

SONIC CONDITIONS FOR SELF-SUSTINED DETONATION WAVE

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Abstract

The generalized sonic conditions for a three-dimensional unsteady self-sustained detonations wave are derived by defining sonic locus as a limiting characteristic surface of the governing hyperbolic equations embedded in the reactive zone at a finite distance behind the shock. Two compatibility conditions are derived by considering Whitham's shock ray co-ordinate system as a front attached co-ordinate, which are necessary to determine the motion of both the lead shock and the sonic surface. The domain of influence of reactive zone is bounded by two surfaces; the lead shock surface and the trailing characteristic surface. The geometry of these two surfaces plays an important role in the underlying dynamics.

Key Words: The generalized sonic conditions, Hyperbolic equation, Shock ray.

Introduction

A detonation wave is a shock wave that triggers exothermic reaction in an explosive as it propagates so that the energy released in the reaction sustains the shock propagation. The original theory of detonation was first developed independently by Zeldovich, von Neumann and Doering in 1940's, known as ZND theory (Fickett and Davis (1979)). ZND theory describes the dynamics of a steady one-dimensional planar detonation in a gaseous explosive. This theory is applicable to self-sustained detonations and over driven detonation both. In a self-sustained detonations motion is sustained entirely by the energy released in their reaction zone while in over driven detonations an additional external support is required to maintain their motion at a nominal speed. In a self-sustained steady one-dimensional 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. Consequently, the leading shock is influenced only by the flow between the shock and the sonic locus. In case of over driven detonations, there exists no sonic locus, the leading shock is influenced by the entire region between the shock and the support.

In modern theory of detonation it has been observed that high explosive detonations are usually curved. Clearly the ZND theory is too simple to account for the observed structure and in the cases where unsteady and multi-dimensional detonations are considered. The equations governing the CJ- detonation are not closed without the condition of sonicity. Understanding of

the nature of sonic conditions in detonations, more general than ZND theory that includes effects of multidimensionality through the shock curvature term is difficult to achieve. Originally, the effect of curvature in the sonic conditions was considered by Wood and Kirkwood (1954) and later was derived rationally in the works of Bdzil (1981), Stewart and Bdzil (1988), (1988), Bdzil, and Stewart (1988). Yao and Stewart (1996) considered an extension of the sonic conditions to include asymptotically small unsteady correction, but their analysis relies partially on the steady concept of sonic locus by assuming that the flow is sonic relative to the lead shock that constrains the sonic locus to always be parallel to the shock. Recently generalized sonic conditions, for a three dimensional unsteady self-sustained detonation wave, are derived by Stewart and Kasimov (2005). They have generalized their results by defining sonic locus as a limiting characteristic surface of the governing hyperbolic equations embedded in the reaction zone at a finite distance behind the shock. 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. Thus, the detonation problem is, in general, a two front problem with both fronts as free boundaries and therefore, sonic conditions must be given by two equations. Kasimov and Stewart (2004) have illustrated the behavior of the sonic locus as a limiting characteristic surface in one-dimensional detonations by means of a numerical simulation. Stewart and Kasimov (2005) have proposed that the sonic conditions for general multidimensional detonations are (1) the condition of local sonicity, that is, for an observer moving with the surface, the particle speed normal to that surface is locally sonic and (2) the compatibility condition in the sonic surface defined as a characteristic surface of the governing reactive Euler equations. These two conditions are direct consequences of the governing hyperbolic equations and hold therefore under quite general circumstances.

In detonation shock dynamics, 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. Stewart and Kasimov (2005) have derived sonic conditions in two dimensional surface attached Bertrand co-ordinates i.e. sonic conditions in the sonic frame attached co-ordinates and in the shock attached frame. Here our aim is also to derive sonic conditions in the three dimensional front attached co-ordinates by introducing Whitham's shock ray co-ordinates system (Whitham (1974)). In section 2, we follow the derivation of the Stewart and Kasimov (2005) to discuss the theory of characteristic surfaces for general system of

quasi-linear hyperbolic partial differential equations and to derive compatibility conditions in the exceptional surface. The compatibility conditions for reactive Euler equations in three dimensions and in particular, the sonic conditions in one dimensional are discussed in section 3. Section 4, is devoted to two dimensional detonations where we specialize the sonic conditions to local frame defined by Witham's shock ray co-ordinate system.

2. Characteristic Surfaces of Hyperbolic Partial Differential Equations and Compatibility Conditions for Reactive Euler Equations.

A general system of quasi-linear hyperbolic equations can be written as

$$(2.1) \quad a_{ij}^k \frac{\partial u_j}{\partial x_k} = b_i$$

where the coefficient a_{ij}^k are functions of the state variable u_j , $j=1, 2, \dots, j$, index i represents the individual equations of motion, x_k are the independent variables, and b_i are the source terms. Multiplying the equations by arbitrary α_i and summing over all the equations

$$(2.2) \quad \alpha_i a_{ij}^k \frac{\partial u_j}{\partial x_k} = m^k \frac{\partial}{\partial x_k} (u_j) = \alpha_i b_i$$

Each term on the left hand side of (2.2) is a directional derivative in space with direction tangents, m , whose components labeled by k , are given by $m^k = \alpha_i a_{ij}^k$. A characteristic surface is defined as a surface such that linear combination (2.2) of directional derivatives expresses changes only in that surface. Then all direction tangents must lie in that surface, and therefore the linear combination (2.2) 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 , i.e.

$$(2.3) \quad m^k \beta_k = \alpha_i \beta_k a_{ij}^k = 0$$

This is the system of J homogeneous linear algebraic equations for α_i , with a nontrivial solution if and only if

$$(2.4) \quad \left| \beta_k a_{ij}^k \right| = 0$$

which is a J^{th} order polynomial that determines a constraint on the direction vector β . If one of the independent variables is time, then constraint on the direction in space time defines the velocity of the characteristic.

