Theory of detonation with an embedded sonic locus

by

D. Scott Stewart Aslan R. Kasimov

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Abstract

We address the problem of generalizing sonic conditions to a three-dimensional unsteady self-sustained detonation wave. The conditions are shown to be the characteristic compatibility conditions on the exceptional surface of the governing hyperbolic system of reactive Euler equations. Two equations are derived that are necessary to determine the motion of both the lead shock and the sonic surface. Detonation with an embedded sonic locus is thus treated as a two-front phenomenon: a reaction zone whose domain of influence is bounded by two surfaces, the lead shock surface and the trailing characteristic surface. The geometry of the two surfaces plays an important role in the underlying dynamics. We also discuss how the sonic conditions of detonation stability theory and detonation shock dynamics can be obtained as special cases of the general sonic conditions.

1 Introduction

A detonation wave is a shock wave that triggers exothermic reactions in an explosive as it propagates so that the energy released in the reactions sustains the shock propagation. Modern theories of detonation originate from the theory first developed independently by Zel'dovich, von Neumann, and Döring in the 1940s (ZND theory, see Fickett and Davis [4] for details) that describes the dynamics of a steady one-dimensional planar detonation in gaseous explosive. The ZND theory is applicable to both self-sustained detonations, that is autonomous waves whose motion is sustained entirely by the energy released in their reaction zone, and overdriven detonations which require an additional external support to maintain their motion at a nominal speed. In self-sustained steady onedimensional planar detonations, which are also called Chapman-Jouguet (CJ) detonations, there exists an embedded sonic locus within or at the end of the reaction zone, such that at that point the flow speed is sonic relative to the shock. In contrast, the lead-shock dynamics of overdriven detonations is influenced by the entire region between the shock and the support (e.g. a piston); no sonic locus exists in such detonations. Without the condition of sonicity, the equations governing the CJ detonation (the mass, momentum, and energy equations) are not closed, since the detonation speed is unknown; the sonicity condition provides the necessary closure. Understanding the nature of the sonic conditions in detonations more general than planar, one-dimensional, steady detonations of the ZND theory, has been very difficult to achieve. It is precisely this task of deriving the general sonic conditions and clarifying their nature that is central to our present investigation.

Research that began in the late 1950s and early 1960s (see, e.g. [4, 2]) has shown that most detonation waves, especially in gases, have a multidimensional cellular structure with transversely propagating shock waves in the reaction zone, and significant unsteady dynamics. In condensed explosives, the detonation is more often observed to be steady, but importantly it has been known for a long time that high-explosive detonation shocks are almost always curved. Clearly, the ZND theory is too simple to account for the observed structure and must be appropriately modified. There exist conceptual problems that cannot be addressed within the framework of the ZND theory if unsteady and multi-dimensional detonations are considered. The principal problem has to do with

^{*}Department of Theoretical and Applied Mechanics, University of Illinois, Urbana-Champaign, Urbana, IL 61801, USA dss@uiuc.edu

[†]Department of Theoretical and Applied Mechanics, University of Illinois, Urbana-Champaign, Urbana, IL 61801, USA kasimov@uiuc.edu

the nature of the sonic condition whose generalization to include unsteady and multi-dimensional effects has been limited so far to linearized problems and quasi-steady detonations.

In the linear stability theory of detonation, the far-field conditions are commonly referred to as "radiation conditions" or "boundedness conditions" depending on specific circumstances such as whether CJ or overdriven detonation is considered (see [3, 6, 8, 12]). The radiation condition is imposed to filter out incoming acoustic perturbations by considering the far-field acoustic solutions of the governing linearized system and to eliminate the incoming waves by setting their amplitude equal to zero. It follows then, that the far-field solutions are linearly dependent and their linear combination forms a far-field constraint on the general solution of the linearized problem. Such a constraint serves as a dispersion relation that allows one to determine the eigenvalues. It turns out (see Section 5 below) that the CJ limit (self-sustained wave) of the radiation condition coincides with the linearized governing equation on the forward characteristic. One can also show that the radiation condition in that case is also a boundedness condition for the solutions of the linearized system at the sonic locus. Thus in the linear stability problem, the general nature of the radiation conditions that provide the dispersion relation is such that they serve as filters of the incoming perturbations and are thus conditions on the forward characteristic surface that acts as an information boundary.

In the theory of Detonation Shock Dynamics (DSD, see Stewart [13] for a general discussion), one treats a quasi-steady *curved* detonation and derives sonic conditions (called generalized sonic conditions) that include effects of multi-dimensionality through the shock curvature term, which is assumed small on the scales of the reaction zone. Originally, the effect of curvature in the sonic conditions was considered by Wood and Kirkwood [15], and later was derived rationally in the works of Bdzil and Stewart (see e.g. Stewart and Bdzil [14]). Yao and Stewart [16] considered an extension of the sonic conditions to include asymptotically small unsteady corrections, but their analysis relies partially on the steady concept of a sonic locus by assuming that the flow is sonic relative to the lead shock, which constrains the sonic locus to be always parallel to the shock. The quasi-steady generalized CJ conditions reflect the fact that in a curved detonation, the flow divergence or convergence acts as a sink or source, respectively, of the energy of the lead shock. Thus for example, in a diverging steady detonation, the sonic condition expresses an exact balance of the heat release and flow divergence as shown by the equation given in Stewart and Bdzil [14]:

$$(\gamma - 1) Q\omega - c^2 (D + U_n) \kappa = 0, \tag{1}$$

where Q is the heat release, γ is the adiabatic exponent, ω is the reaction rate at the sonic point, c is the sound speed, D and U_n are the normal detonation speed and particle velocity at the sonic point relative to the lead shock, and κ is the shock curvature. Equation (1) is obtained from the equation (called Master equation),

$$\frac{\mathrm{d}U_n^2}{\mathrm{d}\lambda} = \frac{2U_n^2 \left[(\gamma - 1) Q\omega - c^2 (D_n + U_n) \kappa \right]}{\omega (c^2 - U_n^2)},\tag{2}$$

(λ is the reaction progress variable) that follows directly from the governing equations by a regularity argument, namely, that for the left-hand side of equation (2) to remain finite, the numerator of the right-hand side has to vanish at the sonic point because the denominator vanishes there, $c^2 = U_n^2$.

For unsteady weakly-curved detonations, the Master equation can again be written in a form similar to equation (2), but the numerator contains more terms (see [16]):

$$\frac{\partial U_n}{\partial n} = \frac{1}{c^2 - U_n^2} \left[(\gamma - 1) Q \omega - c^2 (D + U_n) \kappa + U_n \left(\frac{\partial U_n}{\partial t} + \frac{\partial D}{\partial t} \right) - v \frac{\partial p}{\partial t} \right], \tag{3}$$

where t is time, n is the normal distance from the shock (n < 0 in the reaction zone), v is the specific volume, and p is pressure. A regularity argument is again invoked that requires that the numerator of equation (3) vanish at the sonic point assuming that the denominator vanishes there as well, $c^2 - U_n^2 = 0$. The latter assumption is one of the key elements that distinguishes the present theory from that of Yao and Stewart [16] — we do not define the sonic locus in the shock-attached frame, so that in our theory, $c^2 - U_n^2$ does not necessarily vanish at the sonic locus. In fact, from the characteristic

analysis, we find that $c + U_n = \partial n_* / \partial t = \mathcal{D} - D$, where n_* is the distance between the shock and the sonic locus, \mathcal{D} and D are the speeds of the sonic locus and of the shock, respectively. Thus $c + U_n$ at the sonic locus is equal to the relative speed of the sonic locus and the shock. Therefore, the theory of Yao and Stewart contains an implicit assumption that the sonic locus and the shock are parallel in the characteristic (n,t) plane. In unsteady detonations, a possible imbalance of the heat release and flow divergence is reflected in the unsteadiness of the curved detonation.

Our generalization of the sonic conditions stems from the following observations. In a general unsteady flow that is sufficiently smooth, with a lead detonation shock, one considers all forward propagating characteristic surfaces, which are the envelopes of the forward propagating acoustic wavefronts. For initial conditions that admit smooth evolution, there may exist a limiting forward characteristic surface that never intersects the shock, or intersects the shock only at times that are very long compared to the passage time of particles through the detonation reaction zone. This limiting characteristic is thus identified as a separatrix of the family of forward characteristic surfaces whose motion is toward the shock. On the upstream side of the separatrix, the forward characteristic surfaces flow into the shock in a finite time, while on the downstream side, they flow away from the shock. The region that affects the lead-shock dynamics (the domain of influence) is the region between the shock surface and the limiting characteristic surface so that the evolution of the detonation wave depends only on the data in that region. The limiting sonic surface is then specifically embedded in the reaction zone, usually at a finite distance behind the shock. In Kasimov and Stewart [7], we illustrated both the existence and the behavior of the sonic locus in one-dimensional detonations by means of a numerical simulation.

Thus a general sonic locus is a characteristic surface of the governing hyperbolic equations such that the surface acts as an information boundary that precludes incoming acoustic perturbations from influencing the lead-shock dynamics. Such a definition is in agreement with the limiting cases of the steady detonation, the unsteady linearized theory, as well as the weakly-curved slowly-varying detonation theories that have been derived before. The new concept clarifies the meaning of the sonic locus by emphasizing its nature as a characteristic surface. In particular, since the sonic locus is a boundary of the domain of influence of the reaction zone, it follows immediately that the detonation problem is, in general, a two-front problem with both fronts (the shock and sonic loci) as free boundaries. Therefore, the sonic conditions must be given by two equations, a situation that has not been explicitly emphasized, but is nevertheless a part of all previous theories of detonation. For example, in the planar CJ detonation, the two equations are: (1) the well-known CJ condition, $M_{\rm CJ}=1$, where $M_{\rm CJ}=-U_n/c$ is the local Mach number relative to the shock, and (2) the condition that the sonic point coincides with the end of the reaction zone (for single-step exothermic reaction), $\lambda = 1$. We propose that the sonic conditions for general multi-dimensional detonations are: (1) the condition of local sonicity, that is, for an observer moving with the sonic surface, the particle speed normal to that surface, \mathcal{U}_n , is locally sonic,

$$U_n = -c, (4)$$

and (2) the compatibility condition in the sonic surface defined as a characteristic surface of the governing reactive Euler equations,

$$\rho c \mathbf{n}_* \cdot \left(\frac{D \mathbf{u}}{D t} + \frac{1}{\rho} \nabla p \right) + \rho c^2 \nabla \cdot \mathbf{u} + \frac{D p}{D t} = \rho c^2 \sigma \omega, \tag{5}$$

where \mathbf{n}_* is the unit normal to the sonic surface, \mathbf{u} is the lab-frame particle velocity, $D/Dt = \partial/\partial t + \mathbf{u} \cdot \nabla$ is the material derivative, and σ is the thermicity coefficient. These two conditions are direct consequences of the governing hyperbolic equations and hold therefore under quite general circumstances; no asymptotic ideas are involved.

