is obtained from equations (1) and (2). Upon substituting (35) and (36) into (34), one obtains

$$\left[\frac{\alpha_d}{\rho_d U_d^2}(1 - M_d^2) + \frac{\alpha_f}{\rho_f U_f^2}(1 - M_f^2)\right]$$
$$\times \frac{dP}{dz} = \left(\frac{U_d}{\rho_f U_f^2} - \frac{2}{\rho_f U_f} + \frac{1}{\rho_d U_d}\right.$$
$$\left. + \frac{\alpha_f\kappa_f}{\rho_f}\right)\Gamma_f + \left(\frac{1}{\rho_f U_f^2} - \frac{1}{\rho_d U_d^2}\right)F$$
$$- \frac{\alpha_f T_f\beta_f}{C_{p_f}}\frac{dS_f}{dz} - \frac{\alpha_d T_d S_d}{C_{p_d}}\frac{dS_d}{dz} \quad (37)$$

where M is the Mach number (U/C) and

$$\kappa_f = \frac{\rho_{db} - \rho_c}{\alpha_f\rho_{db}U_d(1 - E)}. \quad (38)$$

Substituting equations (7) and (8) into equation (37), and using the thermodynamic relation: $T\,dS = di - dP/\rho$, one gets:

$$\frac{dP}{dz} = \frac{K_fF + K_r\Gamma_f + K_\varphi\varphi}{\dfrac{\alpha_d}{\rho_d U_d^2}(1 - M_d^2) + \dfrac{\alpha_f}{\rho_f U_f^2}(1 - M_f^2)} \equiv \frac{G}{\Phi} \quad (39)$$

where

$$K_f = \frac{1}{\rho_f U_f^2} - \frac{1}{\rho_d U_d^2} - \frac{\beta_d U_d}{\rho_f^2 C_{p_f} U_f} - \frac{\beta_d U_f}{\rho_d^2 C_{p_d} U_d}, \quad (40)$$

$$K_r = \frac{U_d}{\rho_f U_f^2} - \frac{2}{\rho_f U_f} + \frac{1}{\rho_d U_d} + \frac{\alpha_f\kappa_f}{\rho_f}$$
$$- \frac{\beta_f}{\rho_f^2 C_{p_f} U_f}(\Delta i_d + \tfrac{1}{2} U_r^2) \quad (41)$$

and

$$K_\varphi = \frac{\beta_d}{\rho_d^2 C_{p_d} U_d} - \frac{\beta_f}{\rho_f C_{p_f} U_f} \quad (42)$$

where Γ_f is obtained from equations (16) and (27). We note that if the term in parentheses containing $d\rho_f/dz$ in equation (27) is not set equal to zero, then there will be additional terms in the denominator Φ of equation (39) arising from the state equation (36). As noted above, we set this term to zero on physical grounds, so that $\Gamma_f \to 0$ as $U_r \to 0$. This implies, however, if other fragmentation mechanisms than those due to relative velocity are operative, the choking condition will be different. In the present case, by setting $\Phi = 0$, one obtains the stratified-flow sonic velocity condition [2, 3, 4, 6]:

$$\frac{\alpha_{d_3}}{\rho_d}\left(1 - \frac{U_{eq}^2}{C_d^2}\right) + \frac{\alpha_{f_3}}{\rho_{f_3}}\left(1 - \frac{U_{eq}^2}{C_f^2}\right) = 0 \quad (43)$$

or

$$C_{m_3} = U_{eq} = C_d C_f\left(\frac{\alpha_{d_3}\rho_{f_3} + \rho_d\alpha_{f_3}}{\alpha_{d_3}\rho_{f_3}C_f^2 + \alpha_{f_3}\rho_d C_d^2}\right)^{1/2} \quad (44)$$

where C_f is the speed of sound in the homogeneous (coolant–debris) fluid mixture [6]:

$$C_f^{-2} = \rho_{f_3}\left[\frac{D}{\rho_{db}C_{db}^2} + \frac{(1 - D)\varepsilon_v}{\rho_{v_3}C_{v_3}^2} + \frac{(1 - D)(1 - \varepsilon_v)}{\rho_{c_3}C_{c_3}^2}\right]. \quad (45)$$

