The heat flux can be computed from a nondimensional heat transfer coefficient c_h

$$q_w = c_h \rho \mathrm{u} c_p (T_w - T) , \tag{11.59}$$

which is usually specified by an engineering correlation with the skin friction coefficient, Reynolds and Prandtl numbers, and wall/flow temperature ratio. Note that for high-temperature flows and cold walls, the heat transfer will be from the flow into the duct walls, q_w and $\tilde{q} < 0$.

Combining equations (11.53) and (11.54) with the fundamental relation of thermodynamics, an expression for the entropy gradient is obtained

$$T\frac{\mathrm{d}s}{\mathrm{d}x} = \frac{\tilde{q}}{\rho \mathrm{u}} + \frac{\tilde{\tau}}{\rho} - \sum_k g_i \frac{\mathrm{d}Y_k}{\mathrm{d}x} . \tag{11.60}$$

The adiabatic change equation (9.30) can be used to relate gradients in pressure, density, entropy and species.

$$\frac{\mathrm{d}P}{\mathrm{d}x} = a_f^2 \frac{\mathrm{d}\rho}{\mathrm{d}x} + \mathcal{G}\left(\frac{\tilde{q}}{\mathrm{u}} + \tilde{\tau}\right) + \rho a_f^2 \sum_k \sigma_k \frac{\mathrm{d}Y_k}{\mathrm{d}x} . \tag{11.61}$$

Defining a modified thermicity function

$$\dot{\sigma}' = \sum_k \sigma_k \frac{\mathrm{d}Y_k}{\mathrm{d}x} , \tag{11.62}$$

we can use (11.52) and (11.53) to solve for the gradient in density

$$\frac{\mathrm{d}\rho}{\mathrm{d}x} = -\rho \frac{\dot{\sigma}' + \dfrac{\mathcal{G}}{\rho a_f^2}\left[\dfrac{\tilde{q}}{\mathrm{u}} + (\mathcal{G}+1)\tilde{\tau}\right] - \dfrac{M^2}{A}\dfrac{\mathrm{d}A}{\mathrm{d}x}}{1 - M^2} , \tag{11.63}$$

pressure

$$\frac{\mathrm{d}P}{\mathrm{d}x} = -\rho \mathrm{u}^2 \frac{\dot{\sigma}' + \dfrac{\mathcal{G}}{\rho a_f^2}\left[\dfrac{\tilde{q}}{\mathrm{u}} + (\mathcal{G}+\dfrac{1}{M^2})\tilde{\tau}\right] - \dfrac{1}{A}\dfrac{\mathrm{d}A}{\mathrm{d}x}}{1 - M^2} , \tag{11.64}$$

and velocity

$$\frac{\mathrm{d}\mathrm{u}}{\mathrm{d}x} = \mathrm{u} \frac{\dot{\sigma}' + \dfrac{\mathcal{G}}{\rho a_f^2}\left[\dfrac{\tilde{q}}{\mathrm{u}} + (\mathcal{G}+1)\tilde{\tau}\right] - \dfrac{1}{A}\dfrac{\mathrm{d}A}{\mathrm{d}x}}{1 - M^2} . \tag{11.65}$$

Flow in nozzles

A common and important example of a flow through a variable area duct is the case of converging-diverging nozzle used to accelerate flow from subsonic to supersonic conditions. If we neglect heat transfer and friction, the equations simplify to:

$$\frac{\mathrm{d}\rho}{\mathrm{d}x} = -\rho \frac{\dot{\sigma}' - \dfrac{M^2}{A}\dfrac{\mathrm{d}A}{\mathrm{d}x}}{1 - M^2} , \tag{11.66}$$

$$\frac{\mathrm{d}P}{\mathrm{d}x} = -\rho \mathrm{u}^2 \frac{\dot{\sigma}' - \dfrac{1}{A}\dfrac{\mathrm{d}A}{\mathrm{d}x}}{1 - M^2} \tag{11.67}$$

$$\frac{\mathrm{d}\mathrm{u}}{\mathrm{d}x} = \mathrm{u} \frac{\dot{\sigma}' - \dfrac{1}{A}\dfrac{\mathrm{d}A}{\mathrm{d}x}}{1 - M^2} , \tag{11.68}$$

For an ideal gas, these can be used to compute the temperature gradient

$$\frac{\mathrm{d}T}{\mathrm{d}x} = T\left[\frac{\dot{\sigma}' + (\gamma-1)\dfrac{M^2}{A}\dfrac{\mathrm{d}A}{\mathrm{d}x}}{1-M^2} - \sum_{k=1}^{K}\frac{\mathcal{W}}{\mathcal{W}_k}\frac{\mathrm{d}Y_k}{\mathrm{d}x}\right] \tag{11.69}$$

The species mass fractions gradients are

$$\frac{\mathrm{d}Y_k}{\mathrm{d}x} = \frac{\mathcal{W}_k\dot{\omega}_k}{\rho\mathrm{u}} \tag{11.70}$$

Propagating waves with friction and heat transfer

Equations (11.63) - (11.65) have been formulated in the reference frame of a stationary duct or nozzle and do not apply to the flow behind a propagating detonation or shock wave. In order to formulate the equations correctly for a propagating wave moving with a constant speed U, it is necessary to use a control volume formulation of the integral conservation laws when deriving the differential form of the relationship in a shock-fixed frame; taking into account the effective forces acting on the control volume moving relative to the duct surface. The correlations for friction and convective heat transfer need to evaluated using the appropriate relative velocity Δu between the flow and duct surface.

The key observation is that in a shock-fixed frame of reference, the duct walls are moving relative the wave with speed U. This situation is also encountered when modeling boundary layers behind shock or detonation waves. The conservation of mass and momentum are identical to the stationary frame equations with the substitution $u \rightarrow w = U$ - u. The energy equation contains a work term that corresponds to the work (per unit area) $U\tau_w$ done on the fluid by the moving walls of the duct due to the friction forces at the wall τ_w, moving with speed U. This treatment is necessarily highly approximate as observations of flows behind propagating shocks and detonations demonstrate that immediately behind and for some distance downstream, the flow is highly multidimensional with the effects of friction and heat transfer confined to the relatively thin boundary layers adjacent to the wall. The quasi-one-dimensional flow approximation only makes sense for fully developed flows some distance downstream of the wave. Despite this limitation, this approach has been used to develop correlations for detonation speed as a function of duct size by applying a generalized CJ condition to determine the detonation speed (See Ch. 2 Zhang, 2012).

The equations in the shock-fixed reference frame (flow from left to right) for a constant area duct are:

$$\frac{\mathrm{d}}{\mathrm{d}x}(\rho\mathrm{w}) = 0 \tag{11.71}$$

$$\rho\mathrm{w}\frac{\mathrm{dw}}{\mathrm{d}x} = -\frac{\mathrm{d}P}{\mathrm{d}x} - \tilde{\tau} \tag{11.72}$$

$$\rho\mathrm{w}\frac{\mathrm{d}}{\mathrm{d}x}(h + \frac{\mathrm{w}^2}{2}) = \tilde{q} + U\tilde{\tau} \tag{11.73}$$

$$\mathrm{w}\frac{\mathrm{d}Y_k}{\mathrm{d}x} = \frac{\mathcal{W}_k\dot{\omega}_k}{\rho} \qquad (k = 1, \ldots, K) \tag{11.74}$$

The entropy gradient is

$$T\frac{\mathrm{d}s}{\mathrm{d}x} = \frac{\tilde{q} + U\tilde{\tau}}{\rho\mathrm{w}} + \frac{\tilde{\tau}}{\rho} - \sum_k g_i\frac{\mathrm{d}Y_k}{\mathrm{d}x}\ . \tag{11.75}$$

Inserting this entropy gradient into the adiabatic change equation results in the further transformation of the steady flow equations (11.63) - (11.65) with $\tilde{q}/\mathrm{u} \rightarrow (\tilde{q} + U\tilde{\tau})/\mathrm{w}$.