In Section 2 we work out the theory of the characteristic surfaces for general system of quasilinear hyperbolic partial differential equations and derive compatibility conditions in the exceptional surface. The conditions are specialized to reactive Euler equations in Section 2.2. In Section 3 we discuss the simplest version of the sonic conditions in one spatial dimension to emphasize the connection with the standard theory of characteristics. Section 4 is devoted to two-dimensional detonations where we specialize the sonic conditions to local frames in order to exhibit the connection with the older theories of Detonation Shock Dynamics. The connection of the present work with the theories of detonation stability is a subject of Section 5. We conclude in Section 6.

2 General theory

This section is divided into two subsections. The first is a general discussion and review of properties of characteristic surfaces defined for systems of hyperbolic partial differential equations. We quickly specialize to the reactive, compressible flow equations but the presentation is not restricted to compressible Euler equations and have applications to other hyperbolic systems. The second subsection derives conditions that must be satisfied on a characteristic (sonic) surface, specifically for the reactive Euler equations that are relevant for application to detonation.

2.1 Characteristic surfaces of hyperbolic PDE and compatibility conditions

The analysis given next closely follows that given in von Mises' treatise the "Mathematical Theory of Compressible Fluid Flow", Article 9, [9]. This presentation was developed by G. S. S. Ludford (along with von Mises' wife Hilda Geiringer) to complete the von Mises' monograph after his death. Its teaching was a regular feature of Ludford's famous courses on applied mathematics given at Cornell University. The von Mises' reference is one of the few places one can find the general theory of characteristic surfaces written in a succinct and concise manner, and while classical in its form, it is seldom referenced and not widely known. This powerful presentation in fact becomes the basis for our developments and extensions to generate useful and new three-dimensional results for application to detonations in particular. A useful discussion of characteristic surfaces can also be found in Chapman [1]. Another useful reference is Ovsiannikov [11], where one can find a general characteristic form of equations of inert gas dynamics; the conditions on the acoustic characteristic surfaces are found to be similar to ours, equation (33), when no chemical reactions take place.

Consider a general system of quasi-linear hyperbolic equations written in the form

$$a_{ij}^k \frac{\partial u_j}{\partial x_k} = b_i, \tag{6}$$

where the coefficients a_{ij}^i are functions of the state variables u_j , j = 1, 2, ..., J, index i represents the individual equations of motion, x_k are the independent variables, and b_i are the source terms. Form a linear combination of the equations by multiplying the equations by arbitrary α_i and summing over all equations,

$$\alpha_i a_{ij}^k \frac{\partial u_j}{\partial x_k} \equiv m^k \frac{\partial}{\partial x_k} (u_j) = \alpha_i b_i. \tag{7}$$

Each term on the left-hand side of (7), $\alpha_i a_{ij}^k (\partial u_j/\partial x_k)$, is a directional derivative in space with direction tangents, **m**, whose components, labeled by k, are given by $m^k = \alpha_i a_{ij}^k$. An *exceptional surface* [9], (or more commonly referred to as a characteristic surface) is defined as a surface such that the linear combination (7) of directional derivatives expresses changes only in that surface. Then all direction tangents must lie in that surface and therefore, the linear combination (7) contains no derivatives normal to the surface. If such an exceptional surface exists, then the unit normal vector β to the surface must be orthogonal to all tangent vectors, **m** (see figure 1), that is

$$m^k \beta_k = \alpha_i \beta_k a_{ij}^k = 0. (8)$$

This is a system of J homogeneous linear algebraic equations for α_i , with a non-trivial solution if and only if

$$det|\beta_k a_{ij}^k| = 0, (9)$$

which is a J-th order polynomial that determines a constraint on the direction vector $\boldsymbol{\beta}$. Note that only directions in the space of the independent variables are solved for. If the relation between the

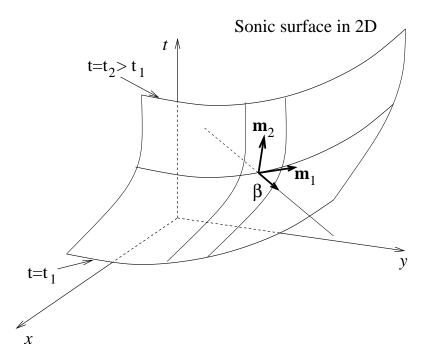


Figure 1: The sonic surface in 2+1 dimensions, which is generated by time evolution of the 2D sonic locus (a line in xy plane) along the third (time t) axis from $t = t_1$ to $t = t_2$.

components of β that there are J such real directions, albeit some can be repeated, then the system is strictly hyperbolic. If one of the independent variables is time, then the constraint on the direction in space-time defines the velocity of the characteristic, which we later denote as the *speed relation*.

The *compatibility condition* is simply the differential relation, (7), found on the characteristic surface. The first step solves for β_k by solving the characteristic polynomial. The second step is, with a chosen direction, one expresses the compatibility relation in the characteristic surface. Since the system of equations for α_i is singular, then the solution for α_i is determined up to an arbitrary constant, i.e the ratio between the α_i is determined in terms of the β_k . Say such a direction β_k^* with a corresponding α_i^* are found. Then the *compatibility condition* is specifically

$$\alpha_i^* a_{ij}^k \frac{\partial u_j}{\partial x_k} = \alpha_i^* b_i. \tag{10}$$

2.2 Compatibility conditions for reactive Euler equations

We now start with reactive Euler equations with a single chemical reaction and closely follow the derivation given in von Mises [9] for the general case of fluid motion for inert flow. Further generalization to a multiple-step chemistry is straightforward. The general equation of state is used in its incomplete form $e = e(p, \rho, \lambda)$.

Note that a simple device is in use. To simplify the algebraic presentation, the equations of motion are assumed to be analyzed at a point instantaneously aligned with the x-axis, which is taken in the direction of the velocity vector $\mathbf{u} = u\mathbf{i} + v\mathbf{j} + w\mathbf{k}$. Therefore, without loss of generality, the material derivative is $d/dt = \partial/\partial t + u\partial/\partial x$. The general condition for the exceptional surfaces is expressed for this special system and subsequently re-written in a frame-invariant notation so that any coordinate system can be used. The notion of an exceptional (characteristic) surface is the one that is based on the physical equations and not the coordinates, and it is simply a matter of expressing the equations and directions indicated in those coordinates.

The equations of motion are written as

$$u\frac{\partial u}{\partial x} + \frac{\partial u}{\partial t} + \frac{1}{\rho} \frac{\partial p}{\partial x} = 0, \tag{11}$$

$$u\frac{\partial v}{\partial x} + \frac{\partial v}{\partial t} + \frac{1}{\rho}\frac{\partial p}{\partial y} = 0, \tag{12}$$

$$u\frac{\partial w}{\partial x} + \frac{\partial w}{\partial t} + \frac{1}{\rho} \frac{\partial p}{\partial z} = 0, \tag{13}$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} + \frac{u}{\rho} \frac{\partial \rho}{\partial x} + \frac{1}{\rho} \frac{\partial \rho}{\partial t} = 0, \tag{14}$$

$$u\frac{\partial p}{\partial x} + \frac{\partial p}{\partial t} - c^2 \left(u \frac{\partial \rho}{\partial x} + \frac{\partial \rho}{\partial t} \right) = \rho c^2 \sigma \omega, \tag{15}$$

$$u\frac{\partial \lambda}{\partial r} + \frac{\partial \lambda}{\partial t} = \omega,\tag{16}$$

where we have used the definition of the thermicity coefficient given by Fickett and Davis [4],

$$\sigma = -\frac{1}{\rho c^2} \frac{e_{\lambda}}{e_p},\tag{17}$$

and the general expression for the sound speed,

$$c^2 = \frac{p - \rho^2 e_\rho}{\rho^2 e_p},\tag{18}$$

where the subscripts of e denote partial differentiation with respect to the arguments.

The state vector u_j is given by $(u_j) = (u, v, w, p, \rho, \lambda)$, with j = 1...6. For the purpose of assigning the a_{ij}^k , we number (11) through (16) by j = 1...6. The generalized independent coordinates are given by the list $(x_k) = (x, y, z, t)$ with k = 1...4. The equations of motion written in the form (6) subsequently identify a_{ij}^k as

$$[a_{11}^{k}] = [u, 0, 0, 1], a_{12}^{k} = 0, a_{13}^{k} = 0, [a_{14}^{k}] = [\frac{1}{\rho}, 0, 0, 0], a_{15}^{k} = 0, a_{16}^{k} = 0,$$

$$a_{21}^{k} = 0, [a_{22}^{k}] = [u, 0, 0, 1], a_{23}^{k} = 0, [a_{24}^{k}] = [0, \frac{1}{\rho}, 0, 0], a_{25}^{k} = 0, a_{26}^{k} = 0,$$

$$a_{31}^{k} = 0, a_{32}^{k} = 0, [a_{33}^{k}] = [u, 0, 0, 1], [a_{34}^{k}] = [0, 0, \frac{1}{\rho}, 0], a_{35}^{k} = 0, a_{36}^{k} = 0,$$

$$[a_{41}^{k}] = [1, 0, 0, 0], [a_{42}^{k}] = [0, 1, 0, 0], [a_{43}^{k}] = [0, 0, 1, 0], a_{44}^{k} = 0, [a_{45}^{k}] = [\frac{u}{\rho}, 0, 0, \frac{1}{\rho}], a_{46}^{k} = 0,$$

$$a_{51}^{k} = 0, a_{52}^{k} = 0, a_{53}^{k} = 0, [a_{54}^{k}] = [u, 0, 0, 1], [a_{55}^{k}] = [-c^{2}u, 0, 0, -c^{2}], a_{56}^{k} = 0,$$

$$a_{61}^{k} = 0, a_{63}^{k} = 0, a_{63}^{k} = 0, a_{64}^{k} = 0, a_{65}^{k} = 0, [a_{66}^{k}] = [u, 0, 0, 1]. \tag{19}$$