However, if fragmentation can occur by mechanisms other than those associated with the relative velocity, additional flashing terms can appear in equation (39), and consequently U_{eq} would be somewhat higher. We note that the sonic velocity calculated by equation (44) is higher than the homogeneous speed of sound in the mixture. Hence the C–J condition must involve the separated-flow speed of sound in order to prevent higher frequency waves from weakening the shock.

7. DETONATION HUGONIOTS AND ZERO-SLIP C–J CONDITIONS

The velocity equilibrium plane, region (3), may be a C–J plane. As discussed above, the pressure at that plane can be specified as a function of two variables: $P_3 = P_3(\bar{v}_3, E)$ where $\bar{v}_3 = 1/\bar{\rho}_3$, and the fragmentation extent, E. The resulting curves in a $(P, \bar{v})$ plot, where E is the parameter, have been termed [4] the partial detonation Hugoniots.

The 4 balance equations are:

$$\alpha_{d_1} U_1 = (1 + \xi)\alpha_{d_3} U_{eq}, \tag{46}$$

$$\alpha_{f_1} \rho_{f_1} U_1 = \rho_{fc_3}\left[1 - \left(1 + \xi\frac{\rho_d}{\rho_{db}}\right)\alpha_{d_3}\right]U_{eq}, \tag{47}$$

$$P_3 - P_1 = \bar{\rho}_1 U_1 (U_1 - U_{eq}), \tag{48}$$

$$E\rho_d \Delta i_d + \frac{\bar{\rho}_1}{2\alpha_{d_1}}(U_1^2 - U_{eq}) = \rho_{f_1}\frac{\alpha_{f_1}}{\alpha_{d_1}}\Delta i_f + \frac{3E\sigma}{r_{db}}. \tag{49}$$

If the fragmentation is completed, $E = 1$, then the two flux balances become:

$$\alpha_{d_1} \rho_d U_1 = D\rho_{db} U_{eq}, \tag{50}$$

$$\alpha_{f_1} \rho_{f_3} U_1 = (1 - D)\rho_{f_3} U_{eq}. \tag{51}$$

If direct contact heat transfer between the phases is negligible, the C–J plane can be determined for every value of E from equations (44) and (45) for the equilibrium sonic velocity, together with equations (46)–(49). If the two phases at the velocity equilibrium plane are considered to be homogeneous, one can find the C–J conditions graphically by drawing a tangent from the initial point $(P_1, \bar{v}_1)$ to the detonation Hugoniot [20]. This method can be used for cases where $E \to 1$. For $E \ll 1$, the two phases are still separated, although there exists no slip between them. The speed of sound is then different from the homogeneous speed of sound, calculated from the slope of the tangent to the Hugoniot.

8. BEHAVIOR IN THE RELAXATION ZONE

8.1. The pressure profile

Referring now to equation (39), when φ is negligible the pressure gradient is given by:

$$\frac{dP}{dz} = \frac{K_f F + K_\Gamma \Gamma_f}{\dfrac{\alpha_d}{\rho_d U_d^2}(1 - M_d^2) + \dfrac{\alpha_f}{\rho_f U_f^2}(1 - M_f^2)}. \tag{52}$$

The denominator is always positive inside the reaction zone, which is characterized by subsonic flow relative to the shock. Hence the sign of the pressure gradient is determined by the numerator.

K_f is always positive $(\rho_d U_d^2 > \rho_f U_f^2$ and β is small), while K_Γ turns out to be negative for all cases investigated. Hence large drag forces will increase the pressures while large fragmentation rates will reduce it.