The compatibility condition is simply the differential relation (2.2) found on the characteristic surface. First solve β_k by solving the characteristic polynomial. The second step is to choose a direction that expresses the compatibility relation in the characteristic surface. Since the system of the 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 . if such a direction β_k^* with a corresponding α_i^* is found, then the compatibility condition is specifically

$$(2.5) \quad \alpha_i^* a_{ij}^k \frac{\partial u_j}{\partial x_k} = \alpha_i^* b_i$$

In particular, to derive compatibility conditions for reactive Euler equations, 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 velocity vector $u = u_i + v_j + w_k$. Therefore, without loss of generality,

the material derivative is $\frac{d}{dt} = \frac{\partial}{\partial t} + u \frac{\partial}{\partial x}$. The general condition for the characteristic surfaces is

expressed for this special system and subsequently rewritten in a frame invariant rotation so that any co-ordinate system can be used. The equations of motion are (Stewart and Kasimov (2005)),

$$(2.6) \quad u \frac{\partial u}{\partial x} + \frac{\partial u}{\partial t} + \frac{1}{\rho} \frac{\partial p}{\partial x} = 0$$

$$(2.7) \quad u \frac{\partial v}{\partial x} + \frac{\partial v}{\partial t} + \frac{1}{\rho} \frac{\partial p}{\partial y} = 0$$

$$(2.8) \quad u \frac{\partial w}{\partial x} + \frac{\partial w}{\partial t} + \frac{1}{\rho} \frac{\partial p}{\partial z} = 0$$

$$(2.9) \quad \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} + \frac{u}{\rho} \frac{\partial \rho}{\partial x} + \frac{1}{\rho} \frac{\partial \rho}{\partial t} = 0$$

$$(2.10) \quad u \frac{\partial p}{\partial x} + \frac{\partial p}{\partial t} - c^2 \left(u \frac{\partial \rho}{\partial x} + \frac{\partial \rho}{\partial t} \right) = \rho c^2 \sigma w$$

$$(2.11) \quad u \frac{\partial \lambda}{\partial x} + \frac{\partial \lambda}{\partial t} = 0$$

where p , ρ , w , c and σ are the pressure, density, reaction progress variable, reaction rate, frozen speed of sound and thermicity coefficient respectively.

The general expression for sound speed and thermicity coefficient are (Fickett and Davis (1979))

$$(2.12) \quad c^2 = \frac{p - \rho^2 e_p}{\rho^2 e_p}$$

and

$$(2.13) \quad \sigma = -\frac{1}{\rho c^2} \frac{e_\lambda}{e_p}$$

where $e = e(p, \rho, \lambda)$ is the general equation of state and the subscripts of e denote partial differentiation equation with respect to arguments.

Denoting $(u, v, w, p, \rho, \lambda)$ by u_j with $j=1,2,3,\dots,6$ and independent variables (x, y, z, t) by x_k with $k=1,2,3,4$, we can write the equations of motion (2.6) to (2.11) in the form (2.1) where a_{ij}^k can be identified easily (Stewart and Kasimov(2005)).

Taking determinants of the characteristic matrix $\beta_k a_{ij}^k$ equal to zero, we have

$$(2.14) \quad -\frac{\beta_o^4}{\rho} \left\{ \beta_o^2 - c^2 (\beta_1^2 + \beta_2^2 + \beta_3^2) \right\} = 0$$

where $\beta_o = u\beta_1 + \beta_4$. The repeated root denoted by $\beta_o = u\beta_1 + \beta_4 = 0$ is associated with the stream surfaces that form the characteristic surface. In addition, there are two other surfaces associated with the roots of the other factor

$$(2.15) \quad \beta_o = \pm c \sqrt{\beta_1^2 + \beta_2^2 + \beta_3^2}$$

To define the compatibility relation we need to solve the equations for α_i . Using the previous definition we obtain the equations

$$(2.16) \quad \alpha_1 \beta_o + \alpha_4 \beta_1 = 0$$

$$(2.17) \quad \alpha_2 \beta_o + \alpha_4 \beta_2 = 0$$

$$(2.18) \quad \alpha_3 \beta_o + \alpha_4 \beta_3 = 0$$

$$(2.19) \quad \frac{1}{\rho} (\alpha_1 \beta_1 + \alpha_2 \beta_2 + \alpha_3 \beta_3) + \alpha_5 \beta_o = 0$$

$$(2.20) \quad \frac{\alpha_4 \beta_o}{\rho} - c^2 \alpha_5 \beta_o = 0$$

$$(2.21) \quad \alpha_6 \beta_o = 0$$

The solution of this system is

$$(2.22) \quad \alpha_1 = -\frac{\alpha_4 \beta_1}{\beta_o}, \quad \alpha_2 = -\frac{\alpha_4 \beta_2}{\beta_o}, \quad \alpha_3 = -\frac{\alpha_4 \beta_3}{\beta_o}, \quad \alpha_5 = \frac{\alpha_4}{\rho c^2}, \quad \alpha_6 = 0$$

The compatibility condition (2.2) may be written as

$$(2.23) \quad \alpha_1 a_{1j}^k \frac{\partial u_j}{\partial x_k} + \alpha_2 a_{2j}^k \frac{\partial u_j}{\partial x_k} + \alpha_3 a_{3j}^k \frac{\partial u_j}{\partial x_k} + \alpha_4 a_{4j}^k \frac{\partial u_j}{\partial x_k} + \alpha_5 a_{5j}^k \frac{\partial u_j}{\partial x_k} = \alpha_5 b_5$$