The 6×6 characteristic matrix, $\beta_k a_{ij}^k$, becomes

$$\begin{bmatrix} \beta_0 & 0 & 0 & \beta_1/\rho & 0 & 0 \\ 0 & \beta_0 & 0 & \beta_2/\rho & 0 & 0 \\ 0 & 0 & \beta_0 & \beta_3/\rho & 0 & 0 \\ \beta_1 & \beta_2 & \beta_3 & 0 & \beta_0/\rho & 0 \\ 0 & 0 & 0 & \beta_0 & -c^2\beta_0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \beta_0 \end{bmatrix},$$
(20)

where $\beta_0 \equiv u\beta_1 + \beta_4$. Setting its determinant equal to zero results in the characteristic equation

$$-\frac{\beta_0^4}{\rho} \left[\beta_0^2 - c^2 (\beta_1^2 + \beta_2^2 + \beta_3^2) \right] = 0.$$
 (21)

A four-fold repeated root is associated with the stream surfaces that form the characteristic surface described by setting $\beta_0 = u\beta_1 + \beta_4 = 0$. In addition, there are two other surfaces associated with the roots of the other factor

$$\beta_0 = \pm c \sqrt{\beta_1^2 + \beta_2^2 + \beta_3^2}. (22)$$

Our focus is on these directions since in a nominally one-dimensional, unsteady flow they would correspond to the forward and backward facing acoustic characteristics (i.e C_+ and C_-) that are called the "Mach lines". We specifically work out the compatibility relation for both of them as they occur in a pair, and later we will use the results for the characteristic surface that would correspond to the forward characteristic as we will explain subsequently.

To display the compatibility relation we need to solve the equations for α_i , namely equation (8), Using the previous definitions one obtains the six equations

$$\alpha_1\beta_0 + \alpha_4\beta_1 = 0$$
, $\alpha_2\beta_0 + \alpha_4\beta_2 = 0$,

$$\begin{split} \alpha_{3}\beta_{0} + \alpha_{4}\beta_{3} &= 0 \,, \quad \frac{1}{\rho} \left(\alpha_{1}\beta_{1} + \alpha_{2}\beta_{2} + \alpha_{3}\beta_{3} \right) + \alpha_{5}\beta_{0} = 0 \,, \\ \frac{\alpha_{4}}{\rho}\beta_{0} - c^{2}\alpha_{5}\beta_{0} &= 0 \,, \quad \alpha_{6}\beta_{0} = 0 \,. \end{split} \tag{23}$$

The solution of this system is, in terms of α_4 (note that $\beta_0 = u\beta_1 + \beta_4 \neq 0$):

$$\alpha_1 = -\frac{\alpha_4 \beta_1}{\beta_0}, \, \alpha_2 = -\frac{\alpha_4 \beta_2}{\beta_0}, \, \alpha_3 = -\frac{\alpha_4 \beta_3}{\beta_0}, \, \alpha_5 = \frac{\alpha_4}{\rho c^2}, \, \alpha_6 = 0.$$
 (24)

The compatibility condition (7) written out long becomes

$$\alpha_1 a_{1j}^k \frac{\partial u_j}{\partial x_k} + \alpha_2 a_{2j}^k \frac{\partial u_j}{\partial x_k} + \alpha_3 a_{3j}^k \frac{\partial u_j}{\partial x_k} + \alpha_4 a_{4j}^k \frac{\partial u_j}{\partial x_k} + \alpha_5 a_{5j}^k \frac{\partial u_j}{\partial x_k} = \alpha_5 b_5. \tag{25}$$

Substituting for the α_i in terms of α_4 leads to equation

$$\frac{-\alpha_4}{\beta_0} \left[\beta_1 a_{1j}^k \frac{\partial u_j}{\partial x_k} + \beta_2 a_{2j}^k \frac{\partial u_j}{\partial x_k} + \beta_3 a_{3j}^k \frac{\partial u_j}{\partial x_k} \right] + \alpha_4 \left[a_{4j}^k \frac{\partial u_j}{\partial x_k} + \frac{1}{\rho c^2} a_{5j}^k \frac{\partial u_j}{\partial x_k} \right] = \frac{\alpha_4}{\rho c^2} b_5. \tag{26}$$

The reader is reminded that each of the terms in the equation represents one of the governing equations. Let us introduce the unit vector

$$\mathbf{n} = \frac{\beta_1 \mathbf{i} + \beta_2 \mathbf{j} + \beta_3 \mathbf{k}}{\sqrt{\beta_1^2 + \beta_2^2 + \beta_2^2}}.$$
 (27)

This unit vector is normal to the tangent plane of the Mach cones, hence normal to the instantaneous realization of the characteristic surface in the physical space.

We also notice that the first three terms in equation (26) represent the first three components of the momentum equation and can be re-written as

$$\frac{-\alpha_4}{\beta_0} \left(\sqrt{\beta_1^2 + \beta_2^2 + \beta_2^2} \right) \mathbf{n} \cdot \left[\frac{D\mathbf{u}}{Dt} + \frac{1}{\rho} \nabla p \right]. \tag{28}$$

The second collection of terms in equation (26) can be re-written as

$$\alpha_4 \left[\frac{1}{\rho} \frac{D\rho}{Dt} + \nabla \cdot \mathbf{u} + \frac{1}{\rho c^2} \left(\frac{Dp}{Dt} - c^2 \frac{D\rho}{Dt} \right) \right]$$
 (29)

and the right-hand side of (26) is

$$\frac{\alpha_4}{\rho c^2} b_5 = \alpha_4 \sigma \omega. \tag{30}$$

Putting it all together leads to the frame-invariant expression of the compatibility condition on the characteristic surface (canceling out the common α_4 and the material derivatives of density, and multiplying through by ρc^2),

$$-\frac{\sqrt{\beta_1^2 + \beta_2^2 + \beta_2^2}}{\beta_0} (\rho c^2) \mathbf{n} \cdot \left[\frac{D\mathbf{u}}{Dt} + \frac{1}{\rho} \nabla p \right] + \left[\rho c^2 \nabla \cdot \mathbf{u} + \frac{Dp}{Dt} \right] = \rho c^2 \sigma \omega. \tag{31}$$

The characteristic equations (22) for the directions show that

$$\frac{\sqrt{\beta_1^2 + \beta_2^2 + \beta_2^2}}{\beta_0} = \pm \frac{1}{c},\tag{32}$$

so that can be used to write the compatibility condition in the form

$$\mp (\rho c)\mathbf{n} \cdot \left[\frac{D\mathbf{u}}{Dt} + \frac{1}{\rho} \nabla p \right] + \left[\rho c^2 (\nabla \cdot \mathbf{u}) + \frac{Dp}{Dt} \right] = \rho c^2 \sigma \omega. \tag{33}$$

The compatibility condition is a differential relation that holds on the characteristic surface. But the other condition is that the motion is confined to be along the space-time characteristic direction defined by *speed relation*

$$u\beta_1 + \beta_4 = \pm c\sqrt{\beta_1^2 + \beta_2^2 + \beta_3^2}. (34)$$

It is important to interpret (34) as well as a frame-invariant relation. The components $(\beta_1, \beta_2, \beta_3)$ can be chosen to be those of a unit normal to the surface and hence $\sqrt{\beta_1^2 + \beta_2^2 + \beta_3^2} = 1$. Also the term $u\beta_1$ has the meaning $\mathbf{u} \cdot \mathbf{n}$. Finally β_4 is the velocity of the characteristic surface normal to itself, $\beta_4 = V_n$ (say). Re-writing the expression above leads to

$$V_n = \mathbf{u} \cdot \mathbf{n} \pm c. \tag{35}$$

In one dimension, this reduces to the familiar equation for the slope of the characteristics $V_n \equiv dx/dt = u \pm c$.

Consider the forward propagating surface that corresponds to the choice of the plus sign in the previous relation (35). Note that the particle velocity in the frame of an observer traveling in the forward surface is $u_n - V_n$ and the speed relation can be written as

$$\frac{u_n - V_n}{c} = -1. ag{36}$$

This means that on this characteristic surface the local normal Mach number is always unity, which is the conventional definition of sonic.

The compatibility and the speed relation, taken together are two pieces of information, namely a differential condition in the sonic surface and a scalar speed relation, that determines the motion of the surface. If we include additional reactions and replace λ by λ_q , q=1,2,...N, where N is the number of reactions, then in the subsequent derivations only the right-hand side of (33) will change since additional reactions only generate additional roots that are multiples of the root associated with the streamline characteristic, but not to the acoustics. The right-hand side of the compatibility condition becomes the sum, $\rho c^2 \sigma_q \omega_q$, over q=1...N, where

$$\sigma_q = -\frac{1}{\rho c^2} \frac{e_{\lambda_q}}{e_p} \tag{37}$$

is the thermicity coefficient and ω_q is the rate of q-th reaction. The sound speed in the governing equations is the frozen sound speed and is still given by (18).

If we specify the result to a detonation wave that is propagating from left to right in positive x direction, then the normal to the characteristic surface embedded in the reaction zone that can possibly intersect the shock points forward. Therefore, we select the plus sign in equation (33). Let us denote the unit normal to the characteristic surface \mathbf{n}_* (in general, the subscript * will refer to a quantity evaluated at the sonic surface). The *compatibility condition* for this surface is then

$$\rho c \mathbf{n}_* \cdot \left(\frac{D \mathbf{u}}{D t} + \frac{1}{\rho} \nabla p \right) + \rho c^2 \nabla \cdot \mathbf{u} + \frac{D p}{D t} = \rho c^2 \sigma \omega, \tag{38}$$

where it is understood that all terms are evaluated at the sonic surface, although we drop subscript * in most of the terms for the sake of clarity. The compatibility condition (38) holds on the exceptional surface at which the flow is locally sonic, that is an observer moving with the surface observes that the flow speed normal to the surface is locally sonic:

$$\mathcal{U}_{n*} = \mathbf{u}_* \cdot \mathbf{n}_* - \mathcal{D} = -c_* \,, \tag{39}$$

where \mathcal{D} is the normal speed of the sonic surface in the lab frame.