According to the R–W equation, Γ_f is proportional to the relative displacement, z_r. Since $z_r \to 0$ close to the shock front $(z \to 0)$, dP/dz will always be positive immediately behind the shock. As the relative velocity approaches zero, the pressure gradient approaches zero as well, unless sonic velocity is also being reached. The stripping rate may be large enough a short distance behind the shock to make the mass transfer term equal to or greater than the drag term, so that the pressure profile exhibits a maximum. We note that different behavior is predicted by the R–W equation, since here Γ_f attains a maximum at the shock front.

8.2. The velocity profiles

Since $dP/dz > 0$ immediately behind the shock front, equation (17) requires that $dU_d/dz < 0$ as $z \to 0$. When $U_r \to 0$, F and dP/dz both approach zero, hence the drop velocity should level off near the velocity equilibrium. Away from the shock front, it is possible for the drops to accelerate relative to the shock.

It is more difficult to predict the fluid velocity behavior. Immediately behind the shock it is possible for the fluid to decelerate relative to the shock, as predicted by Kriebel [8]. Away from the shock where dP/dz is small or negative, one might expect the fluid to accelerate until equilibrium velocity is reached.

8.3. Some qualitative results

Taking the shock front thickness to be that of the region where vapor film collapse occurs, momentum transfer between the fuel drops and the coolant liquid may be non-negligible, in view of the large change in void fraction. Hence it is generally necessary to integrate backwards from the assumed C–J plane to the shock to determine whether a consistent set of assumptions, corresponding to a possible steady detonation, has been made. Calculations of this sort will be presented in a second paper, but here we perform some forward integrations to demonstrate some qualitative features of the problem. For this it is necessary to neglect momentum transfer within the shock zone, which then allows separate mass and momentum jump balances across the shock. For a given undisturbed fuel–coolant mixture ahead of the shock, one can choose a value of the Weber number behind the shock (or equivalently, the shock velocity). The shock jump balances are:

$$[\alpha_i \rho_i U_i] = 0, \quad i = d, f, \tag{53}$$

$$[\alpha_i (P + \rho_i U_i^2)] = 0. \tag{54}$$

The energy equation has been omitted, since the density change due to vapor collapse dominates. Using the conditions immediately behind the shock (region 2) as initial conditions, the equations of the reaction zone are integrated forwards until the equilibrium velocity is reached (region 3). This satisfies the sonic C–J condition for a steady detonation. However useful qualitative information can be readily obtained.