11.9 Stagnation Point and Shock Tube Flows

Stagnation point and shock tube flows can both be used to create reaction zones behind shock waves. In the case of the stagnation stream line, the constraint of the body causes this to occur in a specified and short spatial domain $0 < x < \Delta$ while behind a propagating shock wave, there is no constraint and the reaction zone will extend over a much larger distance behind the shock. An ideal reaction zone behind a propagating shock wave is governed by the reaction zone structure equations with constant stream tube area $A = A_\circ$, i.e., $\alpha = 0$.

The relationship between distance and time in both cases is determined by integrating the flow velocity

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \mathrm{w} \tag{11.76}$$

to relate distance x traveled by the gas particles to time t elapsed when using the time evolution form of the reaction zone equations. This relationship will in general have to be solved simultaneously with the flow variables. In the case of stagnation point flow, the approximate model of linearly decreasing mass flux simplifies the solution of this relationship. The quasi-one-dimensional mass conservation relation can be written

$$\frac{A(x)}{A_\circ}\frac{\mathrm{d}x}{\mathrm{d}t} = \rho_\circ \mathrm{w}_\circ \frac{1}{\rho(t)} \tag{11.77}$$

which can be integrated to obtain the following implict relationship for $x(t)$

$$\int_0^x \frac{A(x')}{A_\circ}\,\mathrm{d}x' = \int_o^t \rho_\circ \mathrm{w}_\circ \frac{\mathrm{d}t'}{\rho(t')}\ . \tag{11.78}$$

Substituting the $A(x)$ relation in (11.42) and carrying out the integration on the left-hand side, we obtain

$$\frac{x}{\Delta} = 1 - \exp\left(-\frac{\mathrm{w}_\circ}{\Delta}\int_o^t \frac{\rho_\circ\,\mathrm{d}t'}{\rho(t')}\right)\ . \tag{11.79}$$

This demonstrates that although the stagnation point is located a finite distance Δ from the shock front, the flow takes an infinitely long time to travel along the stagnation streamline from the shock to the stagnation point. If we suppose that the variation with time of the properties P,ρ, w and $\mathbf{Y}$ is identical for the stagnation point and propagating shock reaction zones, we can further simplify the relationship between the two situations. The distance x_s behind a propagating shock is given by integrating the flow speed w_s relative to the shock

$$\frac{\mathrm{d}x_s}{\mathrm{d}t} = \mathrm{w}_s\ , \tag{11.80}$$

Flow area is constant in the ideal shock tube case, so that

$$\mathrm{w}_s = \mathrm{w}_\circ \rho_\circ/\rho(t) \tag{11.81}$$

or

$$\mathrm{d}x_s = \rho_\circ \mathrm{w}_\circ \frac{\mathrm{d}t}{\rho(t)}\ . \tag{11.82}$$

Substituting in (11.79), we obtain the following relationship between the distance x between the shock and body in a stagnation point flow and postshock distance x_s in a shock tube flow

$$\frac{x}{\Delta} = 1 - \exp\left(-\frac{x_s}{\Delta}\right) \tag{11.83}$$

An example of the results of comparing the reaction zone structure behind a planar shock wave and a stagnation point flow is shown in Fig. 11.11 for a typical case studied in the EAST facility at NASA Ames. The shock or freestream flow speed is 6000 m/s and the initial conditions are a gas composition of 0.96 CO_2 and 0.04 N_2 (mole fractions), pressure of 133 Pa (1 Torr) and temperature of 300 K. The reaction mechanism discussed in Johnston and Brandis (2014) is used to perform the computation although V-T nonequilibrium was not included in this simulation. The comparison for temperature, density and species (only CO_2 is shown but the other species were comparable) is excellent but as we might expect, the pressure at the end of the reaction zone is higher in the stagnation case than the shock tube. The pressure variation throughout the reaction zone is very modest for both the shock and stagnation case so this small (3%) deviation does not affect the overall quality of the comparison. We conclude that transformation (11.83) provides a very useful means to make quantitative comparisons between shock tube and stagnation point flows.

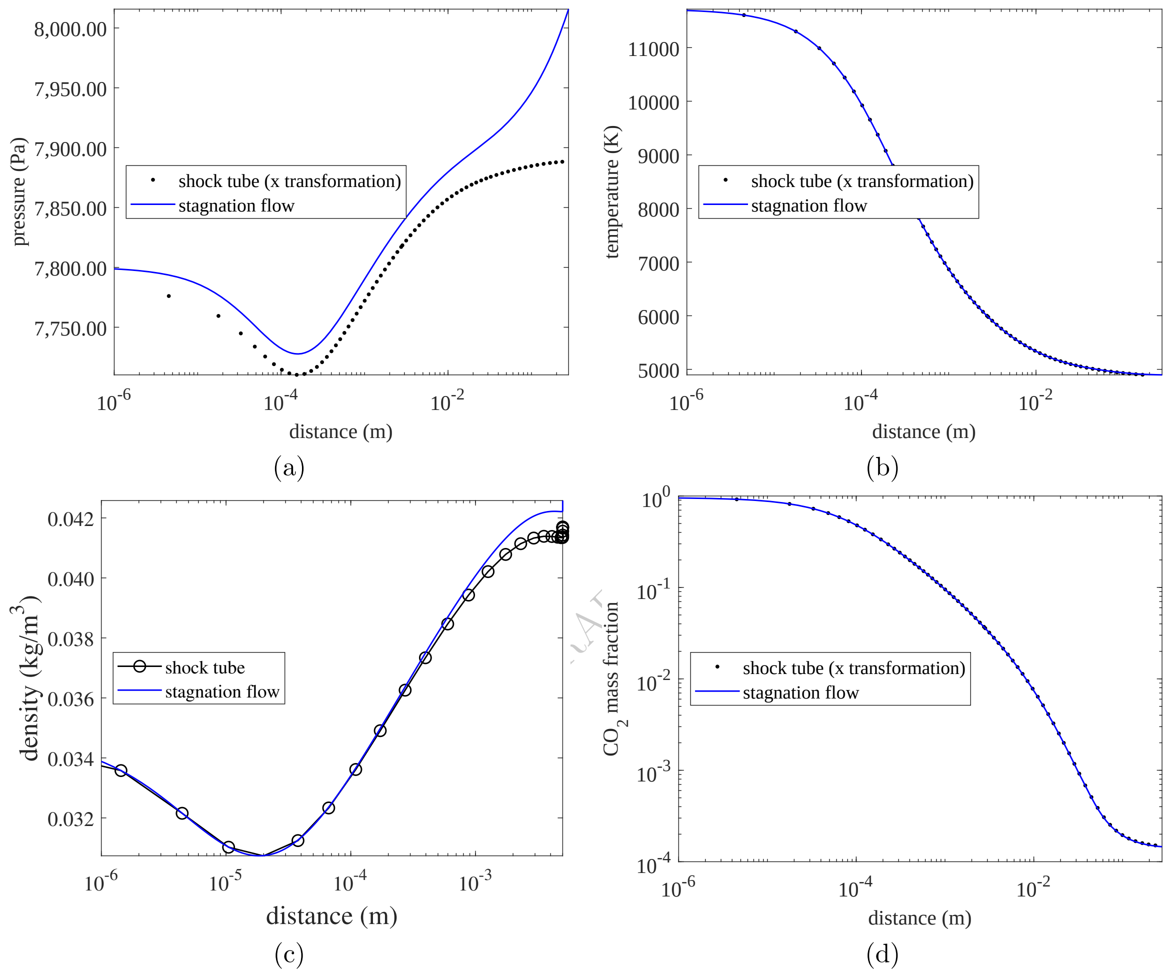

Figure 11.11: Comparison of flow properties evaluated with planar shock and stagnation point models using the transformation methodology of (11.83).