3 One-dimensional sonic conditions

Equation (38) simplifies now to

$$\rho c \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x} \right) + \rho c^2 \frac{\partial u}{\partial x} + \frac{\partial p}{\partial t} + u \frac{\partial p}{\partial x} = \rho c^2 \sigma \omega, \tag{40}$$

which can be rewritten as

$$\frac{dp_*}{dt} + \rho_* c_* \frac{du_*}{dt} = \rho_* c_*^2 \sigma_* \omega_*, \tag{41}$$

where the spatial and temporal derivatives in (40) are combined to form a time derivative along the forward characteristic direction,

$$\frac{d}{dt} = \frac{\partial}{\partial t} + (c_* + u_*) \frac{\partial}{\partial x} = \frac{\partial}{\partial t} + \frac{dx_*}{dt} \frac{\partial}{\partial x}.$$

$$\frac{dx_*}{dt} = c_* + u_*.$$
(42)

As we have mentioned before, the sonic locus is a special characteristic that is a separatrix of two families of characteristic lines, namely those that reach the shock front in finite time and those that do not. It is assumed that the sonic locus exists initially as, for example, in a steady detonation and continues to exist during unsteady evolution. Then the initial condition selects the separatrix from the entire family of forward characteristics for all of which equations (42) and (41) hold. It must be pointed out that it is not, in general, possible to identify the separatrix in an arbitrary initial condition.

One can look at equation (41) as a differential equation that does not involve derivatives normal to the characteristic surface. The sonic locus is an (x,t) curve along a limiting C_+ characteristic (see Figure 2) and the derivative $\partial/\partial x$ does not appear. Indeed, the time derivatives in (41) are the derivatives along the characteristics, that is the derivatives lie in the tangent plane of the characteristic surface.

For one-dimensional detonation with point symmetry (j = 0, 1, 2 correspond to planar, cylindrical, and spherical symmetry, respectively), one easily finds that the compatibility condition is

$$\frac{dp_*}{dt} + \rho_* c_* \frac{du_*}{dt} + \frac{j}{r} \rho_* c_*^2 u_* = \rho_* c_*^2 \sigma_* \omega_*, \tag{43}$$

where r is the radial coordinate, while the speed relation is

$$\frac{dr_*}{dt} = c_* + u_*. \tag{44}$$

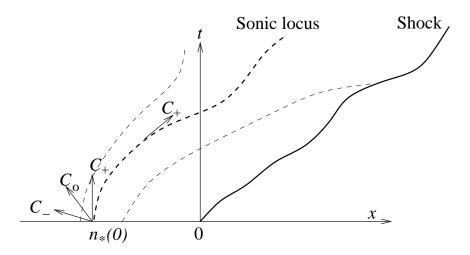


Figure 2: One-dimensional sonic locus as the C_+ characteristic emanating from the initial steady sonic locus.

For a steady one-dimensional planar detonation wave in a mixture with complex reaction network, the compatibility condition reduces to the equation

$$\sigma_q \omega_q = 0, \tag{45}$$

that, together with $c_* + U_* = 0$, defines the sonic locus. For a discussion of the condition in applications to multiple-step reactions in detonation waves, see [4].

4 Sonic conditions of detonation shock dynamics

We call (38) and (39) the *sonic conditions* on the limiting forward characteristic surface and their application to detonation theory is a main result of this paper. Specifically, we consider initial-value problems where there is an initially prescribed detonation shock locus with states behind it that lead subsequently to smooth evolution in the reaction zone for a self-sustained detonation. In this section, we specialize sonic conditions to one- and two-dimensional detonations. We show that when linearized, the compatibility condition reduces to the *radiation condition* of detonation stability theory (see, e.g. [6, 8, 12]). For the two-dimensional, slowly-varying and weakly-curved detonations the compatibility condition reduces to the *thermicity condition* of Detonation Shock Dynamics (DSD theory, see e.g. [16]). In both detonation stability theory and DSD, the governing equations are usually written in a frame of reference attached to the shock front since one is often interested in the shock-front dynamics rather than anything else. For the purpose of comparison with the known sonic conditions, we write our sonic conditions in the shock-attached frame. But before doing that, it is instructive to look at the sonic conditions written in the frame of the sonic locus.

4.1 Sonic conditions in the sonic-frame Bertrand coordinates

We express the sonic conditions in two-dimensional surface-attached Bertrand coordinates which use the normal distance to a prescribed front and the arc-length to a reference point along the front as the intrinsic surface based coordinates, (see e.g. [10, 16]). Since the Bertrand coordinates are developed by the sonic surface, they are perfectly suited to simplify the conditions since only derivatives in the surface and normal to that surface appear. Let (η, ζ) be the normal signed distance to the surface and transverse distance measured along the surface (see figure 3). Let (\mathbf{n}, \mathbf{t}) be the corresponding unit normal and tangent vectors to the sonic surface. The coordinate transformation from

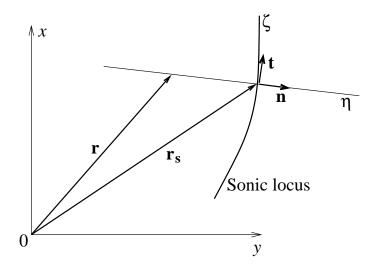


Figure 3: Bertrand frame attached to the sonic locus.

the laboratory frame to the Bertrand frame is defined by

$$\mathbf{r} = \mathbf{r}_s + \eta \mathbf{n},\tag{46}$$

where \mathbf{r} is the lab-frame position of a point in space and $\mathbf{r}_s(\zeta,t)$ is the position of the sonic surface. Then various differential operators in the Bertrand frame are written as follows

$$\nabla = \mathbf{n} \frac{\partial}{\partial \eta} + \frac{\mathbf{t}}{1 + \eta \kappa_*} \frac{\partial}{\partial \zeta},\tag{47}$$

$$\nabla \cdot \mathbf{u} = \frac{\partial u_{\eta}}{\partial \eta} + \frac{1}{1 + \eta \kappa_{*}} \left(\kappa_{*} u_{\eta} + \frac{\partial u_{\zeta}}{\partial \zeta} \right), \quad \mathbf{u} \cdot \nabla = u_{\eta} \frac{\partial}{\partial \eta} + \frac{u_{\zeta}}{1 + \eta \kappa_{*}} \frac{\partial}{\partial \zeta}, \tag{48}$$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t} - \mathcal{D}\frac{\partial}{\partial \mathbf{n}} + \mathcal{S}\frac{\partial}{\partial \zeta},\tag{49}$$

and

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla = \frac{\partial}{\partial t} + (u_{\eta} - \mathcal{D}) \frac{\partial}{\partial \eta} + \left(\mathcal{S} + \frac{u_{\zeta}}{1 + \eta \kappa_{*}} \right) \frac{\partial}{\partial \zeta}, \tag{50}$$

where the lab-frame particle speed is $\mathbf{u} = u_{\eta} \mathbf{n} + u_{\zeta} \mathbf{t}$, κ_* is the curvature of the sonic surface. Note that $\eta = 0$ in the sonic surface and that $u_{\eta} - \mathcal{D} = \mathcal{U}_{\eta}$ is the normal particle velocity relative to the sonic frame. We introduced the rate of strain of the arclength,

$$S = \frac{\partial \zeta}{\partial t},\tag{51}$$

and used the fact that

$$\frac{\partial \mathbf{\eta}}{\partial t} = -\mathcal{D}.\tag{52}$$

Next we calculate the compatibility condition (38) in terms of the new coordinates. Clearly, $\mathbf{n} \cdot \nabla p = \partial p / \partial \eta$, and all other terms are also straightforward, except for $\mathbf{n} \cdot D\mathbf{u}/Dt$. To calculate the latter, we write

$$\mathbf{n} \cdot \frac{D\mathbf{u}}{Dt} = \mathbf{n} \cdot \frac{D}{Dt} \left(u_{\eta} \mathbf{n} + u_{\zeta} \mathbf{t} \right) = \mathbf{n} \cdot \left(\frac{Du_{\eta}}{Dt} \mathbf{n} + u_{\eta} \frac{D\mathbf{n}}{Dt} + \frac{Du_{\zeta}}{Dt} \mathbf{t} + u_{\zeta} \frac{D\mathbf{t}}{Dt} \right) = \frac{Du_{\eta}}{Dt} + u_{\zeta} \mathbf{n} \cdot \left[\frac{\partial \mathbf{t}}{\partial t} + \left(u_{\eta} - \mathcal{D} \right) \frac{\partial \mathbf{t}}{\partial \eta} + \left(\mathcal{S} + u_{\zeta} \right) \frac{\partial \mathbf{t}}{\partial \zeta} \right], \tag{53}$$

where we have used equation (50) and $\mathbf{n} \cdot \mathbf{t} = 0$, $\mathbf{n} \cdot D\mathbf{n}/Dt = 0$. To determine $\mathbf{n} \cdot \partial \mathbf{t}/\partial t$, we differentiate the coordinate transformation, $\mathbf{r} = \mathbf{r}_s + \eta \mathbf{n}$, with respect to time and find

$$0 = \frac{d\mathbf{r}}{dt} = \frac{\partial \mathbf{r}_s}{\partial t} + \frac{\partial \zeta}{\partial t} \frac{\partial \mathbf{r}_s}{\partial \zeta} + \frac{\partial \eta}{\partial t} \mathbf{n} + \eta \left(\frac{\partial \mathbf{n}}{\partial t} + \frac{\partial \zeta}{\partial t} \frac{\partial \mathbf{n}}{\partial \zeta} \right). \tag{54}$$

We evaluate the last result in the sonic surface, at $\eta = 0$, to obtain

$$\frac{\partial \mathbf{r}_s}{\partial t} + \mathcal{S}\mathbf{t} - \mathcal{D}\mathbf{n} = 0, \tag{55}$$

and differentiate the latter with respect to ζ , and noting that $\mathbf{t} = \partial \mathbf{r}_s / \partial \zeta$, we find, using the Frenet formulas,

$$\frac{\partial \mathbf{n}}{\partial \zeta} = \kappa \mathbf{t}, \ \frac{\partial \mathbf{t}}{\partial \zeta} = -\kappa \mathbf{n}, \tag{56}$$

that

$$\mathbf{n} \cdot \frac{\partial \mathbf{t}}{\partial t} = \frac{\partial \mathcal{D}}{\partial \zeta} + \kappa \mathcal{S}. \tag{57}$$