Substituting the values of α_i , we have

$$(2.24) \quad -\frac{\alpha_4}{\beta_o} \left[\beta_1 a_{1j}^k \frac{\partial u_j}{\partial x_k} + \beta_2 a_{2j}^k \frac{\partial u_j}{\partial x_k} + \beta_3 a_{3j}^k \frac{\partial u_j}{\partial x_k} \right] + \alpha_4 \left[a_{4j}^k \frac{\partial u_j}{\partial x_k} + \frac{1}{\rho c^2} a_{5j}^k \frac{\partial u_j}{\partial x_k} \right]$$

$$= \frac{\alpha_4 b_5}{\rho c^2}$$

Each of the terms in equation (2.24) represents one of the governing equations. Let us introduce the unit vector

$$(2.25) \quad \mathbf{n} = \frac{\beta_1 \mathbf{i} + \beta_2 \mathbf{j} + \beta_3 \mathbf{k}}{\sqrt{\beta_1^2 + \beta_2^2 + \beta_3^2}}$$

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

The collection of the terms in (2.24) can be written as

$$(2.26) \quad -\frac{\alpha_4}{\beta_o} \left(\sqrt{\beta_1^2 + \beta_2^2 + \beta_3^2} \right) \mathbf{n} \cdot \left[\frac{D\mathbf{u}}{Dt} + \frac{1}{\rho} \nabla p \right]$$

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

Simplifying (2.26) and then multiplying by ρc^2 , we have

$$(2.27) \quad -\frac{\sqrt{\beta_1^2 + \beta_2^2 + \beta_3^2}}{\beta_o} (\rho c^2) \mathbf{n} \cdot \left[\frac{D\mathbf{u}}{Dt} + \frac{1}{\rho} \nabla p \right] + \left[\rho c^2 \nabla \cdot \mathbf{u} + \frac{Dp}{Dt} \right] = \rho c^2 \sigma \omega$$

This is the frame invariant expression of the compatibility condition on the characteristic surface.

Using (2.15) in (2.27) we may write compatibility condition in the form

$$(2.28) \quad m(\rho c)n \cdot \left[\frac{D\mathbf{u}}{Dt} + \frac{1}{\rho} \nabla p \right] + \left[\rho c^2 (\nabla \cdot \mathbf{u}) + \frac{Dp}{Dt} \right] = \rho c^2 \sigma \omega$$

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

$$(2.29) \quad u\beta_1 + \beta_4 = \pm c \sqrt{\beta_1^2 + \beta_2^2 + \beta_3^2}$$

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 $u \cdot \mathbf{n}$. β_4 is the velocity of the characteristic surface normal to itself, i.e. $\beta_4 = V_n$ (say). Thus, from (2.29)

$$(2.30) \quad V_n = \mathbf{u} \cdot \mathbf{n} \pm c$$

In one dimension, this reduces to the familiar equation for the slope of the characteristics

$$V_n = \frac{dx}{dt} = u \pm c$$

Consider the forward propagating surface corresponding to the plus sign in (2.30). The particle velocity in the frame of an observer travelling in the forward surface is $u_n - V_n$ and the speed relation can be rewritten as

$$(2.31) \quad \frac{u_n - V_n}{c} = -1$$

This means on this characteristic surface the local normal Mach number is always unity, which is the definition of sonic. Thus, (2.28) gives differential condition in the sonic surface and a scalar speed relation (2.31) determine the motion of the surface.

Suppose a detonation wave is propagating along the positive x-direction, then the normal to the characteristic surface embedded in the reaction zone, which can possibly intersect the shock points forward. Therefore we select the plus sign in (2.28). Let \mathbf{n}^* be the unit normal to the characteristic surface. The compatibility condition for this surface is

$$(2.32) \quad \rho c_n \left[\frac{D\mathbf{u}}{Dt} + \frac{1}{\rho} \nabla p \right] + \left[\rho c^2 (\nabla \cdot \mathbf{u}) + \frac{Dp}{Dt} \right] = \rho c^2 \sigma \omega$$

where all the terms of the equation (2.32) are evaluated at the sonic surface. The compatibility condition (2.32) 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.

In one-dimensional motion, the compatibility condition (2.32) reduces to the equation

$$(2.33) \quad \rho c \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x} \right) + \rho c^2 \frac{\partial u}{\partial x} + \frac{\partial p}{\partial t} + u \frac{\partial p}{\partial x} = \rho c^2 \sigma \omega$$

which can be re-written as?

$$(2.34) \quad \frac{dp_*}{dt} + \rho_* c_* \frac{du_*}{dt} = \rho_* c_*^2 \sigma_* \omega_*$$

where

$$(2.35) \quad \frac{d}{dt} = \frac{\partial}{\partial t} + (u_* + c_*) \frac{\partial}{\partial x} = \frac{\partial}{\partial t} + \frac{dx_*}{dt} \frac{\partial}{\partial x}, \quad \frac{dx_*}{dt} = u_* + c_*$$

* refer to a quantity evaluated at sonic surfaces.

The time derivatives in (2.34) are the derivatives along the characteristics i.e. the derivatives lie in the tangent plane of the characteristic surface.

The compatibility condition for one dimensional detonation with point symmetry (j= 0, 1, 2) is

$$(2.36) \quad \frac{dp_*}{dt} + \rho_* c_* \frac{du_*}{dt} + \frac{j}{r} \rho_* c_*^2 u_* = \rho_* c_*^2 \sigma_* \omega_*$$

where r is the radial co-ordinate, while speed reaction is

$$(2.37) \quad \frac{dr_*}{dt} = c_* + u_*$$

3. Whitham's Shock Ray Co-ordinates System

We introduce here the Whitham's shock ray co-ordinates as a shock attached reference frame. In analogy to the Huyghens principle, orthogonal trajectories of successive shock surfaces, called "shock rays" serve as co-ordinate lines of the normal co-ordinate ξ . With each point X on the shock ray, we associate a unit normal vector $n(X)$ and a scalar wave speed $\hat{D}(X)$ as follows: $n(X)$ is the unit tangent to the shock ray at X and $\hat{D}(X)$ is the value of the front normal velocity in x at the instant when the shock passes the point.