11.10 Curvature-Area Relation

A simple explanation of the curvature-area relationship for propagating waves can be motivated by examining the conservation of mass relationship for the flow behind the wave

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \, . \tag{11.84}$$

Modeling the wave front as a spherical or cylindrical surface of radius R_s moving with a speed $U = dR_s/dt$, the conservation equations can be written in terms of a radial coordinate r

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho \mathrm{u}}{\partial r} + \frac{j}{r}\rho \mathrm{u} = 0 \, , \tag{11.85}$$

where $j = 1$ for cylindrical waves and $j = 2$ for spherical waves. Transform to wave-fixed coordinates using the relations

$$x = R_s(t) - r \tag{11.86}$$

$$\mathrm{w} = U(t) - \mathrm{u} \tag{11.87}$$

to obtain

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho \mathrm{w}}{\partial x} + \frac{j}{R_s(t) - x}\rho(U - \mathrm{w}) = 0 \, . \tag{11.88}$$

The quasi-steady, slightly-curved approximate form of this equation can be deduced with the aid of the following order of magnitude estimates

$$x \sim \Delta \, ; \quad t_{\text{slow}} \sim \rho / \frac{\partial \rho}{\partial t} \text{ and } R_s / \frac{\partial R_s}{\partial t} \, ; \quad t_{\text{fast}} \sim \frac{\mathrm{w}}{\Delta} \tag{11.89}$$

Estimating the size of each term in Eqn. (11.84), we find that in order to obtain the quasi-steady form of the equations we must have

$$t_{\text{slow}} >> t_{\text{fast}} \tag{11.90}$$

so that the evolution of the wave speed is slow compared to the transit time of fluid elements through the reaction zone. In the limit as $t_{\text{fast}}/t_{\text{slow}} \to 0$, the partial derivative with respect to time in (11.88) can be neglected and we can approximate R_s as a constant. Physically we are making the assumption that the reaction takes place much faster than the wave speed is changing so that in the wave-fixed frame the reaction zone structure is steady to a first approximation.

To further simplify the mass conservation equation, we need to suppose that the reaction zone length is small

$$R_s >> \Delta \tag{11.91}$$

so that the last term in (11.88) can be expanded to yield the approximate expression

$$\frac{\partial \rho \mathrm{w}}{\partial x} + \frac{j}{R_s}\rho(U - \mathrm{w})(1 + \frac{x}{R_s} + \dots) = 0 \tag{11.92}$$

which as $x/R_s \to 0$, yields

$$\frac{\partial \rho \mathrm{w}}{\partial x} + \rho \mathrm{w}\frac{j}{R_s}(\frac{U}{\mathrm{w}} - 1) = 0 \tag{11.93}$$

Comparing this with the quasi-one-dimensional steady mass conservation equation, we can identify the logarithmic area derivative as

$$\alpha = \frac{1}{A}\frac{\mathrm{d}A}{\mathrm{d}t} = \frac{j}{R_s}(\frac{U}{\mathrm{w}} - 1) \tag{11.94}$$

This is the result used for the simplest version of the quasi-one-dimensional, quasi-steady reaction zone structure model of curved detonation waves. The history of this model is given in Bdzil and Stewart (2007), who provide a rigorous derivation with extensions to multidimensional flow and illustrations of applications to high explosives.

The effect of wave curvature on stream tube expansion at first glance appears contradictory. There are two ways to explain this. The first is that radial flow u induced by the shock wave is in the direction of the shock motion U, for expanding waves this means that the flow moves in the $+r$ direction into increasing stream tube area. For converging waves, the flow moves in the $-r$ direction into decreasing stream tube area. The second explanation, is to consider the motion relative to curved shock front propagating into an uniform region at rest. Considering the flow in a small region (the red box outlined in Fig. 11.12 surrounding the central un-deflected streamline, the deflection of the adjacent streamlines creates divergence due to the obliquity of the shock at locations on the surface away from the central streamline. This deflection is a consequence of the oblique shock jump conditions and the decomposition of the velocity in normal and transverse components. For unsteady flow, the approximate mass balance equation in shock fixed coordinates

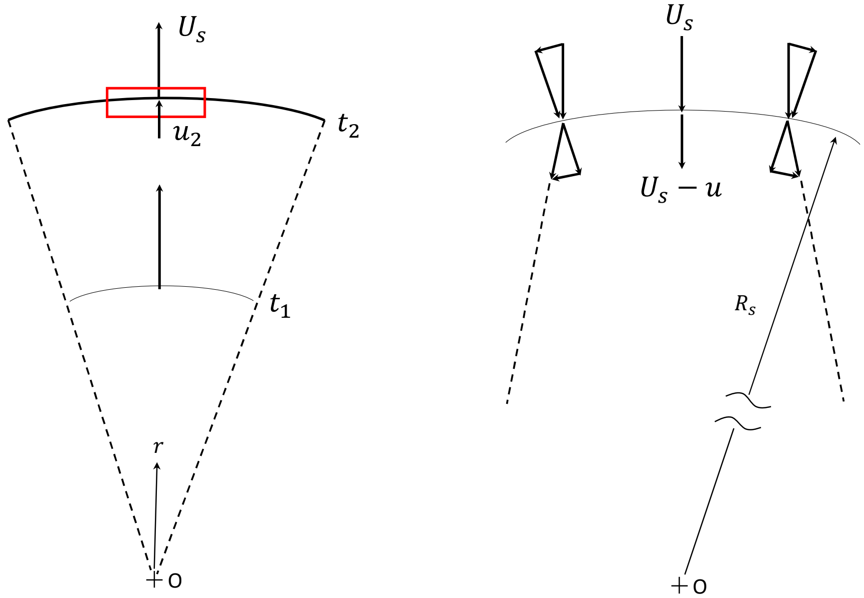

Figure 11.12: Explanation of relationship between wave curvature and stream tube expansion for a decaying blast wave.

is

$$\frac{\partial \rho}{\partial t} + w\frac{\partial \rho}{\partial x} = -\rho\frac{\partial w}{\partial x} - \frac{j\,\mathrm{u}}{R_s} \tag{11.95}$$

11.11 Shock Change Relations - Planar Waves

The growth or decay of shock waves in a reactive flow can be analyzed by focusing on the processes just behind the wave front to obtain an evolution equation for the wave strength, known as the *shock change equation*.

Versions of the shock change or acceleration wave formalism has been derived independently by a number of researchers over the past century as discussed by Becker (1972) and Chen and Gurtin (1971). The results have been used to analyze the growth and decay of shock waves in inhomogeneous (Nunziato and Walsh, 1972, 1973) and chemically reacting flows (Nunziato, 1973, Kennedy and Nunziato, 1976). Fickett and Davis (1979, p. 101) discuss the application to detonations and the implications for steady flow in the reaction zone. Recently, Radulescu (2020) derived expressions for shock propagation in quasi-one dimensional flows, gave explicit expressions for nonreactive perfect gases and discussed the relationship to the shock dynamics approximation of Whitham. Extension to fully three-dimensional shock fronts was given by Rabie and Wackerle (1978) defining the local shock shape with principle radii of curvature. Emanuel (2013) discusses in great detail the computation of computing spatial derivatives at curved shock in a perfect gas, there is brief mention of unsteadiness but no consideration of reaction processes. Hornung (1972), **?** has derived and used the steady version of the curved shock relationships with reaction and a general equation of state to explain (Hornung, 2010) features in the relaxation region behind shock waves on blunt bodies in hypervelocity flows. Hornung's approach has been applied to combusting flows to analyze the reaction zone behind steady oblique detonation waves (Kaneshige, 1999, Hung and Shepherd, 2005) and unsteady one- (Eckett et al., 2000) and two-dimensional detonation waves (Arienti and Shepherd, 2005).

These derivations usually consider the upstream conditions to be uniform, with the exception of (Nunziato and Walsh, 1972), and the flow to be at rest. In order to treat the interaction of a shock waves with an expansion wave, as occurs when a detonation wave reflects from a contact surface or end wall, it is necessary to consider how both the upstream unsteadiness and spatial nonuniformity enter into the relationship between wave acceleration and flow gradients downstream of the shock.