Then collecting all terms in (53), we find that

$$\mathbf{n} \cdot \frac{D\mathbf{u}}{Dt} = \frac{Du_{\eta}}{Dt} + u_{\zeta} \frac{\partial \mathcal{D}}{\partial \zeta} - \kappa u_{\zeta}^{2}. \tag{58}$$

What is left is to collect terms in (38), which results in the following equation

$$\rho c \left(\frac{Du_{\eta}}{Dt} + u_{\zeta} \frac{\partial \mathcal{D}}{\partial \zeta} - \kappa u_{\zeta}^{2} + \frac{1}{\rho} \frac{\partial p}{\partial \eta} \right) +$$

$$\rho c^{2} \left(\frac{\partial u_{\eta}}{\partial \eta} + \kappa_{*} u_{\eta} + \frac{\partial u_{\zeta}}{\partial \zeta} \right) + \frac{Dp}{Dt} = \rho c^{2} \sigma \omega.$$
(59)

Expanding the material derivative according to equation (50) and rearranging derivatives along the same directions, we obtain

$$\frac{\partial p}{\partial t} + \rho c \frac{\partial u_{\eta}}{\partial t} + \kappa_* \rho c^2 u_{\eta} + (c + u_{\eta} - \mathcal{D}) \left(\frac{\partial p}{\partial \eta} + \rho c \frac{\partial u_{\eta}}{\partial \eta} \right) + \rho c^2 \frac{\partial u_{\zeta}}{\partial \zeta} + \rho c u_{\zeta} \left(\frac{\partial \mathcal{D}}{\partial \zeta} - \kappa_* u_{\zeta} \right) + (\mathcal{S} + u_{\zeta}) \left(\frac{\partial p}{\partial \zeta} + \rho c \frac{\partial u_{\eta}}{\partial \zeta} \right) = \rho c^2 \sigma \omega.$$
(60)

An important observation now is that in the sonic surface the flow is locally sonic with

$$c + u_{\mathsf{n}} - \mathcal{D} = 0, \tag{61}$$

which is the speed relation. Therefore, all normal-derivative terms in the compatibility condition (60) drop out resulting in equation

$$\frac{\partial p}{\partial t} + \rho c \frac{\partial u_{\eta}}{\partial t} + \kappa_* \rho c^2 u_{\eta} = \rho c^2 \sigma \omega - R_*, \tag{62}$$

where the terms that explicitly depend on the transverse variation are lumped into R_* , given by

$$R_* = \rho c^2 \frac{\partial u_{\zeta}}{\partial \zeta} + \rho c u_{\zeta} \left(\frac{\partial \mathcal{D}}{\partial \zeta} - \kappa_* u_{\zeta} \right) + \left(\mathcal{S} + u_{\zeta} \right) \left(\frac{\partial p}{\partial \zeta} + \rho c \frac{\partial u_{\eta}}{\partial \zeta} \right).$$

The reader is reminded that everything in equation (62) is evaluated in the sonic surface.

By definition, the compatibility condition must not contain derivatives along the normal to the characteristic surface in (ζ, η, t) space. Since our coordinate frame is local, that is attached to the characteristic surface, then the time derivative in (62) does indeed lie in the surface, similar to the time derivative along the C_+ characteristic in one dimension. Furthermore, ζ - derivative is also in

the surface, as ζ is the arclength. The only derivative that is *off* the characteristic surface in (ζ, η, t) space is $\partial/\partial \eta$ and that derivative is indeed absent in equation (62). If R_* can be neglected, equation (62) is similar to the thermicity condition of the old Detonation Shock Dynamics theories with an important difference that here U_{η} and \mathcal{D} are the particle velocity in the *sonic* frame and normal speed of the *sonic* surface, respectively; in the older theories of DSD, the same variables are calculated in the *shock-attached* frame. The approximate form, that neglects R_* is valid only in the limit of weak curvature, slow time, and small transverse variation. Equation (62) is an exact relation that is valid for general two-dimensional detonations with an embedded sonic surface, provided only that the Bertrand coordinates are invertible, which is true if the radius of curvature of the sonic locus is large compared to the length of the reaction zone.

4.2 Sonic conditions of DSD theory: formulation in the shock-attached frame

The linear stability problem and the DSD problem were originally formulated in shock-attached coordinates; in the first case, this dates back to the first rigorous analysis given by Erpenbeck [3], in the second case, the shock-attached coordinates were used because the goal of DSD theory is to determine the dynamics of the shock front [14, 16].

Here we revisit the formulation of DSD in the shock-attached coordinates and use Bertrand coordinates attached to the shock. Let (n, ξ) be the normal and transverse coordinates and let (\mathbf{n}, \mathbf{t}) represent the corresponding unit normal and tangent vectors in the shock frame; then the coordinate transformation is given by

$$\mathbf{r} = \mathbf{r}_s(\xi, t) + n\mathbf{n}(\xi, t). \tag{63}$$

The time-derivative in the shock-attached frame is represented as

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t} - D\frac{\partial}{\partial n} + S\frac{\partial}{\partial \xi},$$

the velocity in the lab frame is $\mathbf{u} = u_n \mathbf{n} + u_{\xi} \mathbf{t}$, D is the normal shock speed, $S = \partial \xi / \partial t$ is the stretch rate of the arc-length along the shock, and $U_n = u_n - D$ is the normal particle speed relative to the shock. The material derivative is then

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + U_n \frac{\partial}{\partial n} + \left(S + \frac{u_{\xi}}{1 + n_{\star} \kappa} \right) \frac{\partial}{\partial \xi}.$$
 (64)

Differential operators involving ∇ are similar to those in the sonic frame, (47-48), only now the velocity is expressed in the shock frame. A slight complication arises from the fact that the unit normal, \mathbf{n}_* , in (38) is that to the sonic surface, which in general is different from \mathbf{n} , the unit normal to the shock. Therefore, the shock-frame compatibility condition will contain terms, proportional to $\mathbf{n}_* \cdot \mathbf{n}$, which need to be evaluated.

Let

$$\mathbf{n}_* = a_n \mathbf{n} + a_{\xi} \mathbf{t},\tag{65}$$

where the components, $a_n = \mathbf{n}_* \cdot \mathbf{n}$ and $a_{\xi} = \mathbf{n}_* \cdot \mathbf{t}$, will be determined below (see equations (77)). Then, $\mathbf{n}_* \cdot \nabla p = a_n \partial p / \partial n + a_{\xi} \partial p / \partial \xi$, and

$$\mathbf{n}_* \cdot \frac{D\mathbf{u}}{Dt} = \mathbf{n}_* \cdot \frac{D}{Dt} \left(u_n \mathbf{n} + u_{\xi} \mathbf{t} \right) = \frac{Du_n}{Dt} \mathbf{n}_* \cdot \mathbf{n} + u_n \mathbf{n}_* \cdot \frac{D\mathbf{n}}{Dt} + \frac{Du_{\xi}}{Dt} \mathbf{n}_* \cdot \mathbf{t} + u_{\xi} \mathbf{n}_* \cdot \frac{D\mathbf{t}}{Dt}.$$
(66)

We now calculate each term on the right-hand side of this equation. Consider

$$\mathbf{n}_* \cdot \frac{D\mathbf{n}}{Dt} = a_{\xi} \mathbf{t} \cdot \frac{D\mathbf{n}}{Dt} = a_{\xi} \mathbf{t} \cdot \left[\frac{\partial \mathbf{n}}{\partial t} + \left(S + \frac{u_{\xi}}{1 + n_* \kappa} \right) \frac{\partial \mathbf{n}}{\partial \xi} \right]. \tag{67}$$

By time-differentiating the coordinate transformation (63) and evaluating the result at the shock we find that

$$\frac{\partial \mathbf{r}_s}{\partial t} + S\mathbf{t} - D\mathbf{n} = 0. \tag{68}$$

Differentiating this result with respect to ξ and using $\mathbf{t} = \partial \mathbf{r}_s / \partial \xi$, we find

$$\frac{\partial \mathbf{t}}{\partial t} + \left(\frac{\partial S}{\partial \xi} - \kappa D\right) \mathbf{t} - \left(\frac{\partial D}{\partial \xi} + \kappa S\right) \mathbf{n} = 0, \tag{69}$$

from which it follows that

$$\mathbf{t} \cdot \frac{\partial \mathbf{n}}{\partial t} = -\mathbf{n} \cdot \frac{\partial \mathbf{t}}{\partial t} = -\frac{\partial D}{\partial \xi} - \kappa S \tag{70}$$

and

$$\frac{\partial S}{\partial \xi} - \kappa D = 0. \tag{71}$$

Using equation (70) and the Frenet formula, $\partial \mathbf{n}/\partial \xi = \kappa \mathbf{t}$, we find that equation (67) results in

$$\mathbf{n}_* \cdot \frac{D\mathbf{n}}{Dt} = a_{\xi} \left(-\frac{\partial D}{\partial \xi} + \frac{\kappa u_{\xi}}{1 + n_* \kappa} \right). \tag{72}$$

Similarly, we find

$$\mathbf{n}_* \cdot \frac{D\mathbf{t}}{Dt} = a_n \mathbf{n} \cdot \left[\frac{\partial \mathbf{t}}{\partial t} + \left(S + \frac{u_{\xi}}{1 + n_* \kappa} \right) \frac{\partial \mathbf{t}}{\partial \xi} \right] = a_n \left(\frac{\partial D}{\partial \xi} - \frac{\kappa u_{\xi}}{1 + n_* \kappa} \right). \tag{73}$$

Equation (66) becomes

$$\mathbf{n}_* \cdot \frac{D\mathbf{u}}{Dt} = a_n \frac{Du_n}{Dt} + a_\xi \frac{Du_\xi}{Dt} + \left(u_n a_\xi - u_\xi a_n\right) \left(-\frac{\partial D}{\partial \xi} + \frac{\kappa u_\xi}{1 + n_* \kappa}\right). \tag{74}$$

Collecting all terms, we obtain that the shock-frame compatibility condition is

$$\frac{\partial p}{\partial t} + (c + U_n) \frac{\partial p}{\partial n} + \rho c \left[\frac{\partial u_n}{\partial t} + (c + U_n) \frac{\partial u_n}{\partial n} \right] + \frac{\kappa}{1 + n_* \kappa} \rho c^2 u_n = \rho c^2 \sigma \omega - R, \tag{75}$$

where κ (without the * subscript) is the local curvature of the shock, n_* is the normal distance from the shock to the sonic surface, and all terms are evaluated in the sonic surface. By R in the right-hand side of (75) we denote the following collection of terms

$$R = \left(S + \frac{u_{\xi}}{1 + n_{*}\kappa}\right) \left(\frac{\partial p}{\partial \xi} + \rho c \frac{\partial u_{n}}{\partial \xi}\right) + \frac{\rho c^{2}}{1 + n_{*}\kappa} \frac{\partial u_{\xi}}{\partial \xi} + c\left(a_{n} - 1\right) \left(\frac{\partial p}{\partial n} + \rho \frac{Du_{n}}{Dt}\right) + ca_{\xi} \left(\frac{\partial p}{\partial \xi} + \rho \frac{Du_{\xi}}{Dt}\right) + \rho c\left(u_{n}a_{\xi} - u_{\xi}a_{n}\right) \left(-\frac{\partial D}{\partial \xi} + \frac{\kappa u_{\xi}}{1 + n_{*}\kappa}\right).$$

$$(76)$$

From the derivations below (see equation (84)), the coefficients a_n and a_ξ in (76) are given by

$$a_n = \left[1 + \left(\frac{1}{1 + n_* \kappa} \frac{\partial n_*}{\partial \xi}\right)^2\right]^{-1/2}, \ a_{\xi} = -\frac{a_n}{1 + n_* \kappa} \frac{\partial n_*}{\partial \xi},\tag{77}$$

so that small transverse variation implies smallness of $a_n - 1$ and a_{ξ} .