Calculations of this sort were carried out with Sn/H_2O mixtures with equal volumes of tin, water and steam in the unreacted mixture. The following parameters were chosen: $C_D = 2$ and 10; initial drop diameter $= 1$, 3 and 5 cm; and the R–W stripping equation (34). Sample results are shown in Figs. (4)–(7). More details are given elsewhere [4]. It is found that the flow variables change rapidly in a relatively thin region behind the shock. This active region is followed by a long tail, where changes are slow. The effective reaction zone length, L_e can be defined as the distance from the shock front to the plane where $E = (1 - e^{-1})$ E_{final}. This length is about 20% of the length at which the relative velocity is nearly zero say, $(U_r/U_{ro} = $
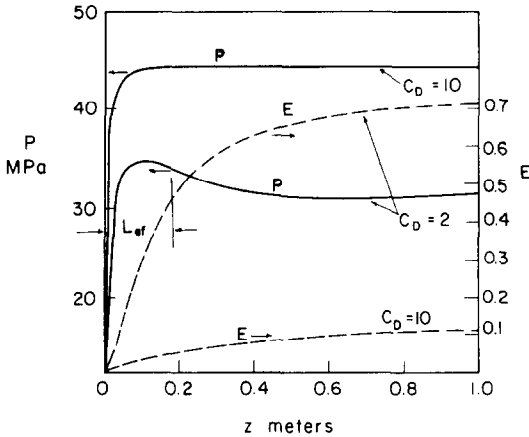
FIG. 4. The effect of C_D on the pressure and fragmentation profiles. $T_b = 3$; $\alpha_{d_1} = 1/3$; $v_{v_1} = 0.5$; $We = 10^5$. Sn/H$_2$O.
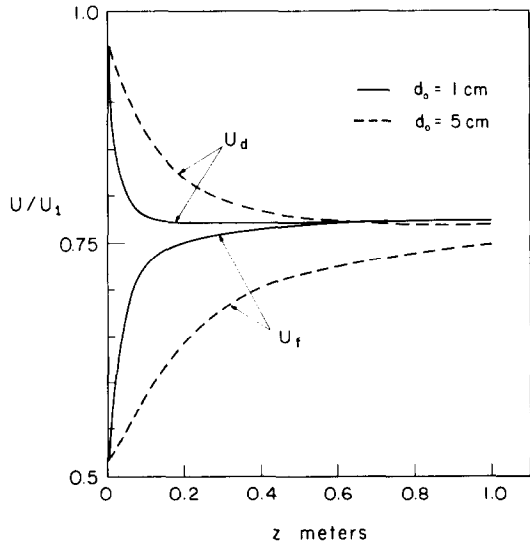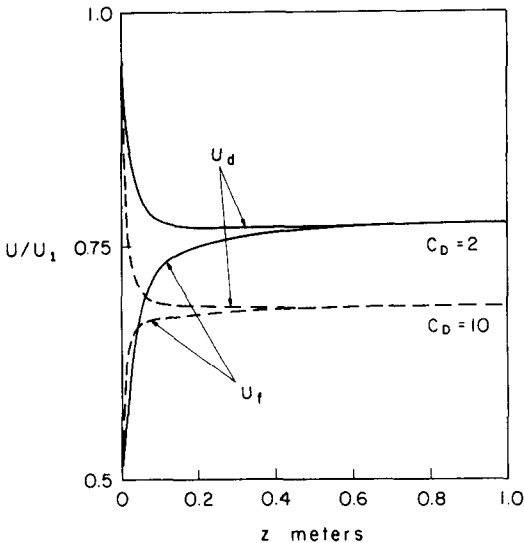

FIG. 5. The effect of C_D on the velocity profile. (Conditions as for Fig. 4.)

FIG. 6. The effect of drop diameter on the pressure profile. (Conditions as for Fig. 4.)
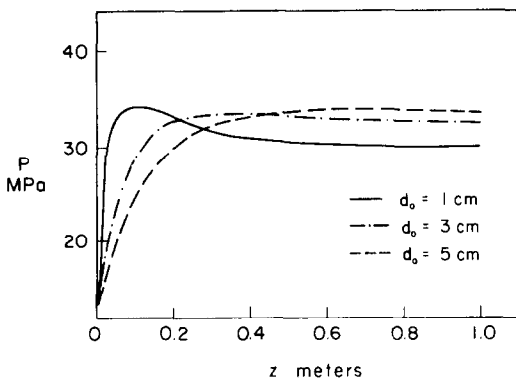

FIG. 7. The effect of drop diameter on the velocity profile. (Conditions as for Fig. 4.)

0.005), and one or two orders of magnitude smaller than the zero-slip length, calculated with Stokes drag when $Re < 1$.

From these calculations the following observations can be made:

(1) Significant fragmentation is predicted with $C_D = 2$ and $T_b = 3$. However, it is difficult to achieve sonic conditions ($M_3 = 1$) and reasonable reaction lengths ($L_e < 0.1$ m) in this case.

(2) Larger values of C_D, still with $T_b = 3$, reduce the predicted reaction length and increase the final pressure. However, the stripping rate becomes negligibly small and the equilibrium velocity is decreased.

(3) For large drops there is less stripping and the reaction zone length is larger. Hence fine initial mixing is important.

(4) High fragmentation rates tend to decrease the final pressure, increase the final velocity and decrease the reaction length. Hence, small break-up times favor the possibility of a quasi-steady detonation wave passing through the fuel–coolant mixture.