Assumptions

The fundamental idea of the shock change relation is to compute the time rate of change of the properties on each side of the shock from both the shock jump conditions and the governing partial differential equations of fluid motion. Requiring these independent computations to be compatible results in a system of equations that we solve to determine the rate of change of shock speed and through the jump conditions any other post-shock property in terms of the gradients in the flow.

We make some restrictive assumptions in deriving and solving these equations.

1. The shock wave is an ideal surface of discontinuity in the flow, so that the ideal shock jump conditions are applicable and relate fluid properties upstream (state 1) and downstream (state 2) of the shock in an unsteady flow with spatial gradients.

2. The flow upstream and downstream of the shock is consider as inviscid, i.e., the effects of molecular transport are neglected, but can be reacting through chemical or physical mechanisms like energy transfer between the various degrees of freedom.

3. The flow is considered to be adiabatic and one-dimensional. The extension to multi-dimensional flows with unsteadiness is significantly more involved (Emanuel, 2013) than the one-dimensional treatment. For simplicity, we have intentionally kept the focus of the present work on the effect of gradients and unsteadiness in the upstream flow for planar flows.

Shock Motion

The shock velocity can be expressed in terms of the time derivative of the location $X(t)$ of the surface of discontinuity representing the ideal shock

$$U = \frac{\mathrm{d}X}{\mathrm{d}t} \; . \tag{11.96}$$

Flow properties $f(x,t)$ adjacent to the shock can be expressed as limits approaching the surface of discontinuity

$$f_1 = \lim_{x \to X^-} f(x,t) = \lim_{\epsilon \to 0} f(X(t) - \epsilon, t) = f_1(X(t), t) \; , \tag{11.97}$$

$$f_2 = \lim_{x \to X^+} f(x,t) = \lim_{\epsilon \to 0} f(X(t) + \epsilon, t) = f_2(X(t), t) \; . \tag{11.98}$$

The time rate of change of the properties adjacent to the shock must be computed in a reference frame moving with the shock. From (11.97) and (11.96), we have

$$\left(\frac{\mathrm{d}f}{\mathrm{d}t}\right)_{\mathcal{S}} = \frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} \; , \tag{11.99}$$

Consistent with the limiting proceses used in (11.97) we define the partial derivatives at the shock front by limiting process, computing the derivatives in the bulk fluid away from the shock and finding the limiting value as the the shock front is approached from either the upstream or downstream side

$$\left(\frac{\mathrm{d}f_i}{\mathrm{d}t}\right)_{\mathcal{S}} = \lim_{x\to X^\pm}\left(\frac{\partial f}{\partial t}\right) + U \lim_{x\to X^\pm}\left(\frac{\partial f}{\partial x}\right) = \frac{\partial f_i}{\partial t} + U\frac{\partial f_i}{\partial x} \ . \tag{11.100}$$

The equations of fluid motion can be written in terms of the convective or substantial derivative

$$\frac{\mathrm{D}f}{\mathrm{D}t} = \frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} \ . \tag{11.101}$$

From (11.99), the relationship of convective and shock frame time derivatives at the shock front can be expressed as

$$\left(\frac{\mathrm{d}f_i}{\mathrm{d}t}\right)_{\mathcal{S}} = \frac{\mathrm{D}f_i}{\mathrm{D}t} + (U - u_i)\,\frac{\partial f_i}{\partial x} \tag{11.102}$$

In terms of the convective derivatives, the equations of motion are

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\rho\frac{\partial u}{\partial x} \tag{11.103}$$

$$\rho\frac{\mathrm{D}u}{\mathrm{D}t} = -\frac{\partial P}{\partial x} \tag{11.104}$$

$$\frac{\mathrm{D}P}{\mathrm{D}t} = a_f^2\frac{\mathrm{D}\rho}{\mathrm{D}t} + \rho a_f^2\dot{\sigma} \tag{11.105}$$

$$\frac{\mathrm{D}Y_k}{\mathrm{D}t} = \dot{\Omega}_k \qquad k = 1,\ldots,K \tag{11.106}$$

The frozen sound speed is defined as

$$a_f^2 = \left(\frac{\partial P}{\partial \rho}\right)_{s,\mathbf{Y}} \tag{11.107}$$

and the thermicity is defined as

$$\dot{\sigma} = \sum_{k=1}^{K}\sigma_k\frac{\mathrm{D}Y_k}{\mathrm{D}t} \tag{11.108}$$

$$= \boldsymbol{\sigma}\cdot\frac{\mathrm{D}\mathbf{Y}}{\mathrm{D}t} \tag{11.109}$$

The variables Y_k represent the internal state variables such as mass fraction that are associated with reaction or relaxation processes that evolve according to reaction rates $\dot{\Omega}_k$. The thermicity coefficients σ_k are response functions associated with isentropic changes in the internal state variables

$$\sigma_k = \frac{1}{\rho a_f^2}\left(\frac{\partial P}{\partial Y_k}\right)_{s,\rho,Y_{i\neq k}} \tag{11.110}$$

Compatibility Conditions at Shock Front

Eliminating density from (11.105) using (11.103) and transform to shock coordinates, we obtain a pair of relationships coupling the time rate of change of properties at the shock to spatial gradients and reaction.

$$\left(\frac{\mathrm{d}P}{\mathrm{d}t}\right)_{\mathcal{S}} + (u - U)\,\frac{\partial P}{\partial x} + \rho a_f^2\frac{\partial u}{\partial x} - \rho a_f^2\dot{\sigma} = 0 \ , \tag{11.111}$$

$$\rho\left(\frac{\mathrm{d}u}{\mathrm{d}t}\right)_{\mathcal{S}} + \rho\,(u - U)\,\frac{\partial u}{\partial x} + \frac{\partial P}{\partial x} = 0 \ . \tag{11.112}$$

Eliminating $\partial P/\partial x$ from (11.111) and (11.112) we obtain

$$\left(\frac{\mathrm{d}P}{\mathrm{d}t}\right)_{\mathcal{S}} + \rho w \left(\frac{\mathrm{d}u}{\mathrm{d}t}\right)_{\mathcal{S}} - \rho a_f^2 \left(\dot{\sigma} - \eta \frac{\partial u}{\partial x}\right) = 0 \; , \tag{11.113}$$

where we have made the subsitution $w = U - u$ and defined the *sonic parameter*

$$\eta = 1 - (w/a_f)^2 \; . \tag{11.114}$$

The compatibility conditions apply equally upstream and downstream of the shock. In what follows, we will assume the upstream state is specified and evaluate all terms in (11.113) at the state downstream of the shock.

The upstream states enter in through the jump conditions, in the laboratory reference frame these are:

$$[\rho] = [\rho u]/U \tag{11.115}$$
$$[P] = [\rho(U-u)] \tag{11.116}$$
$$[h] = [(U-u)^2]/2 \tag{11.117}$$

where $[f]$ is the change or jump $f_2 - f_1$ of any property across the wave. Because we are assuming an ideal shock wave, the jump conditions have a unique solution for a given upstream state $(u_1, P_1, \rho_1, \mathbf{Y}_1)$ and wave speed U. The shock speed and upstream flow velocity do not enter into the jump conditions (11.115) independently but through the combination $w_1 = U - u_1$. For a given upstream state and shock speed, a unique solution exists to the downstream state.

$$P_2 = P_2(w_1, P_1, \rho_1, \mathbf{Y}_1) \tag{11.118}$$
$$w_2 = w_2(w_1, P_1, \rho_1, \mathbf{Y}_1) \tag{11.119}$$
$$\rho_2 = \rho_2(w_1, P_1, \rho_1, \mathbf{Y}_1) \tag{11.120}$$