Note that the operator $\partial/\partial t + (c + U_n)\partial/\partial n$ in (75), in general is *not* the time derivative along the sonic locus unlike the one in (62). In the sonic frame, we had $\mathcal{U}_{n*} = -c_*$ exactly as a speed relation. But now it is no longer true that $c_* + U_{n*} = 0$! In one dimension, we could write $c_* + U_{n*} = dn_*/dt$, in which case the operator $\partial/\partial t + (c + U_n)\partial/\partial n$ does indeed become a total derivative along the sonic locus. But in general two-dimensional detonation wave, the derivative $\partial/\partial t + (c + U_n)\partial/\partial n$ does not lie in the tangent plane of the sonic locus; only if the transverse variations can be neglected is the derivative in the sonic surface.

The speed relation expressed in the shock-attached coordinates is derived next. Let the equation

$$\Psi(x, y, t) = 0 \tag{78}$$

represent the level set of the sonic surface in the laboratory frame. Then its unit normal and normal speed are given by

$$\mathbf{n}_* = \frac{\nabla \psi}{|\nabla \psi|} \quad \text{and} \quad \mathcal{D} = -\frac{1}{|\nabla \psi|} \frac{\partial \psi}{\partial t},$$
 (79)

respectively, so that the general speed relation (39) can be re-written as

$$\frac{\partial \mathbf{\psi}}{\partial t} + c |\nabla \mathbf{\psi}| + \mathbf{u} \cdot \nabla \mathbf{\psi} = 0. \tag{80}$$

An interesting form of the speed relation is obtained from (80) by noting that $|\nabla \psi| = \mathbf{n}_* \cdot \nabla \psi$,

$$\frac{\partial \mathbf{\psi}}{\partial t} + (\mathbf{u} + c \,\mathbf{n}_*) \cdot \nabla \mathbf{\psi} = 0, \tag{81}$$

a transport equation that underscores propagation of the sonic surface in the direction of $\mathbf{u} + c\mathbf{n}_*$ with the normal speed $|\mathbf{u} + c\mathbf{n}_*|$. The derivative $\mathcal{L} = \partial/\partial t + (\mathbf{u} + c\mathbf{n}_*) \cdot \nabla$ is a directional time derivative normal to the sonic surface (which is the ray direction), so that equation (81) is an expression of constancy of ψ in the sonic surface.

In the shock-attached frame, (n, ξ, t) , the level-set equation can be written as

$$\Psi \equiv n - n_*(\xi, t) = 0, \tag{82}$$

where n_* is the normal distance from the shock to the sonic surface. Then we obtain that

$$\nabla \psi = \mathbf{n} - \frac{1}{1 + n_* \kappa} \frac{\partial n_*}{\partial \xi} \mathbf{t}, \quad \frac{\partial \psi}{\partial t} = -D - \frac{\partial n_*}{\partial t} - S \frac{\partial n_*}{\partial \xi}, \tag{83}$$

and

$$\mathbf{n}_* = \frac{1}{|\nabla \psi|} \left(\mathbf{n} - \frac{1}{1 + n_* \kappa} \frac{\partial n_*}{\partial \xi} \mathbf{t} \right). \tag{84}$$

Be reminded, that in these expressions κ is the curvature of the shock. Substituting these formulas into equation (80), we obtain the speed relation in the shock-attached frame,

$$\frac{\partial n_*}{\partial t} + \left(S + \frac{u_{\xi}}{1 + n_* \kappa}\right) \frac{\partial n_*}{\partial \xi} = U_n + c \sqrt{1 + \left(\frac{1}{1 + n_* \kappa} \frac{\partial n_*}{\partial \xi}\right)^2}.$$
 (85)

Again, this is an exact relation that expresses the speed relation for the sonic surface written in the shock-attached Bertrand coordinates in terms of the shock properties, that is the curvature κ and the stretch S, and the flow state in the sonic surface, $n_*(\xi,t)$, U_n , u_{ξ} , and c. Thus we have two equations, (75) and (85) that represent the sonic conditions in the shock-attached Bertrand frame.

Equation (85) can be rewritten as

$$c + U_n = \frac{\partial n_*}{\partial t} + \left(S + \frac{u_{\xi}}{1 + n_* \kappa}\right) \frac{\partial n_*}{\partial \xi} + c \left[1 - \sqrt{1 + \left(\frac{1}{1 + n_* \kappa} \frac{\partial n_*}{\partial \xi}\right)^2}\right], \tag{86}$$

from which one can see that the speed relation is similar to the equation of the forward characteristic in one dimension, (42), which in the shock-attached frame is $c + U_n = dn_*/dt$, but involves more terms, all due to the transverse variation.

Next we make certain approximations in order to simplify the sonic conditions (75) and (85) and to see their connection with the older formulations of DSD. Let us assume, that the shock curvature is small, $\kappa = o(1)$, and the transverse flow speed and transverse variations are also small, $u_{\xi} = o(1)$, $\partial/\partial \xi = o(1)$. Then retaining only the leading order terms, from equation (85), we obtain that

$$\frac{\partial n_*}{\partial t} = U_n + c_*. \tag{87}$$

Retaining only leading order curvature terms in equation (75), we obtain that

$$\frac{\partial p}{\partial t} + \rho c \frac{\partial u_n}{\partial t} + \kappa \rho c^2 u_n - \rho c^2 \sigma \omega = 0, \tag{88}$$

where the time derivative is now

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t} + (c + U_n) \frac{\partial}{\partial n} = \frac{\partial}{\partial t} + \frac{\partial n_*}{\partial t} \frac{\partial}{\partial n}.$$

The time derivative in (88) must be taken along the sonic locus, that is the state variables, p and u_n , must first be evaluated at the sonic locus and only then their derivatives be taken.

5 Sonic conditions of detonation stability theory

In this section, we show that the linearized version of the compatibility condition reduces to the radiation conditions of detonation stability theory (see, e.g. [6, 8, 12]). Here we derive the one- and two-dimensional radiation conditions.

One-dimensional radiation condition follows directly from equation (41) by straightforward linearization. Let us denote the steady base state by an overbar and perturbations about the base state by a prime, e.g. $p = \bar{p}(n) + p'(n,t)$, etc. Then the perturbed sonic state is given by

$$p_* = \bar{p}_* + p'(n_*, t), \ u_* = \bar{u}_* + u'(n_*, t), \tag{89}$$

$$\rho_* = \bar{\rho}_* + \rho'(n_*, t), \ \lambda_* = \bar{\lambda}_* + \lambda'(n_*, t), \tag{90}$$

where we can take $n_* = \bar{n}_*$ since the correction to the sonic locus, $n'_* = n_* - \bar{n}_*$, that results from the use of the speed relation,

$$\dot{n}'_* = c'_* + U'_{n_*},\tag{91}$$

contributes only higher order terms to expansions (89) and (90). The resultant radiation condition is

$$\frac{dp'}{dt} + \bar{\rho}_* \bar{c}_* \frac{du'}{dt} = \bar{\rho}_* \bar{c}_*^2 \bar{\sigma}_* \omega', \tag{92}$$

where we have taken into account that $\bar{\omega}_* = 0$ and where ω' is the perturbation of the reaction rate.

In the special case of an ideal gas, the equation of state is $p = \rho RT$, $e = pv/(\gamma - 1) - \lambda Q$, so that $\rho c^2 \sigma = (\gamma - 1) Q \rho$. For simple-depletion kinetics with $\nu = 1$, and normal-mode perturbations, $p' = \bar{p}'(n) \exp(\alpha t)$, etc., the radiation condition (92) reduces to

$$\alpha \left(\bar{p}'_* + \bar{\rho}_* \bar{c}_* \bar{u}'_*\right) + (\gamma - 1) Q \bar{\rho}_* k \exp\left(-E/\bar{p}_* \bar{v}_*\right) \bar{\lambda}'_* = 0, \tag{93}$$

which is exactly the CJ limit of the radiation condition derived by Lee and Stewart [8].