Let $X = X_0(\mathfrak{S})$ the parameterize the initial shock surface; then \mathfrak{S}^i ($i = 1, 2$) label the shock rays emanating from this reference front, so that

$$(3.1) \quad \underline{\mathfrak{S}} = \text{constant along shock rays}$$

We specify the normal co-ordinate ξ by the following statements. (Struik (1950), Millman and Parker (1977)), Klein and Stewart (1993)

1. At any given time τ , the arc length ds of a line element on a shock ray at a point \bar{x} is

$$(3.2) \quad ds = \hat{D}(X)d\xi$$

2. A point $\bar{x}(\xi, \mathfrak{S}, \tau)$ with $(\xi, \mathfrak{S}) = \text{constant}$ moves in time along a ray at the speed \hat{D} i.e.

$$(3.3) \quad ds = \hat{D}(X)d\tau$$

3. $\xi = 0$ on the shock surface.

Thus, we have

$$(3.4) \quad \frac{\partial X}{\partial \xi}(\xi, \underline{\mathfrak{S}}, \tau) \frac{\partial X}{\partial \tau}(\xi, \underline{\mathfrak{S}}, \tau) = \left(\hat{D} n \right) (X(\xi, \underline{\mathfrak{S}}, \tau))$$

and all the metric functions associated with the co-ordinate transformation will depend only on the combination of variables $(\underline{\mathfrak{S}}, \xi + \tau)$. The \mathfrak{S}^i ($i= 1, 2$) are a set of tangential co-ordinates in the surface $\xi = \text{constant}$.

Take upper and lower roman indices cover the range $\{1, 2\}$, while Greek indices cover $\{0, 1, 2\}$ and use the summation convention for the respective ranges of the indices. For convenience, we define

$$(3.5) \quad \mathfrak{S}^0 = \xi$$

The vectors

$$(3.6) \quad \mathbf{g}_0 = \frac{\partial \mathbf{X}}{\partial \xi} = \left(\hat{\mathbf{D}} \mathbf{n} \right) (\underline{\mathfrak{S}}, \xi + \tau) \quad \text{and} \quad \mathbf{g}_i = \frac{\partial \mathbf{X}}{\partial \mathfrak{S}^i} (\underline{\mathfrak{S}}, \xi + \tau)$$

Form the local co-variant basis $\{\mathbf{g}_0, \mathbf{g}_1, \mathbf{g}_2\}$ associated with the mapping $(\xi, \underline{\mathfrak{S}}) \rightarrow \mathbf{X}$.

The co-variant basis determines the co-variant metric coefficient

$$(3.7) \quad \mathbf{g}_{\nu, \mu} = (\mathbf{g}_\mu \cdot \mathbf{g}_\nu) = \begin{bmatrix} \hat{\mathbf{D}}^2 & 0 \\ 0 & \mathbf{g}_{ij} \end{bmatrix}$$

The yet unknown coefficients (\mathbf{g}_{ij}) , ($i, j = 1, 2$) characterize the transverse parametrization.

The zeros in (3.7) arise because $(\mathbf{g}_0 : \mathbf{n} \perp \mathbf{g}_i)$

Associated with the covariant basis $\{\mathbf{g}_\nu\}$, is its dual $\{\mathbf{g}^\nu\}$, the contravariant basis. It is defined by

$$(3.8) \quad \mathbf{g}^\mu \cdot \mathbf{g}_\nu = \delta_\nu^\mu$$

where δ_ν^μ is the Kronecker delta.

An alternative but equivalent definition of the contravariant basis is given by

$$(3.9) \quad \mathbf{g}^o = \text{grad}(\xi) = \left(\frac{1}{\hat{D}} \mathbf{n} \right) (\mathfrak{S}, \xi + \tau) \text{ and } \mathbf{g}^i = \text{grad}(\mathfrak{S}^i)$$

The Jacobian determinant of the co-ordinate mapping is

$$(3.10) \quad J = \mathbf{g}_o \cdot (\mathbf{g}_1 \times \mathbf{g}_2) = \sqrt{\det(\mathbf{g}_{\nu\mu})} = \hat{D} \hat{A} \text{ with } \hat{A} = \sqrt{\det(\mathbf{g}_{ij})}$$

The Jacobian relates volume elements in the physical space to volume elements in the co-ordinate space through $dV = J d\xi d\mathfrak{S}^1 d\mathfrak{S}^2$. The physical meaning of \hat{A} as a ray tube area function.

The velocity relative to the moving co-ordinate frame i.e. relative to a point $(\xi, \mathfrak{S}) = \text{constant}$ is

$$(3.11) \quad \mathbf{U} = u^\nu \mathbf{g}_\nu = \hat{u} \mathbf{x} + u^i \mathbf{g}_i$$

where the $\{u^\nu\}$ are the contravariant velocity components. The contravariant velocity co-

ordinate is $u^o = \frac{\hat{u}}{\hat{D}}$ while \hat{u} is the physical value of the normal velocity relative to the shock

attached reference frame. From (3.4), the velocity in an inertial frame is

$$(3.12) \quad \mathbf{U} = \left(\hat{u} + \hat{D} \right) \mathbf{n} + u^i \mathbf{g}_i$$

The gradient operator reads as

$$(3.13) \quad \text{grad} = \mathbf{g}^\nu \frac{\partial}{\partial \mathfrak{S}^\nu} = \frac{1}{\hat{D}} \mathbf{n} \frac{\partial}{\partial \xi} + \mathbf{g}^i \frac{\partial}{\partial \mathfrak{S}^i}$$

Beginning with a formulation in terms of Cartesian co-ordinates $(t, x^\nu), (\nu = 0, 1, 2)$, we write

$$(3.14) \quad \frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \text{grad}.$$

The co-ordinate transformation $(t, x^v) \rightarrow (\tau, \mathfrak{I}^v)$ implies that

$$(3.15) \quad \frac{\partial}{\partial \tau} = \frac{\partial}{\partial t} + \frac{\partial X}{\partial \tau} \cdot \text{grad}$$

such that

$$(3.15) \quad \frac{D}{D\tau} = \frac{\partial}{\partial \tau} + \left(\mathbf{u} - \frac{\partial X}{\partial \tau} \right) \frac{\partial X}{\partial \tau} \cdot \text{grad}$$