For frozen (nonreactive) shock waves, the composition does not change across the wave

$$\mathbf{Y}_2 = \mathbf{Y}_1 \; . \tag{11.121}$$

For reactive shock waves that result in equilibrium downstream states

$$\mathbf{Y}_2 = \mathbf{Y}_2^{eq}(P_2, \rho_2; \mathbf{Y}_1) \tag{11.122}$$

Changes in downstream state can be related to small changes in the upstream state through differentiation of the jump conditions:

$$\mathrm{d}P_2 = \left(\frac{\partial P_2}{\partial w_1}\right)_{P_1,\rho_1,\mathbf{Y}_1} \mathrm{d}w_1 + \left(\frac{\partial P_2}{\partial P_1}\right)_{w_1,\rho_1,\mathbf{Y}_1} \mathrm{d}P_1 + \left(\frac{\partial P_2}{\partial \rho_1}\right)_{w_1,P_1,\mathbf{Y}_1} \mathrm{d}\rho_1 + \sum_{k=1}^{K} \left(\frac{\partial P_2}{\partial Y_{1,k}}\right)_{w_1,P_1,Y_{1,i\neq k}} \mathrm{d}Y_{1,k} \; , \tag{11.123}$$

$$\mathrm{d}w_2 = \left(\frac{\partial w_2}{\partial w_1}\right)_{P_1,\rho_1,\mathbf{Y}_1} \mathrm{d}w_1 + \left(\frac{\partial w_2}{\partial P_1}\right)_{w_1,\rho_1,\mathbf{Y}_1} \mathrm{d}P_1 + \left(\frac{\partial w_2}{\partial \rho_1}\right)_{w_1,P_1,\mathbf{Y}_1} \mathrm{d}\rho_1 + \sum_{k=1}^{K} \left(\frac{\partial w_2}{\partial Y_{1,k}}\right)_{w_1,P_1,Y_{1,i\neq k}} \mathrm{d}Y_{1,k} \; . \tag{11.124}$$

The changes in the velocities w_1 and w_2 depend both on the lab frame velocity and shock speed

$$\mathrm{d}w_1 = \mathrm{d}U - \mathrm{d}u_1 \; , \tag{11.125}$$
$$\mathrm{d}w_2 = \mathrm{d}U - \mathrm{d}u_2 \; . \tag{11.126}$$

Using these results, the two unsteady terms in (11.113) can be computed

$$\begin{aligned}\left(\frac{\mathrm{d}P_2}{\mathrm{d}t}\right)_{\mathcal{S}} &= \left(\frac{\partial P_2}{\partial w_1}\right)_{P_1,\rho_1,\mathbf{Y}_1}\left[\frac{\mathrm{d}U}{\mathrm{d}t} - \left(\frac{\mathrm{d}u_1}{\mathrm{d}t}\right)_{\mathcal{S}}\right] + \left(\frac{\partial P_2}{\partial P_1}\right)_{w_1,\rho_1,\mathbf{Y}_1}\left(\frac{\mathrm{d}P_1}{\mathrm{d}t}\right)_{\mathcal{S}} \\ &+ \left(\frac{\partial P_2}{\partial \rho_1}\right)_{w_1,P_1,\mathbf{Y}_1}\left(\frac{\mathrm{d}\rho_1}{\mathrm{d}t}\right)_{\mathcal{S}} + \sum_{k=1}^{K}\left(\frac{\partial P_2}{\partial Y_{1,k}}\right)_{w_1,P_1,Y_{1,i\neq k}}\left(\frac{\mathrm{d}Y_{1,k}}{\mathrm{d}t}\right)_{\mathcal{S}},\end{aligned} \tag{11.127}$$

$$\begin{aligned}\left(\frac{\mathrm{d}u_2}{\mathrm{d}t}\right)_{\mathcal{S}} &= \left[1 - \left(\frac{\partial w_2}{\partial w_1}\right)_{P_1,\rho_1,\mathbf{Y}_1}\right]\frac{\mathrm{d}U}{\mathrm{d}t} + \left(\frac{\partial w_2}{\partial w_1}\right)_{P_1,\rho_1,\mathbf{Y}_1}\left(\frac{\mathrm{d}u_1}{\mathrm{d}t}\right)_{\mathcal{S}} - \left(\frac{\partial w_2}{\partial P_1}\right)_{w_1,\rho_1,\mathbf{Y}_1}\left(\frac{\mathrm{d}P_1}{\mathrm{d}t}\right)_{\mathcal{S}} \\ &- \left(\frac{\partial w_2}{\partial \rho_1}\right)_{w_1,P_1,\mathbf{Y}_1}\left(\frac{\mathrm{d}\rho_1}{\mathrm{d}t}\right)_{\mathcal{S}} - \sum_{k=1}^{K}\left(\frac{\partial w_2}{\partial Y_{1,k}}\right)_{w_1,P_1,Y_{1,i\neq k}}\left(\frac{\mathrm{d}Y_{1,k}}{\mathrm{d}t}\right)_{\mathcal{S}}\end{aligned} \tag{11.128}$$

Derivatives and Hugoniot Thermodynamics

For unsteady and/or spatially nonuniform upstream flows it is necessary to compute the six partial derivatives. For a perfect gas model of the equation of state, the derivatives can be computed analytically from the explicit solutions for the jump conditions. For more complex equations of state, it may be necessary to use numerical methods in the Shock and Detonation Toolbox (**?**) or analysis based on differentiating the jump conditions and solving the resulting system of equations Kao (2008). These derivatives depend only on the instantaneous upstream state and solutions to the jump condition so they are properties of the fluid state and thermodynamic properties. An additional complication is that for spatially nonuniform flows, the partial derivatives will vary from point to point in the flow and even if analytical solutions are available, these must be evaluated at each point in the flow.

For spatially uniform upstream flow, only two of the derivatives are required and for steady, spatially uniform upstream flow, only one derivative is needed because the solutions to the jump conditions can be parameterized by a single variable. This is the conventional approach used (Fickett and Davis, 1979, Radulescu, 2020) to derive the shock change equation.

Perfect gas The perfect gas model of a shock wave has explicit solutions for nondimensional property ratios in terms of the upstream Mach number $M_1 = w_1/a_1$ and specific heat ratio γ. Pressure derivatives can be evaluated from the pressure jump equation solution in the form

$$P_2 = \frac{2}{\gamma+1}\rho_1 w_1^2 - P_1\frac{\gamma-1}{\gamma+1} \tag{11.129}$$

The derivatives of pressure can be expressed as

$$\left(\frac{\partial P_2}{\partial w_1}\right)_{P_1,\rho_1} = \frac{P_1}{a_1}\frac{4\gamma}{\gamma+1}M_1 \tag{11.130}$$

$$\left(\frac{\partial P_2}{\partial P_1}\right)_{w_1,\rho_1} = -\frac{\gamma-1}{\gamma+1} \tag{11.131}$$

$$\left(\frac{\partial P_2}{\partial \rho_1}\right)_{w_1,P_1} = \frac{2a_1^2}{\gamma+1}M_1^2 \tag{11.132}$$

$$\tag{11.133}$$

where $M_1 = w_1/a_1$ and we have suppressed the dependence on $\mathbf{Y}$ which we assume to be constant. The velocity jump solution can be expressed as

$$w_2 = \frac{\gamma-1}{\gamma+1}w_1 + \frac{P_1}{\rho_1}\frac{2\gamma}{\gamma+1}\frac{1}{w_1} \tag{11.134}$$

and the derivatives are

$$\left(\frac{\partial w_2}{\partial w_1}\right)_{P_1,\rho_1} = \frac{\gamma-1}{\gamma+1} - \frac{2}{\gamma+1}\frac{1}{M_1^2} \tag{11.135}$$

$$\left(\frac{\partial w_2}{\partial P_1}\right)_{w_1,\rho_1} = \frac{2\gamma}{\gamma+1}\frac{a_1}{P_1}\frac{1}{M_1} \tag{11.136}$$

$$\left(\frac{\partial w_2}{\partial \rho_1}\right)_{w_1,P_1} = -\frac{2}{\gamma+1}\frac{a_1}{\rho_1}\frac{1}{M_1} \tag{11.137}$$

$$\tag{11.138}$$

Real fluids Analytic expressions for the derivatives in terms of thermodynamic properties can be obtained by using the technique described in (Kao, 2008, p. 157) of differentiating the jump conditions with appropriate constraints and solving a set of linear equations. The results can be simplified by using the following thermodynamic definitions. The Grüneisen parameter is defined as

$$\mathcal{G} = \frac{1}{\rho}\left(\frac{\partial P}{\partial e}\right)_\rho \tag{11.139}$$

and is related to the derivative of enthalpy w.r.t. pressure by

$$\left(\frac{\partial h}{\partial P}\right)_\rho = \frac{1}{\rho}\frac{\mathcal{G}+1}{\mathcal{G}} . \tag{11.140}$$