If the depletion factor is distinct from unity, that is $\omega = k (1 - \lambda)^{\nu} \exp(-E/p\nu)$ with $\nu < 1$, then the reaction-rate perturbation away from the sonic locus is

$$\omega' = \left(\frac{\partial \bar{\omega}}{\partial \bar{p}}\right) p' + \left(\frac{\partial \bar{\omega}}{\partial \bar{v}}\right) v' + \left(\frac{\partial \bar{\omega}}{\partial \bar{\lambda}}\right) \lambda'. \tag{94}$$

As $\bar{\lambda} \to 1$ one finds that $\left(\partial \bar{\omega}/\partial \bar{\lambda}\right) \sim \left(1-\bar{\lambda}\right)^{\nu-1} \to \infty$, so the last term in the previous expansion is non-uniform as the sonic locus is approached, clearly a result of the base-state reaction rate vanishing at the sonic locus. Near the sonic locus the reaction rate perturbation is

$$\omega' = \omega(\lambda_*) - \omega(\bar{\lambda}_*) = k(-\lambda')^{\mathsf{v}} \exp(-E/\bar{p}_*\bar{v}_*), \tag{95}$$

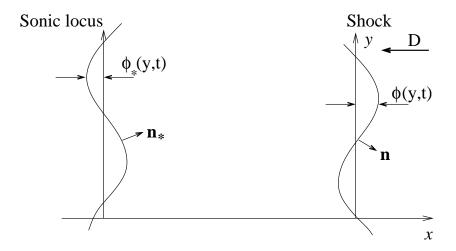


Figure 4: Perturbation of a two-dimensional steady detonation with an embedded sonic locus.

which is a *non-linear* function of λ' , another indication of non-uniformity of solutions of the original linearized system of Euler equations. If all perturbations in expansions (89) and (90) are assumed to be $O(\varepsilon)$ with $\varepsilon \to 0$, then the left-hand side of (92) is also $O(\varepsilon)$, while the right-hand side is $O(\varepsilon^{\mathsf{v}})$. It follows then, that although in the main-reaction layer (i.e. the region behind the shock, but away from the sonic locus), the perturbations are $O(\varepsilon)$, they are no longer $O(\varepsilon)$ as the sonic locus is approached (that is in the transonic layer). This potential non-uniformity has to be dealt with by considering the linear stability problem separately in the main-reaction layer and the transonic layer, a problem that is beyond the scope of the present paper.

Consider now a two-dimensional detonation wave with an embedded sonic locus subject to a small perturbation of the shock locus, $\phi(y,t)$, as shown in figure 4. Most treatments of detonation stability employ a Cartesian frame of reference attached to the perturbed shock so that the coordinate transformation from the lab frame is

$$x = x^{l} - Dt - \phi\left(y^{l}, t\right), \ y = y^{l}. \tag{96}$$

Here x^l and y^l are the lab-frame coordinates, D is the steady-state detonation speed, and ϕ is the small shock-displacement in the x direction. Thus the shock is always fixed at x = 0 and the reaction zone is at x < 0, while the unperturbed medium is at x > 0. The differential operators in the moving frame are now

$$\nabla = \frac{\partial}{\partial x}\mathbf{i} + \left(\frac{\partial}{\partial y} - \phi_y \frac{\partial}{\partial x}\right)\mathbf{j} \text{ and } \frac{D}{Dt} = \frac{\partial}{\partial t} + U_1 \frac{\partial}{\partial x} + u_2 \frac{\partial}{\partial y} - u_2 \phi_y \frac{\partial}{\partial x}, \tag{97}$$

where $U_1 = u_1 - D - \partial \phi / \partial t$ and u_2 are the x- and y- components of the particle speed relative to the perturbed shock, respectively.

Notice that the displacement of the sonic locus, $\phi_*(y,t)$, is not the same as ϕ and therefore, the unit normal, \mathbf{n}_* , to the sonic locus differs from \mathbf{n} , the unit normal to the shock. To the leading order in the displacements, the unit normals are given by

$$\mathbf{n} = \mathbf{i} - \frac{\partial \phi}{\partial y} \mathbf{j}, \ \mathbf{n}_* = \mathbf{i} - \frac{\partial \phi_*}{\partial y} \mathbf{j}. \tag{98}$$

It is easy to show that the small transverse component of \mathbf{n}_* contributes only second-order terms to the compatibility condition. Indeed, let $\phi = \phi' = o(1)$, $\phi_* = \phi'_* = o(1)$, and linearize the state variables about the steady state, as e.g. $p = \bar{p}(x) + p'(x,t)$, $\mathbf{u} = (\bar{u}_1 + u'_1)\mathbf{i} + u'_2\mathbf{j}$, etc., similar to the one-dimensional case; the primed quantities are small corrections to the base state. Retaining only

linear terms in perturbations, we find that

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \bar{U}_1 \frac{\partial}{\partial x} + \left(U_1' \frac{\partial}{\partial x} + u_2' \frac{\partial}{\partial y} \right), \tag{99}$$

$$\mathbf{n}_{*} \cdot \frac{D\mathbf{u}}{Dt} = \left(\mathbf{i} - \frac{\partial \phi_{*}'}{\partial y}\mathbf{j}\right) \cdot \left[\frac{\partial}{\partial t} + \bar{U}_{1}\frac{\partial}{\partial x} + \left(U_{1}'\frac{\partial}{\partial x} + u_{2}'\frac{\partial}{\partial y}\right)\right] \left(\bar{u}_{1}\mathbf{i} + \mathbf{u}'\right) = \\ \bar{U}_{1}\frac{\partial \bar{u}_{1}}{\partial x} + \left(\frac{\partial u_{1}'}{\partial t} + \bar{U}_{1}\frac{\partial u_{1}'}{\partial x} + U_{1}'\frac{\partial \bar{u}_{1}}{\partial x}\right), \tag{100}$$

$$\mathbf{n}_* \cdot \nabla p = \frac{\partial \bar{p}}{\partial x} + \frac{\partial p'}{\partial x}, \ \nabla \cdot \mathbf{u} = \frac{\partial \bar{u}_1}{\partial x} + \left(\frac{\partial u_1'}{\partial x} + \frac{\partial u_2'}{\partial y}\right), \tag{101}$$

and

$$\frac{Dp}{Dt} = \bar{U}_1 \frac{\partial \bar{p}}{\partial x} + \left(\frac{\partial p'}{\partial t} + U_1' \frac{\partial \bar{p}}{\partial x} + \bar{U}_1 \frac{\partial p'}{\partial x} \right). \tag{102}$$

Before linearization of the compatibility condition, it is convenient to rewrite it as

$$\rho c \left(\mathbf{n}_* \cdot \frac{D\mathbf{u}}{Dt} + c \nabla \cdot \mathbf{u} \right) + \frac{Dp}{Dt} + c \mathbf{n}_* \cdot \nabla p = \rho c^2 \sigma \omega. \tag{103}$$

We then find that

$$\mathbf{n}_* \cdot \frac{D\mathbf{u}}{Dt} + c\nabla \cdot \mathbf{u} = \left(\frac{\partial u_1'}{\partial t} + \bar{c}\frac{\partial u_2'}{\partial y}\right) + \left(c' + U_1'\right)\frac{\partial \bar{u}_1}{\partial x}$$
(104)

and

$$\frac{Dp}{Dt} + c\mathbf{n}_* \cdot \nabla p = \frac{\partial p'}{\partial t} + \left(c' + U_1'\right) \frac{\partial \bar{p}}{\partial x},\tag{105}$$

so that the linearized compatibility condition becomes

$$\frac{\partial p'}{\partial t} + \bar{\rho}_* \bar{c}_* \frac{\partial u_1'}{\partial t} + \bar{\rho}_* \bar{c}_*^2 \frac{\partial u_2'}{\partial v} = \bar{\rho}_* \bar{c}_*^2 \bar{\sigma}_* \omega', \tag{106}$$

or, in terms of the normal modes $(p' \rightarrow p' \exp(\alpha t + iky), \text{ etc.})$,

$$\alpha \left(p' + \bar{\rho}_* \bar{c}_* u_1' \right) + ik \bar{\rho}_* \bar{c}_*^2 u_2' = \bar{\rho}_* \bar{c}_*^2 \bar{\sigma}_* \omega'. \tag{107}$$

In deriving (104) and (105), we took advantage of the fact that $\bar{c}_* + \bar{U}_{1*} = 0$ and

$$\frac{\partial \bar{p}}{\partial x} + \bar{\rho}_* \bar{c}_* \frac{\partial \bar{u}_1}{\partial x} = 0, \tag{108}$$

where the latter result follows directly from the steady momentum equation, provided that

$$\lim_{n \to \bar{n}_*} (\bar{c} + \bar{U}_1) \frac{\partial \bar{u}_1}{\partial x} = 0, \tag{109}$$

a condition that is indeed satisfied for any reaction order v > 0, as one can easily check. Even if v < 1/2, when $\lim_{n \to \bar{n}_*} \partial \bar{u}_1/\partial x = \infty$, one can show that condition (109) still holds, because $\bar{c} + \bar{U}_1 \sim \sqrt{1-\bar{\lambda}}$, while $\partial \bar{u}_1/\partial x \sim (1-\bar{\lambda})^{v-1/2}$ as $\bar{\lambda} \to 1$.

If one sets the right-hand side of (107) to zero, then one obtains the CJ limit of the radiation condition of Short and Stewart [12]. But of course, equation (107) is more general as it includes a general rate term and holds for a general equation of state.

5.1 The compatibility condition as a boundedness condition

We now prove that for detonations with depletion factor v > 1/2, the linearized compatibility condition

$$\frac{dp'}{dt} + \bar{\rho}_* \bar{c}_* \left(\frac{dU'}{dt} + \frac{dD'}{dt} \right) - (\gamma - 1) Q \bar{\rho}_* \omega' = 0.$$
 (110)

is necessary for the linear stability problem to have solutions bounded at $n \to \bar{n}_*$.

Indeed, the one-dimensional Euler equations written in the shock-attached frame

$$v_t + Uv_n - vU_n = 0, \tag{111}$$

$$U_t + UU_n + vp_n = -D_t, (112)$$

$$p_t + Up_n + \gamma p U_n = (\gamma - 1)Q\rho\omega, \tag{113}$$

$$\lambda_t + U\lambda_n = \omega, \tag{114}$$

can be linearized so that the following set of linear equations is obtained

$$v_t' + \bar{U}v_n' + \bar{v}_n U' - \bar{v}U_n' - \bar{U}_n v' = 0, \tag{115}$$

$$U'_t + \bar{U}U'_n + \bar{U}_nU' + \bar{v}p'_n + \bar{p}_nv' = -D'_t, \tag{116}$$

$$p'_{t} + \bar{U}p'_{n} + \bar{p}_{n}U' + \gamma\bar{p}U'_{n} + \gamma\bar{U}_{n}p' - (\gamma - 1)Q(\bar{\rho}\omega' + \bar{\omega}\rho') = 0,$$
(117)

$$\lambda_t' + \bar{U}\lambda_n' + \bar{\lambda}_n U' = \omega', \tag{118}$$

where the perturbations are assumed to be small deviations from the corresponding steady-state values. Adding equation (117) and equation (116) multiplied by $\bar{\rho}\bar{c}$, one obtains

$$\left[\frac{\partial}{\partial t} + (\bar{U} + \bar{c})\frac{\partial}{\partial n}\right] p' + \bar{\rho}\bar{c}\left[\frac{\partial}{\partial t} + (\bar{U} + \bar{c})\frac{\partial}{\partial n}\right] (U' + D') - (\gamma - 1)Q\bar{\rho}\omega' + (\bar{p}_n + \bar{\rho}\bar{c}\bar{U}_n)U' + \gamma\bar{U}_n p' + \bar{\rho}\bar{c}\bar{p}_n v' - (\gamma - 1)Q\bar{\omega}\rho' = 0.$$
(119)

The first two terms are seen to form time derivatives along the steady C_+ characteristic direction, $\partial/\partial t + (\bar{U} + \bar{c}) \partial/\partial n$, so that the first line of (119) tends to the compatibility condition in the limit $n \to \bar{n}_*$ (so that $\bar{U} + \bar{c} \to 0$). All terms in the second line vanish as $n \to \bar{n}_*$ provided that $\nu > 1/2$ (so that the spatial derivatives of the base state vanish at the sonic locus) and that all perturbations remain uniformly bounded. Thus our statement is proved.