Due to (3.4), (3.12) and (3.13), we have

$$(3.17) \quad \frac{D}{Dt} = \frac{\partial}{\partial \tau} + \left(\hat{\mathbf{u}} \mathbf{n} + \mathbf{u}^j \mathbf{g}_j \right) \cdot \left(\frac{1}{\hat{D}} \mathbf{n} \frac{\partial}{\partial \xi} + \mathbf{g}^i \frac{\partial}{\partial \mathfrak{I}^i} \right)$$

Since $\mathbf{n} \perp \mathbf{g}^i$ and $\mathbf{g}_i \mathbf{g}^i = \delta_j^i$, we obtain

$$(3.18) \quad \frac{D}{D\tau} = \frac{\partial}{\partial \tau} + \frac{\hat{\mathbf{u}}}{\hat{D}} \frac{\partial}{\partial \xi} + \mathbf{u}^i \frac{\partial}{\partial \mathfrak{I}^i}$$

For the divergence of a vector field \mathbf{W} (say), we have

$$(3.19) \quad \text{div} \mathbf{W} = \frac{1}{J} \frac{\partial}{\partial \mathfrak{I}^v} \left(J \mathbf{W}^v \right)$$

This relation is a standard expression. Replacing $J \mathbf{W}^\lambda = J \mathbf{g}^\lambda \cdot \mathbf{W}$, we observe that

$$J \mathbf{g}^\lambda = \mathbf{g}_\mu \times \mathbf{g}_\nu$$

We consider here (λ, μ, ν) to be cyclic permutation of $(0, 1, 2, \dots)$. Thus we obtain

$$(3.20) \quad \text{div} \mathbf{W} = \mathbf{g}^\lambda \frac{\partial \mathbf{W}}{\partial \mathfrak{I}^\lambda} + \frac{1}{J} \mathbf{W} \cdot \sum_{\lambda=0}^2 \frac{\partial}{\partial \mathfrak{I}^\lambda} (\mathbf{g}_\mu \times \mathbf{g}_\nu)$$

Carrying out the differentiation of the product in the sum of the second term and observing the

definition $g_\nu = \frac{\partial X}{\partial \mathfrak{S}^\nu}$ and that (λ, μ, ν) are cyclic permutation of $\{0, 1, 2\}$ we find that

$$(3.21) \quad \frac{\partial}{\partial \mathfrak{S}^\lambda} (J g^\lambda) = \sum_{\lambda=0}^2 \frac{\partial}{\partial \mathfrak{S}^\lambda} (g_\mu \times g_\nu) = 0$$

Hence

$$(3.22) \quad \text{div} W = g^\lambda \frac{\partial W}{\partial \mathfrak{S}^\lambda}$$

Writing $W = w^0 \hat{D}n + w^i g_i$ and using (3.22) for normal components and (3.19) for tangential component we get

$$(3.23) \quad \text{div} W = \frac{1}{\hat{D}} \frac{\partial}{\partial \xi} \left(\hat{D} w^0 \right) + \hat{D} w^0 \text{div} n + \frac{1}{J} \frac{\partial}{\partial \mathfrak{S}^i} (J w^i)$$

If $W = \mathbf{U}$ from (3.11) and $\text{div} (n) = k$, curvature of the surface $\xi = \text{constant}$, then flow divergence is given by

$$(3.24) \quad \text{div} (\mathbf{U}) = \frac{1}{\hat{D}} \frac{\partial}{\partial \xi} \left(\hat{u} + \hat{D} \right) + k \left(\hat{u} + \hat{D} \right) + \frac{1}{J} \frac{\partial}{\partial \mathfrak{S}^i} (J u^i)$$

In two dimensions, the co-variant and contravariant bases are,

$$(3.25) \quad \{g_0, g_1\} = \left\{ \hat{D}n + \hat{A}t \right\} \quad \text{and} \quad \{g^0, g^1\} = \left\{ \frac{n}{\hat{D}} + \frac{1}{\hat{A}} t \right\}$$

where t is a unit tangent vector pointing toward increasing \mathfrak{S} . Let length \hat{A} of g_1 determines an arc length increment along a surface $\xi = \text{constant}$ via

$$(3.26) \quad ds = \hat{A} d\mathfrak{S}$$

The two functions $(\hat{D}, \hat{A}) \left(\bar{\mathfrak{S}}, \bar{\xi} + \hat{\tau} \right)$ completely describe the metric of the ray co-ordinate system.

Basic differential geometric calculations using (3.19), (3.22) and (3.25) show that \hat{A} evolve along a shock ray according to

$$(3.27) \quad \frac{1}{\hat{A}} \frac{\partial \hat{A}}{\partial \hat{\xi}} = \hat{k} \hat{D}, \quad \frac{1}{\hat{A}} \frac{\partial n}{\partial \mathfrak{S}^i} = \hat{k} t$$

4. Sonic Conditions in Sonic Frame

Applying the various differential operators derived in section 3 above in the ray co-ordinate system we express the compatibility conditions in three dimensional surface attached with Whitham's ray co-ordinate. The compatibility condition (2.32) may be written as,