An alternative definition of sound speed is

$$a^2 = \frac{\left(\frac{\partial h}{\partial \rho}\right)_P}{\frac{1}{\rho} - \left(\frac{\partial h}{\partial P}\right)_\rho} . \tag{11.141}$$

The derivative of enthalpy w.r.t. density can be expressed as

$$\left(\frac{\partial h}{\partial \rho}\right)_P = -\frac{a^2}{\rho}\frac{1}{\mathcal{G}} . \tag{11.142}$$

Spatially uniform, steady flows

The solutions to the jump conditions can be parameterized by a single upstream variable such as shock velocity $U = w_1$ or shock Mach number $M_1 = U/a_1$; parameterizing in terms of a downstream variable such w_2 is often used in simple wave analysis in the form of a $P_2(u_2)$ relation to aid in graphical pressure-velocity solutions.

The derivative relations for this case simplify to

$$\left(\frac{\mathrm{d}P_2}{\mathrm{d}t}\right)_\mathcal{S} = \left(\frac{\partial P_2}{\partial w_1}\right)_{P_1,\rho_1,\mathbf{Y}_1}\frac{\mathrm{d}U}{\mathrm{d}t} , \tag{11.143}$$

$$\left(\frac{\mathrm{d}u_2}{\mathrm{d}t}\right)_\mathcal{S} = \left[1 - \left(\frac{\partial w_2}{\partial w_1}\right)_{P_1,\rho_1,\mathbf{Y}_1}\right]\frac{\mathrm{d}U}{\mathrm{d}t} \tag{11.144}$$

Taking the ratio of these terms

$$\left(\frac{\mathrm{d}u_2}{\mathrm{d}P_2}\right)_\mathcal{H} = \frac{\left(\frac{\mathrm{d}u_2}{\mathrm{d}t}\right)_\mathcal{S}}{\left(\frac{\mathrm{d}P_2}{\mathrm{d}t}\right)_\mathcal{S}} = \frac{1 - \left(\frac{\partial w_2}{\partial w_1}\right)_{P_1,\rho_1,\mathbf{Y}_1}}{\left(\frac{\partial P_2}{\partial w_1}\right)_{P_1,\rho_1,\mathbf{Y}_1}} \tag{11.145}$$

The subscript $\mathcal{H}$ indicates that the derivative is a relationship obtained by constraining the variables to the Hugoniot or shock adiabat, i.e., the solution to the jump conditions. Graphically, the interpretation of this derivative is the co-slope of the Hugoniot solution in $P-u$ coordinates. Substituting into (11.113) we obtain

$$\frac{\mathrm{d}P_2}{\mathrm{d}t} = \rho_2 a_{2,f}^2 \frac{\dot{\sigma} - \eta \dfrac{\partial u_2}{\partial x}}{1 + \rho_2 w_2 \left(\dfrac{\mathrm{d}u_2}{\mathrm{d}P_2}\right)_{\mathcal{H}}} \tag{11.146}$$

In terms of shock velocity, this relationship is

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \rho_2 a_{2,f}^2 \frac{\dot{\sigma} - \eta \dfrac{\partial u_2}{\partial x}}{\left(\dfrac{\mathrm{d}P_2}{\mathrm{d}U}\right)_{\mathcal{H}} \left[1 + \rho_2 w_2 \left(\dfrac{\mathrm{d}u_2}{\mathrm{d}P_2}\right)_{\mathcal{H}}\right]} \tag{11.147}$$

where the notation $(\ )_{\mathcal{H}}$ indicates derivatives on the ordinary shock adiabat or Hugoniot with $u_1 = 0$, and constant values of $(P_1, \rho_1, \mathbf{Y}_1))$ in the spatially uniform upstream state.

For a perfect gas, the terms can be expressed in terms of the shock Mach number using the results of the previous section. For example

$$\left(\frac{\partial u_2}{\partial P_2}\right)_{P_1,\rho_1} = \frac{\left(\dfrac{\partial u_2}{\partial w_1}\right)_{P_1,\rho_1}}{\left(\dfrac{\partial P_2}{\partial w_1}\right)_{P_1,\rho_1}} \tag{11.148}$$

$$= \frac{1}{2\rho_1 a_1} \frac{M_1^2 + 1}{M_1^3} \tag{11.149}$$

and the denominator of (11.146) is

$$1 + \rho_1 w_1 \left(\frac{\partial u_2}{\partial P_2}\right)_{P_1,\rho_1} = \frac{3}{2} + \frac{1}{2M_1^2} \tag{11.150}$$

Note that the denominator is bounded between 2 and 1.5 for $1 \leq M_1 \leq \infty$. The parameter η can be expressed in terms of the shock Mach number

$$\eta = 1 - M_2^2 = \frac{\gamma+1}{2\gamma} \frac{M_1^2 - 1}{M_1^2 - \dfrac{\gamma - 1}{2\gamma}} \tag{11.151}$$

and $0 \leq \eta \leq (\gamma+1)/2\gamma$ for $1 \leq M_1 \leq \infty$. A case of special interest is the nonreacting, $\dot{\sigma} = 0$ shock. The shock change equation can be written in nonndimensional form as

$$\frac{1}{\rho_1 a_1^2} \frac{\mathrm{d}P_2}{\mathrm{d}t} = -\frac{\rho_2 a_2^2}{\rho_1 a_1^2} \frac{\eta \dfrac{\partial u_2}{\partial x}}{1 + \rho_2 w_2 \left(\dfrac{\mathrm{d}u_2}{\mathrm{d}P_2}\right)_{\mathcal{H}}} \tag{11.152}$$

For a perfect gas, simplifies to

$$\frac{\mathrm{d}P_2/P_1}{\mathrm{d}t} = -\gamma \frac{P_2}{P_1} \frac{\eta \dfrac{\partial u_2}{\partial x}}{1 + \rho_2 w_2 \left(\dfrac{\mathrm{d}u_2}{\mathrm{d}P_2}\right)_{\mathcal{H}}} \tag{11.153}$$

Another useful representation of the shock change equation is to express the velocity gradient in terms of the rate of change of the shock velocity by rearranging (11.147) and formulating dP_2/dw_1 in terms of the shock Mach number

$$\frac{\mathrm{d}P_2}{\mathrm{d}w_1} = \rho_1 a_1 \frac{4}{\gamma+1} M_1 \tag{11.154}$$

to obtain

$$\frac{\partial u}{\partial x} = -\frac{4M_1}{(\gamma+1)\eta}\frac{P_1}{P_2}\left(1+\rho_2 w_2 \left(\frac{\mathrm{d}u_2}{\mathrm{d}P_2}\right)_{\mathcal{H}}\right)\frac{\mathrm{d}M_1}{\mathrm{d}t} \tag{11.155}$$

This relationship can be written in term of a nondimensional function $F(M,\gamma)$

$$\frac{\partial u}{\partial x} = -F(M,\gamma)\frac{\mathrm{d}M_1}{\mathrm{d}t} \tag{11.156}$$