6 Conclusions

In this work we have introduced a general definition of a sonic locus for multi-dimensional unsteady self-sustained detonation waves and discussed its properties under important limiting conditions that are relevant to detonation stability theories and asymptotic theories of slowly evolving weakly curved detonations. We have shown that previously known sonic conditions of steady detonation theory, linear stability theory, and detonation shock dynamics are all limiting cases of our generalized conditions. Importantly, self-sustained detonations are shown to be two-front phenomena with the lead shock and the limiting characteristic surface (as the sonic locus) as free boundaries. The sonic conditions that we have derived are closure equations that together with the Euler equations and Rankine-Hugoniot conditions complete the set of governing equations for self-sustained detonations.

An important ingredient of the present theory is that the sonic surface is assumed to exist initially; we simply take it as given in the initial conditions. The initial condition could be, for example, a steady detonation wave in which a sonic surface can be defined unambiguously, and a clear exact case is that of the steady CJ detonation or a weakly perturbed detonation that corresponds to theories

relevant to detonation instability or detonation shock dynamics, both of which are perturbation theories that assume either deviations from a plane CJ state or weak spatial and temporal variation from plane states. Many important initial conditions, for example, in initiation problems, will not have an initial sonic locus. But as the detonation forms and becomes a self-sustained wave, the sonic locus will appear somewhere in the flow. From that point on, the detonation dynamics is described by our theory provided only that the sonic locus persists in the flow, which is the case if the flow evolution is smooth.

Clearly, appearance of strong discontinuities within the reaction zone, such as shock waves, can destroy a sonic surface in which case the present theory may not be applicable. It is indeed the case in gas-phase detonations that strong transverse shock fronts almost always exist which can interact with the sonic surface. Yet, the situations is quite different in condensed explosives in which smooth reaction zones are more common. In any case, the range of phenomena that the present theory can address is considerable, and even in the case of cellular detonations, the onset of cellular dynamics and propagation of weakly unstable detonations may be phenomena that the present theory is applicable to. Some applications of the theory to weakly curved and slowly evolving detonations as well as to the stability problems in explosives described by complex equation of state and rate law can be found in [5] and in forthcoming papers.

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1020	Bhattacharjee, P., and D. N. Riahi	Effect of rotation on surface tension driven flow during protein crystallization – <i>Microgravity Science and Technology</i> 14 , 36–44 (2003)	Apr. 2003
1021	Fried, E.	The configurational and standard force balances are not always statements of a single law — <i>Proceedings of the Royal Society</i> (submitted)	Apr. 2003
1022	Panat, R. P., and K. J. Hsia	Experimental investigation of the bond coat rumpling instability under isothermal and cyclic thermal histories in thermal barrier systems – <i>Proceedings of the Royal Society of London A</i> 460 , 1957–1979 (2003)	May 2003
1023	Fried, E., and M. E. Gurtin	A unified treatment of evolving interfaces accounting for small deformations and atomic transport: grain-boundaries, phase transitions, epitaxy – <i>Advances in Applied Mechanics</i> , in press (2003)	May 2003
1024	Dong, F., D. N. Riahi, and A. T. Hsui	On similarity waves in compacting media – <i>Horizons in Physics</i> , in press (2003)	May 2003
1025	Liu, M., and K. J. Hsia	Locking of electric field induced non-180° domain switching and phase transition in ferroelectric materials upon cyclic electric fatigue — <i>Applied Physics Letters</i> 83 , 3978–3980 (2003)	May 2003
1026	Liu, M., K. J. Hsia, and M. Sardela Jr.	In situ X-ray diffraction study of electric field induced domain switching and phase transition in PZT-5H— <i>Journal of the American Ceramics Society</i> (submitted)	May 2003
1027	Riahi, D. N.	On flow of binary alloys during crystal growth – Recent Research Development in Crystal Growth, in press (2003)	May 2003
1028	Riahi, D. N.	On fluid dynamics during crystallization — Recent Research Development in Fluid Dynamics, in press (2003)	July 2003
1029	Fried, E., V. Korchagin, and R. E. Todres	Biaxial disclinated states in nematic elastomers — <i>Journal of Chemical Physics</i> 119 , 13170–13179 (2003)	July 2003
1030	Sharp, K. V., and R. J. Adrian	Transition from laminar to turbulent flow in liquid filled microtubes — <i>Physics of Fluids</i> (submitted)	July 2003
1031	Yoon, H. S., D. F. Hill, S. Balachandar, R. J. Adrian, and M. Y. Ha	Reynolds number scaling of flow in a Rushton turbine stirred tank: Part I — Mean flow, circular jet and tip vortex scaling — <i>Chemical Engineering Science</i> (submitted)	Aug. 2003
1032	Raju, R., S. Balachandar, D. F. Hill, and R. J. Adrian	Reynolds number scaling of flow in a Rushton turbine stirred tank: Part II — Eigen-decomposition of fluctuation — <i>Chemical Engineering Science</i> (submitted)	Aug. 2003
1033	Hill, K. M., G. Gioia, and V. V. Tota	Structure and kinematics in dense free-surface granular flow – <i>Physical Review Letters</i> , in press (2003)	Aug. 2003

List of Recent TAM Reports (cont'd)

No.	Authors	Title	Date
1034	Fried, E., and S. Sellers	Free-energy density functions for nematic elastomers — <i>Journal of the Mechanics and Physics of Solids</i> 52 , 1671–1689 (2004)	Sept. 2003
1035	Kasimov, A. R., and D. S. Stewart	On the dynamics of self-sustained one-dimensional detonations: A numerical study in the shock-attached frame — <i>Physics of Fluids</i> (submitted)	Nov. 2003
1036	Fried, E., and B. C. Roy	Disclinations in a homogeneously deformed nematic elastomer — <i>Nature Materials</i> (submitted)	Nov. 2003
1037	Fried, E., and M. E. Gurtin	The unifying nature of the configurational force balance – <i>Mechanics of Material Forces</i> (P. Steinmann and G. A. Maugin, eds.), in press (2003)	Dec. 2003
1038	Panat, R., K. J. Hsia, and J. W. Oldham	Rumpling instability in thermal barrier systems under isothermal conditions in vacuum — <i>Philosophical Magazine</i> , in press (2004)	Dec. 2003
1039	Cermelli, P., E. Fried, and M. E. Gurtin	Sharp-interface nematic-isotropic phase transitions without flow – <i>Archive for Rational Mechanics and Analysis</i> (submitted)	Dec. 2003
1040	Yoo, S., and D. S. Stewart	A hybrid level-set method in two and three dimensions for modeling detonation and combustion problems in complex geometries— <i>Combustion Theory and Modeling</i> (submitted)	Feb. 2004
1041	Dienberg, C. E., S. E. Ott-Monsivais, J. L. Ranchero, A. A. Rzeszutko, and C. L. Winter	Proceedings of the Fifth Annual Research Conference in Mechanics (April 2003), TAM Department, UIUC (E. N. Brown, ed.)	Feb. 2004
1042	Kasimov, A. R., and D. S. Stewart	Asymptotic theory of ignition and failure of self-sustained detonations — <i>Journal of Fluid Mechanics</i> (submitted)	Feb. 2004
1043	Kasimov, A. R., and D. S. Stewart	Theory of direct initiation of gaseous detonations and comparison with experiment – <i>Proceedings of the Combustion Institute</i> (submitted)	Mar. 2004
1044	Panat, R., K. J. Hsia, and D. G. Cahill	Evolution of surface waviness in thin films via volume and surface diffusion — <i>Journal of Applied Physics</i> (submitted)	Mar. 2004
1045	Riahi, D. N.	Steady and oscillatory flow in a mushy layer — <i>Current Topics in Crystal Growth Research</i> , in press (2004)	Mar. 2004
1046	Riahi, D. N.	Modeling flows in protein crystal growth – <i>Current Topics in Crystal Growth Research</i> , in press (2004)	Mar. 2004
1047	Bagchi, P., and S. Balachandar	Response of the wake of an isolated particle to isotropic turbulent cross-flow — <i>Journal of Fluid Mechanics</i> (submitted)	Mar. 2004
1048	Brown, E. N., S. R. White, and N. R. Sottos	Fatigue crack propagation in microcapsule toughened epoxy — <i>Journal of Materials Science</i> (submitted)	Apr. 2004
1049	Zeng, L., S. Balachandar, and P. Fischer	Wall-induced forces on a rigid sphere at finite Reynolds number — <i>Journal of Fluid Mechanics</i> (submitted)	May 2004
1050	Dolbow, J., E. Fried, and H. Ji	A numerical strategy for investigating the kinetic response of stimulus-responsive hydrogels — <i>Journal of the Mechanics and Physics of Solids</i> (submitted)	June 2004
1051	Riahi, D. N.	Effect of permeability on steady flow in a dendrite layer — <i>Journal of Porous Media</i> (submitted)	July 2004
1052	Cermelli, P., E. Fried, and M. E. Gurtin	Transport relations for surface integrals arising in the formulation of balance laws for evolving fluid interfaces — <i>Journal of Fluid Mechanics</i> (submitted)	Sept. 2004
1053	Stewart, D. S., and A. R. Kasimov	Theory of detonation with an embedded sonic locus— <i>SIAM Journal on Applied Mathematics</i> (submitted)	Oct. 2004