$$(4.1) \quad \rho c n \left[n \left(\frac{\partial}{\partial t} + \frac{\hat{u}}{\hat{D}} \frac{\partial}{\partial \hat{\xi}} + u^i \frac{\partial}{\partial \mathfrak{S}^i} \right) \left(\hat{u} + \hat{D} \right) + g_i \left(\frac{\partial}{\partial t} + \frac{\hat{u}}{\hat{D}} \frac{\partial}{\partial \hat{\xi}} + u^i \frac{\partial}{\partial \mathfrak{S}^i} \right) u^i \right. \\ \left. + \left(\hat{u} + \hat{D} \right) \left\{ \left(1 + \frac{\hat{u}}{\hat{D}} \right) \frac{\partial n}{\partial \hat{\xi}} + u^i \frac{\partial n}{\partial \mathfrak{S}^i} \right\} + u^i \left\{ \left(1 + \frac{\hat{u}}{\hat{D}} \right) \frac{\partial g_i}{\partial \hat{\xi}} + u^i \frac{\partial g_i}{\partial \mathfrak{S}^i} \right\} \right. \\ \left. + \frac{1}{\rho} \left(\frac{n}{\hat{D}} \frac{\partial}{\partial \hat{\xi}} + g^i \frac{\partial}{\partial \mathfrak{S}^i} \right) p \right] + \rho c^2 \left\{ \frac{n}{\hat{D}} \frac{\partial}{\partial \hat{\xi}} \left(\hat{u} + \hat{D} \right) + k \left(\hat{u} + \hat{D} \right) + \frac{\partial}{\partial \mathfrak{S}^i} \left(J u^i \right) \right\} \\ + \left(\frac{\partial}{\partial t} + \frac{\hat{u}}{\hat{D}} \frac{\partial}{\partial \hat{\xi}} + u^i \frac{\partial}{\partial \mathfrak{S}^i} \right) p = \rho c^2 \sigma \omega$$

Since $n \cdot g_i = 0$, we have

$$(4.2) \quad n \cdot \frac{\partial g_i}{\partial \hat{\xi}} = -g_i \frac{\partial n}{\partial \hat{\xi}}, \quad n \cdot \frac{\partial g_i}{\partial \mathfrak{S}^i} = -g_i \frac{\partial n}{\partial \mathfrak{S}^i}, \quad n \cdot \frac{\partial n}{\partial \hat{\xi}} = 0$$

From (4.1) and (4.2), we get

$$(4.3) \quad \rho c \left(\frac{\partial}{\partial t} + \frac{\hat{u}}{\hat{D}} \frac{\partial}{\partial \xi} + u^i \frac{\partial}{\partial \mathfrak{S}^i} \right) \left(\hat{u} + \hat{D} \right) + \rho c u^i \left(1 + \frac{\hat{u}}{\hat{D}} \right) \left(g_i \cdot g^i \frac{\partial \hat{D}}{\partial \mathfrak{S}^i} \right) \\ + \rho c u^i u^i \left(-g_i \cdot k g^i \right) + \frac{c}{\hat{D}} \frac{\partial p}{\partial \xi} + \frac{\rho c^2}{\hat{D}} \frac{\partial}{\partial \xi} \left(\hat{u} + \hat{D} \right) + \rho c^2 k \left(\hat{u} + \hat{D} \right) + \frac{\rho c^2}{J} \frac{\partial}{\partial \mathfrak{S}^i} \left(J u^i \right) \\ + \left(\frac{\partial}{\partial t} + \frac{\hat{u}}{\hat{D}} \frac{\partial}{\partial \xi} + u^i \frac{\partial}{\partial \mathfrak{S}^i} \right) p = \rho c^2 \sigma \omega$$

Rearranging the terms, we get

$$(4.4) \quad \rho c \left(\frac{\partial}{\partial t} + \frac{\hat{u}}{\hat{D}} \frac{\partial}{\partial \xi} + u^i \frac{\partial}{\partial \mathfrak{S}^i} \right) \left(\hat{u} + \hat{D} \right) + \rho c u^i \left(1 + \frac{\hat{u}}{\hat{D}} \right) \frac{\partial \hat{D}}{\partial \mathfrak{S}^i} - \rho c u^i u^i k + \frac{c}{\hat{D}} \frac{\partial p}{\partial \xi} \\ + \frac{\rho c^2}{\hat{D}} \frac{\partial}{\partial \xi} \left(\hat{u} + \hat{D} \right) + \rho c^2 K \left(\hat{u} + \hat{D} \right) + \frac{\rho c^2}{J} \frac{\partial}{\partial \mathfrak{S}^i} \left(J u^i \right) \\ + \left(\frac{\partial}{\partial t} + \frac{\hat{u}}{\hat{D}} \frac{\partial}{\partial \xi} + u^i \frac{\partial}{\partial \mathfrak{S}^i} \right) p = \rho c^2 \sigma \omega$$

In two dimension,

$$(4.5) \quad \frac{1}{J} \frac{\partial}{\partial \mathfrak{S}^i} \left(J u^i \right) = \frac{1}{\hat{A} \hat{D}} \frac{\partial}{\partial \mathfrak{S}^i} \left(\hat{A} \hat{D} u^i \right) = \frac{\partial u^i}{\partial \mathfrak{S}^i} + \frac{1}{\hat{D}} \frac{\partial \hat{D}}{\partial \mathfrak{S}^i} + \frac{u^i}{\hat{A}} \frac{\partial \hat{A}}{\partial \mathfrak{S}^i}$$

Thus, the compatibility condition in this case becomes

$$(4.6) \quad \rho c \left\{ \left(\frac{\partial}{\partial t} + \frac{\hat{u}}{\hat{D}} \frac{\partial}{\partial \xi} + u^i \frac{\partial}{\partial \zeta^i} \right) (\hat{u} + \hat{D}) + u^i \left(1 + \frac{\hat{u}}{\hat{D}} \right) \frac{\partial \hat{D}}{\partial \zeta^i} - k u^i u^i + \frac{1}{\rho \hat{D}} \frac{\partial p}{\partial \xi} \right\}$$

$$+ \rho c^2 \left\{ \frac{1}{\hat{D}} \frac{\partial}{\partial \xi} (\hat{u} + \hat{D}) + k (\hat{u} + \hat{D}) + \frac{\partial u^i}{\partial \zeta^i} \right\} + \left(\frac{\partial}{\partial t} + \frac{\hat{u}}{\hat{D}} \frac{\partial}{\partial \xi} + u^i \frac{\partial}{\partial \zeta^i} \right) p$$

$$+ \frac{1}{\hat{D}} u^i \frac{\partial \hat{D}}{\partial \zeta^i} + \frac{u^i}{\hat{A}} \frac{\partial \hat{A}}{\partial \zeta^i} = \rho c^2 \sigma \omega$$