Using the perfect gas jump conditions, after some algebraic manipulation the function F can be expressed as

$$F = \frac{2}{\gamma+1}\frac{(3M_1^2+1)}{M_1(M_1^2-1)} \tag{11.157}$$

See Radulescu (2020) for discussion of applications of this form of the equation to blast decay problems. The function $F(M)$ is strongly varying as a function of shock Mach number, as shown Fig. 11.13 The limiting

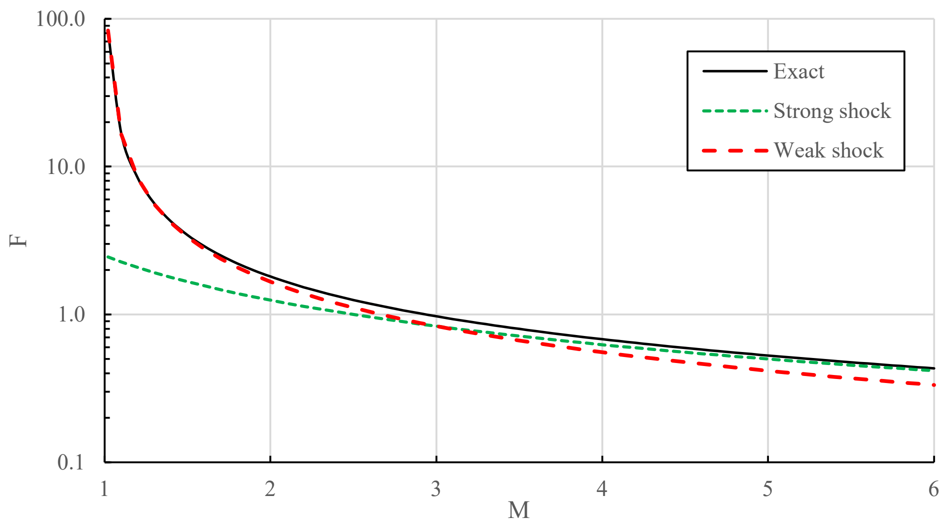

Figure 11.13: Shock change relation function $F(M)$ for a perfect gas, $\gamma = 1.4$.

behavior for weak and strong shock waves is

$$\lim_{M_1\to 1} F \sim \frac{4}{\gamma+1}\frac{1}{M_1-1} \tag{11.158}$$

$$\lim_{M_1\to\infty} F \sim \frac{6}{\gamma+1}\frac{1}{M_1} \tag{11.159}$$

Note that the weak shock approximation is useful for a much large range of shock Mach numbers than the strong shock approximation and has the correct M_1 dependence at both limits. The weak shock approximation for F has a maximum relative error of 25% over the range $1 \leq M_1 \leq 5$ for $\gamma = 1.4$.

Spatially nonuniform, nonsteady flows

Substituting (11.127) and (11.128) into (11.113), the most general form of a shock change relationship is obtained

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \frac{\rho_2 a_{2,f}^2 \left[\dot{\sigma} - \eta \dfrac{\partial u_2}{\partial x}\right] - \sum\limits_{\mathrm{ns}}}{\left(\dfrac{\mathrm{d}P_2}{\mathrm{d}w_1}\right)_{P_1,\rho_1,\mathbf{Y}_1} + \rho_2 w_2 \left[1 - \left(\dfrac{\mathrm{d}w_2}{\mathrm{d}w_1}\right)_{P_1,\rho_1,\mathbf{Y}_1}\right]} . \tag{11.160}$$

All of the effects associated with the nonsteady and nonuniform upstream state have been lumped into a single term

$$\begin{aligned}
\sum_{\mathrm{ns}} = &- \left[\left(\frac{\partial P_2}{\partial w_1}\right)_{P_1,\rho_1,\mathbf{Y}_1} - \rho_2 w_2 \left(\frac{\partial w_2}{\partial w_1}\right)_{P_1,\rho_1,\mathbf{Y}_1}\right] \left(\frac{\mathrm{d}u_1}{\mathrm{d}t}\right)_{\mathcal{S}} \\
&+ \left[\left(\frac{\partial P_2}{\partial P_1}\right)_{w_1,\rho_1,\mathbf{Y}_1} - \rho_2 w_2 \left(\frac{\partial w_2}{\partial P_1}\right)_{w_1,\rho_1,\mathbf{Y}_1}\right] \left(\frac{\mathrm{d}P_1}{\mathrm{d}t}\right)_{\mathcal{S}} \\
&+ \left[\left(\frac{\partial P_2}{\partial \rho_1}\right)_{w_1,P_1,\mathbf{Y}_1} - \rho_2 w_2 \left(\frac{\partial w_2}{\partial \rho_1}\right)_{w_1,P_1,\mathbf{Y}_1}\right] \left(\frac{\mathrm{d}\rho_1}{\mathrm{d}t}\right)_{\mathcal{S}} \\
&+ \sum_{k=1}^{K} \left[\left(\frac{\partial P_2}{\partial Y_k}\right)_{w_1,P_1,Y_{1,i\neq k}} - \rho_2 w_2 \left(\frac{\partial w_2}{\partial Y_{1,k}}\right)_{w_1,P_1,Y_{1,i\neq k}}\right] \left(\frac{\mathrm{d}Y_{1,k}}{\mathrm{d}t}\right)_{\mathcal{S}}
\end{aligned} \tag{11.161}$$

Nonuniformity and unsteadiness enters into (11.160) not only through the explicit derivatives of the upstream state in (11.161) but also through the dependence of downstream states and the derivatives of the shock jump conditions on the local upstream state. For nonreacting flows, the equations can be further simplified since $\dot{\sigma} = 0$ and the consideration of composition or internal state $\mathbf{Y}$ can be dropped from the differentiation process and upstream state. This approach was successfully applied by Schoeffler and Shepherd (2022, 2023) to modelling the acceleration of shock waves generated by detonation reflection.

Equilibrium Shock States

In some situations, the reaction proceeds sufficiently rapidly behind the shock front that an equilibrium state is reached a short distance Δ behind the shock front. If the thickness of the reaction zone is much smaller than any other length scale L, i.e., $\Delta \ll L$, then the shock wave can be idealized as a surface between an arbitrary upstream state and a chemically equilibrium downstream state. This case can be idealized as the composition changing instantaneously to keep the state in chemical equilibrium as the pressure and density vary. For a specified upstream state, the downstream composition will be determined by simultaneously solving the chemical equilibrium condition with the jump conditions for mass, momentum and energy. The equilibrium composition is only a function of the local thermodynamic state, for example (P, ρ) so that

$$\mathbf{Y}_2 = \mathbf{Y}^{eq}(P, \rho; \mathbf{Y}_1) \tag{11.162}$$

The dependence on the upstream composition can be supressed if the elemental composition of the upstream state does not vary with space or time. This will be the case in reacting flows with initially uniform composition as long as species diffusion does not create significant variations in elemental composition. For this case

$$\mathbf{Y}_2 = \mathbf{Y}^{eq}(P_2, \rho_2) \tag{11.163}$$

The composition $\mathbf{Y}_2$ will shift as (P, ρ) vary downstream of the shock and the time rate of change of composition will be

$$\frac{\mathrm{D}\mathbf{Y}}{\mathrm{D}t} = \left(\frac{\partial \mathbf{Y}^{eq}}{\partial P}\right)_{\rho} \frac{\mathrm{D}P}{\mathrm{D}t} + \left(\frac{\partial \mathbf{Y}^{eq}}{\partial \rho}\right)_{P} \frac{\mathrm{D}\rho}{\mathrm{D}t} \tag{11.164}$$

Subsituting into the adiabatic change relationship (11.105) we obtain

$$\frac{\mathrm{D}P}{\mathrm{D}t} = a_f^2 \frac{\mathrm{D}\rho}{\mathrm{D}t} + \rho a_f^2 \boldsymbol{\sigma} \cdot \left(\frac{\partial \mathbf{Y}^{eq}}{\partial P} \right)_\rho \frac{\mathrm{D}P}{\mathrm{D}t} + \rho a_f^2 \boldsymbol{\sigma} \cdot \left(\frac{\partial \mathbf{Y}^{eq}}{\partial \rho} \right)_P \frac{\mathrm{D}\rho}{\mathrm{D}t} \tag{11.165}$$