9. CONCLUDING DISCUSSION

We have concerned ourselves here with strongly supercritical steady detonations, proposed by Board and Hall, for which fragmentation by local boiling is excluded, and only hydrodynamic mechanisms, such as boundary-layer stripping and/or Taylor instability, need be considered. Pressures of this sort have not been observed experimentally.

An examination of the indeterminacy condition for a protected shock shows that the dependent variables may assume isolated values at the end of the fragmentation zone which make the pressure gradient indeterminate. However, in contrast to the subcritical pressure case, where an increase in void fraction leads

to a reduction in heat transfer, and hence to a decrease in void fraction, there is no obvious feedback mechanism to return the perturbed system to the isolated singularities. Hence it is suggested that they are unstable to small perturbations, and that truly steady supercritical detonations are achieved only when the fragmentation zone is terminated by an equilibrium Chapman–Jouguet plane (zero velocity and temperature difference between fuel and coolant). A similar conclusion has been stated by Scott and Berthoud. This is not impossible of achievement, since the drag coefficient depends upon the Reynolds number, so that velocity equilibrium may occur within a finite distance. On the other hand, the required reaction zone lengths are quite unrealistic, as suggested by approximate calculations using $T_b = 3$. This is not to say, however, that *slowly-varying* detonations are unfeasible. To examine this possibility a numerical solution of the unsteady conservation equations, using singular perturbation methods, is required. Furthermore, if $T_b \sim 0.4$, as reported by Patel and Theofanous, even the steady detonation cannot be dismissed from consideration.

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SUR L'EXISTENCE DE DETONATIONS THERMIQUES PLANES, SUPERCRITIQUES ET STATIONNAIRES

Résumé—On considère les conditions d'existence de détonations fortement supercritiques et stationnaires proposées par Board et Hall. On exclue la fragmentation par ébullition locale et seuls les mécanismes hydrodynamiques, comme le stripping de la couche-limite et ou l'instabilité de Taylor, peuvent être actifs. Des détonations supercritiques stationnaires sont réalisées lorsque la zone de fragmentation est terminée par un équilibre plan de Chapman–Jouguet (vitesse nulle et différence de température nulle entre le carburant et le réfrigérant). De fortes contraintes sont aussi nécessaires.

A. SHARON and S. G. BANKOFF

ÜBER DIE EXISTENZ STATIONÄRER ÜBERKRITISCHER EBENER THERMISCHER DETONATIONEN

Zusammenfassung—Es werden die von Board und Hall vorgeschlagenen Bedingungen für die Existenz überkritischer stationärer Detonationen behandelt. Fragmentation durch örtliches Sieden wird ausgeschlossen, und nur hydrodynamische Mechanismen wie zum Beispiel Grenzschichtablösung und/oder Taylor-Instabilität sollen wirksam sein. Wirkliche stationäre überkritische Detonationen können nur dann erzieltwerden, wenn die Fragmentationszone durch eine Chapman–Jouguet Gleichgewichts-Ebene (Geschwindigkeit gleich null und Temperaturunterschied zwischen Treibstoff und Kühlmedium) abgeschlossen wird. Starke, seitliche Zwangsbedingungen sind ebenfalls notwendig.

О СУЩЕСТВОВАНИИ СТАЦИОНАРНЫХ СВЕРХКРИТИЧЕСКИХ ПЛОСКИХ ТЕПЛОВЫХ ДЕФОРМАЦИЙ

Аннотация — Рассматриваются описанные Бордом и Холлом условия существования сверхкритических стационарных детонаций. Диспергирование под влиянием локального кипения не учитывается и предполагается, что имеют место только расслоение пограничного слоя и тэйлоровская неустойчивость. Стационарная сверхкритическая детонация достигается только в том случае, когда зона диспергирования ограничена равновесной плоскостью Чепмана Жюге (нулевая скорость и разность температур топлива и теплоносителя). Необходимы также жесткие боковые ограничители.