Again rearranging the terms of (4.6) we have

$$(4.7) \quad \frac{\partial p}{\partial t} + \rho c \frac{\partial}{\partial t} (\hat{u} + \hat{D}) + k \rho c^2 (\hat{u} + \hat{D}) + \left(\frac{c + \hat{u}}{\hat{D}} \right) \left\{ \frac{\partial p}{\partial \xi} + \rho c \frac{\partial}{\partial \xi} (\hat{u} + \hat{D}) \right\}$$

$$+ \rho c^2 \frac{\partial u^i}{\partial \zeta^i} + u^i \left\{ \frac{\partial p}{\partial \zeta^i} + \rho c \frac{\partial}{\partial \zeta^i} (\hat{u} + \hat{D}) \right\} + \rho c u^i \left\{ \left(1 + \frac{\hat{u}}{\hat{D}} \right) \frac{\partial \hat{D}}{\partial \zeta^i} + u^i k \right\}$$

$$+ \frac{1}{\hat{A}} \rho c^2 u^i \frac{\partial \hat{A}}{\partial \zeta^i} + \frac{1}{\hat{D}} \rho c^2 u^i \frac{\partial \hat{D}}{\partial \zeta^i} = \rho c^2 \sigma \omega$$

In the sonic surface the flow is locally sonic i.e. $c + \hat{u} = 0$

$$(4.8) \quad \frac{\partial p}{\partial t} + \rho c \frac{\partial}{\partial t} (\hat{u} + \hat{D}) + k_* \rho c^2 (\hat{u} + \hat{D}) = \rho c^2 \sigma \omega - R_*$$

where

$$R_* = \rho c^2 \frac{\partial u^i}{\partial \zeta^i} + \rho c u^i \left\{ \left(1 + \frac{\hat{u}}{\hat{D}} \right) \frac{\partial \hat{D}}{\partial \zeta^i} - u^i k \right\} + u^i \left\{ \frac{\partial p}{\partial \zeta^i} + \rho c \frac{\partial}{\partial \zeta^i} (\hat{u} + \hat{D}) \right\}$$

$$+\frac{1}{\hat{A}}\rho c^2 u^i \frac{\partial \hat{A}}{\partial \zeta^i} + \frac{1}{\hat{D}}\rho c^2 u^i \frac{\partial \hat{D}}{\partial \zeta^i}$$

In (4.8) everything is evaluated in the sonic surface. Equation (4.8) is an exact relation that is valid for the general two dimensional detonations with an embedded sonic surface. Similar relation has been obtained by Stewart and Kasimov (2005) by considering Bertrand co-ordinate system.

5. Sonic Conditions in the Shock - attached Frame

The linear stability problem and the detonation shock problem wave originally formulated in shock attached co-ordinate because the goal of detonation shock dynamic theory is to determine the dynamics of the shock front (Erpenbeck (1964), Stewart and Bdzil (1988), Yao and Stewart (1996)).

In this case difference arises from the fact that n_* in (2.32) is uni normal to the sonic surface which in general is different from n , the unit normal to the shock. Therefore, the shock frame compatibility condition will contain terms proportional to $n_* \cdot n$ which need to be evaluated.

Let

$$(5.1) \quad n_* = a_\xi n + a_\zeta g_i$$

where the components

$$(5.2) \quad a_\xi = n_* \cdot n \quad \text{and} \quad a_\zeta = n_* \cdot g_i$$

Taking differential operators similar to those in the sonic frame and \hat{u}_n is the normal speed relative to the shock.

$$(5.3) \quad n_* \frac{DU}{Dt} = a_\xi \frac{D}{Dt} \left(\hat{u}_n + \hat{D} \right) + a_\zeta \frac{Du^i}{Dt} + a_\xi \left(\hat{u}_n + \hat{D} \right) \left(1 + \frac{\hat{u}_n}{\hat{D}} \right) \left(n \cdot \frac{\partial n}{\partial \xi} \right)$$

$$\begin{aligned}
 &+a_{\xi}\left(\hat{u}_n+\hat{D}\right)u^i\left(n.\frac{\partial n}{\partial \mathfrak{S}^i}\right)+a_{\mathfrak{S}}\left(\hat{u}_n+\hat{D}\right)\left(1+\frac{\hat{u}_n}{\hat{D}}\right)\left(g_i.\frac{\partial n}{\partial \xi}\right) \\
 &+a_{\mathfrak{S}}\left(\hat{u}_n+\hat{D}\right)u^i\left(g_i.\frac{\partial n}{\partial \mathfrak{S}^i}\right)+a_{\xi}u^i\left(1+\frac{\hat{u}_n}{\hat{D}}\right)\left(n.\frac{\partial g_i}{\partial \xi}\right)+a_{\xi}u^i u^i\left(n.\frac{\partial g_i}{\partial \mathfrak{S}^i}\right) \\
 &+a_{\mathfrak{S}}u^i\left(1+\frac{\hat{u}_n}{\hat{D}}\right)\left(g_i.\frac{\partial g_i}{\partial \xi}\right)+a_{\mathfrak{S}}u^i u^i\left(g_i.\frac{\partial g_i}{\partial \mathfrak{S}^i}\right)
 \end{aligned}$$

Since

$$\frac{\partial n}{\partial \xi}=-g^i \frac{\partial \hat{D}}{\partial \xi}, \quad n.\frac{\partial n}{\partial \xi}=0$$

$$n.\frac{\partial n}{\partial \mathfrak{S}^i}=n.(kg^i)=kg_i.n=0$$

Equation (6.3) takes the form

$$\begin{aligned}
 (5.4) \quad n_* \frac{DU}{Dt} &= a_{\xi} \frac{D}{Dt} \left(\hat{u}_n + \hat{D} \right) + a_{\mathfrak{S}} \frac{Du^i}{Dt} + \left(a_{\mathfrak{S}} \left(\hat{u}_n + \hat{D} \right) - u^i a_{\xi} \right) \\
 &\quad \left(- \left(1 + \frac{\hat{u}_n}{\hat{D}} \right) \frac{\partial \hat{D}}{\partial \mathfrak{S}^i} + u^i k \right)
 \end{aligned}$$

and

$$(5.5) \quad \rho c n_* \left(\frac{1}{\rho} \nabla p \right) = c \left(\frac{a_{\xi}}{\hat{D}} \frac{\partial p}{\partial \xi} + \frac{a_{\mathfrak{S}}}{\hat{D}} \frac{\partial p}{\partial \mathfrak{S}^i} \right)$$

Thus, compatibility condition in two dimensions may be written as

$$\begin{aligned}
 (5.6) \quad & \rho c a_{\xi} \frac{D}{Dt} \left(\hat{u}_n + \hat{D} \right) + \rho c a_{\zeta} \frac{D u^i}{Dt} + \rho c \left(a_{\xi} \left(\hat{u}_n + \hat{D} \right) - u^i a_{\xi} \right) \\
 & \left(- \left(1 + \frac{\hat{u}_n}{\hat{D}} \right) \frac{\partial \hat{D}}{\partial \zeta} + u^i k \right) + c \left(\frac{a_{\xi}}{\hat{D}} \frac{\partial p}{\partial \xi} + \frac{a_{\zeta}}{\hat{D}} \frac{\partial p}{\partial \zeta^i} \right) + \rho c^2 \left\{ \frac{1}{\hat{D}} \frac{\partial}{\partial \xi} \left(\hat{u}_n + \hat{D} \right) \right. \\
 & \left. + k \left(\hat{u}_n + \hat{D} \right) + \frac{\partial u^i}{\partial \zeta^i} + \frac{u^i}{\hat{D}} \frac{\partial \hat{D}}{\partial \zeta^i} + \frac{u^i}{\hat{A}} \frac{\partial \hat{A}}{\partial \zeta^i} \right\} \\
 & + \frac{\partial p}{\partial t} + \frac{\hat{u}_n}{\hat{D}} \frac{\partial p}{\partial \xi} + u^i \frac{\partial p}{\partial \zeta^i} = \rho c^2 \sigma \omega
 \end{aligned}$$

Rearranging the terms of (6.6) we may write

$$\begin{aligned}
 (5.7) \quad & \frac{\partial p}{\partial t} + \left(\frac{c + \hat{u}_n}{\hat{D}} \right) \frac{\partial p}{\partial \xi} + \rho c \left(\frac{\partial}{\partial t} \left(\hat{u}_n + \hat{D} \right) + \left(\frac{c + \hat{u}_n}{\hat{D}} \right) \frac{\partial}{\partial \xi} \left(\hat{u}_n + \hat{D} \right) \right) \\
 & + k \rho c^2 \left(\hat{u}_n + \hat{D} \right) = \rho c^2 \sigma \omega + R
 \end{aligned}$$

where

$$\begin{aligned}
 (5.8) \quad & R = u^i \left(\frac{\partial p}{\partial \zeta^i} + \frac{\partial \left(\hat{u}_n + \hat{D} \right)}{\partial \zeta^i} \right) + \rho c^2 \frac{\partial u^i}{\partial \zeta^i} + c \left(a_{\xi} - 1 \right) \left(\frac{1}{\hat{D}} \frac{\partial p}{\partial \xi} + \rho \frac{D}{Dt} \left(\hat{u}_n + \hat{D} \right) \right) \\
 & c a_{\zeta} \left(\frac{1}{\hat{D}} \frac{\partial p}{\partial \zeta^i} + \rho \frac{D u^i}{Dt} \right) + \rho c \left(a_{\zeta} \left(\hat{u}_n + \hat{D} \right) - u^i a_{\xi} \right) \left(- \left(1 + \frac{\hat{u}_n}{\hat{D}} \right) \frac{\partial \hat{D}}{\partial \zeta^i} + u^i k \right)
 \end{aligned}$$

$$+\rho c^2 u^i \left(\frac{1}{\hat{D}} \frac{\partial \hat{D}}{\partial \hat{\mathcal{S}}^i} + \frac{1}{\hat{A}} \frac{\partial \hat{A}}{\partial \hat{\mathcal{S}}^i} \right)$$

The equation (5.7) is the shock frame compatibility condition where k 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.

To simplify the sonic conditions and to see connection with the older formulation we make certain approximation i.e. neglecting transverse variations in the derivative in the sonic surface, we obtain the from (5.7)

$$(5.9) \quad \left(\frac{\partial}{\partial t} + \left(\frac{c^* + u_n}{\hat{D}} \right) \frac{\partial}{\partial \xi} \right) p + \rho c^* \left(\frac{\partial}{\partial t} + \left(\frac{c^* + u_n}{\hat{D}} \right) \frac{\partial}{\partial \xi} \right) (u_n + \hat{D}) + k \rho c^{*2} (u_n + \hat{D}) = \rho c_*^2 \omega \sigma$$

or

$$(5.10) \quad \frac{Dp}{Dt} + \rho c^* \frac{D}{Dt} (u_n + \hat{D}) + k \rho c^{*2} (u_n + \hat{D}) = \rho c_*^2 \omega \sigma$$

where

$$(5.11) \quad \frac{D}{Dt} = \frac{\partial}{\partial t} + \left(\frac{c_* + u_n}{\hat{D}} \right) \frac{\partial}{\partial \xi} = \frac{\partial}{\partial t} + \frac{\partial n_*}{\partial t} \frac{\partial}{\partial \xi}$$

and

$$(5.12) \quad \frac{\partial n_*}{\partial t} = \left(\frac{c^* + u_n}{\hat{D}} \right)$$

is a speed relation. The time derivative in (5.10) must be taken along the sonic locus.

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