Simplifying, we obtain the equilibrium form of the adiabatic change equation

$$\frac{\mathrm{D}P}{\mathrm{D}t} = a_{eq}^2 \frac{\mathrm{D}\rho}{\mathrm{D}t} \tag{11.166}$$

where the equilibrium sound speed is defined as

$$a_{eq}^2 = a_f^2 \frac{1 + \rho \boldsymbol{\sigma} \cdot \left(\dfrac{\partial \mathbf{Y}^{eq}}{\partial \rho} \right)_P}{1 - \rho a_f^2 \boldsymbol{\sigma} \cdot \left(\dfrac{\partial \mathbf{Y}^{eq}}{\partial P} \right)_\rho} \tag{11.167}$$

An alternative expression for the equilibrium sound speed is simply

$$a_{eq}^2 = \left(\frac{\partial P}{\partial \rho} \right)_{s, \mathbf{Y}^{eq}} . \tag{11.168}$$

With these changes implemented and repeating the derivation, the shock change relation (11.160) for equilibrium shocks is transformed to

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \frac{-\rho_2 a_{2,eq}^2 \eta \dfrac{\partial u_2}{\partial x} - \displaystyle\sum_{\mathrm{ns}}}{\left(\dfrac{\mathrm{d}P_2}{\mathrm{d}w_1} \right)_{P_1, \rho_1, \mathbf{Y}_1} + \rho_2 w_2 \left[1 - \left(\dfrac{\mathrm{d}w_2}{\mathrm{d}w_1} \right)_{P_1, \rho_1, \mathbf{Y}_1} \right]} . \tag{11.169}$$

where all downstream (post-shock) states and derivatives are computed using the assumption of complete chemical equilibrium. In particular, the sonic parameter will be based on the equilibrium rather than frozen sound speed, $\eta = 1 - w_2^2/a_{2,eq}^2$. If the elemental composition is varying upstream of the shock, there will be an additional term in the adiabatic change equation the shock change equation will have corresponding modifications.

Although the thermicity no longer explicitly appears in the shock change relation for an equilibrium shock, this result is not equivalent to setting the thermicity or species time derivatives to zero. The components σ_k of the thermicity and the rate of change of the species do not vanish in an equilibrium, spatially and time-dependent flow. They key is the evolution of the composition is assumed to always occur sufficiently rapidly that the rate of change of the composition precisely keeps step with the changes in the thermodynamic state. This situation is more general and can apply throughout a flow as long as the chemical reactions are sufficiently rapid compared to the rate of change of the thermodynamic state. This is often the case in the expansion wave immediately following a detonation although the applicability of this approximation depends both on the specific mixture as well as the location within flow. A detailed examination of these chemical nonequilibrium issues for the Taylor-Zeldovich model of detonation propagation was made by Cooper (see Ch. 6 of Cooper, 2004) and the implications for modeling the impulse of detonation waves are discussed by Wintenberger (see Ch. 4 and App. B of Wintenberger, 2004).

Application to Detonation and the CJ Condition

The shock change equation illustrates how shock waves are affected by chemical reaction and flow divergence. Exothermic chemical reactions $\dot{\sigma} > 0$, and favorable velocity gradients $\partial \mathrm{u}/\partial x < o$ will cause the shock pressure to increase, i.e., the shock strengthens. Endothermic chemical reactions $\dot{\sigma} < 0$, or unfavorable velocity gradients $\partial \mathrm{u}/\partial x > o$ will cause the shock pressure to decrease, i.e., the shock weakens.

If the flow is to be steady, then the energy exchange processes must be exactly balanced by the spatial gradients in the flow

$$\dot{\sigma} - \eta \frac{\partial \mathrm{u}}{\partial x} = 0 \tag{11.170}$$

This is the basis of computing steady detonation wave structure for the ZND model.

The hydrodynamic model of a detonation considers the reaction zone to sufficiently thin that we can consider the detonation wave to behave as a reactive shock wave that can be treated as a jump from reactants to equilibrium products. The postshock state then refers to properties in the completely reacted equilibrium products hence the thermicity term vanishes, $\dot{\sigma} = 0$. The appropriate shock adiabat is the equilibrium detonation adiabat $\mathcal{H}$ with a corresponding velocity-pressure relation $\mathrm{u}_{\mathcal{H}}(P)$. The adiabatic change relation between pressure and density for an equilibrium flow is

$$\frac{\mathrm{D}P}{\mathrm{D}t} = a_e^2 \frac{\mathrm{D}\rho}{\mathrm{D}t} , \tag{11.171}$$

and using the equations of motion as above, this is

$$\frac{\mathrm{D}P}{\mathrm{D}t} = -\rho a_e^2 \frac{\partial \mathrm{u}}{\partial x} , \tag{11.172}$$

where a_e is the equilibrium sound speed. The derivative of the pressure just behind the detonation wave $\mathcal{D}$ is

$$\left.\frac{\mathrm{d}P}{\mathrm{d}t}\right|_{\mathcal{D}} = -\frac{\rho a_e^2}{1 + \rho_1 U \left(\dfrac{\mathrm{du}}{\mathrm{d}P}\right)_{\mathcal{D}}} \eta_e \frac{\partial \mathrm{u}}{\partial x} \tag{11.173}$$

where $(\mathrm{du}/\mathrm{d}P)_{\mathcal{D}}$ is computed using the equilibrium detonation products. The sonic parameter is now based on the equilibrium sound speed

$$\eta_e = 1 - \frac{(U - \mathrm{u})^2}{a_e^2} \tag{11.174}$$

The unsteady evolution of an overdriven detonation towards the CJ state can be explained using (11.173). Since the flow is subsonic behind an overdriven detonation wave or shock, $\eta > 0$ and the wave will decay, $\left.\frac{\mathrm{d}P}{\mathrm{d}t}\right)_{\mathcal{D}} < 0$ if it is followed by an expansion wave with $\partial \mathrm{u}/\partial x > 0$. As the wave approaches the CJ condition, $\eta \longrightarrow 0$ and the influence of gradients behind the wave diminish. Therefore, the wave will tend to a steady wave $\left.\frac{\mathrm{d}P}{\mathrm{d}t}\right)_{\mathcal{D}} \to 0$ with $U - \mathrm{u} \to a_e$ at large times as long as the wave remains sufficiently thin and the reaction zone is relatively insensitive to the unsteadiness in thermodynamic state behind the shock front. This provides an alternative justification for the CJ condition to the conventional explanation of the CJ condition as the minimum wave speed consistent with the steady flow jump conditions.

11.12 Shock Change Relations - Curved Waves

Shock change relations can be extended to curved shock waves in two or three dimensions. The approach is extend the previous treatment using the same considerations as developed for the quasi-steady model of reaction zone structure behind curved propagating waves, Section 11.10. We will first consider blast waves with unifrom surface curvature independent of position on the wave and then consider the extension to a more general case of nonuniform curvature.

Uniform Curvature

Modeling the flow as one-dimensional in a planar ($j = 0$), cylindrical ($j = 1$), or spherical ($j = 2$) coordinate system, the conservation of mass equation can be written as in terms of a radial coordinate r

$$\frac{1}{\rho}\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\frac{\partial \mathrm{u}}{\partial r} - \frac{j}{r}\mathrm{u} \tag{11.175}$$

For a shock wave of radius R_s moving with a speed $U = dR_s/dt$, the methodology used for the planar shock change equation can be extended to a curved wave. For the case of a unifrom, stationary upstream the followin versions of the shock change relation can be derived

$$\rho w\left(\frac{\mathrm{d}u}{\mathrm{d}t}\right)_{\mathcal{S}} + \left(\frac{\mathrm{d}P}{\mathrm{d}t}\right)_{\mathcal{S}} = \rho a^2\left(-\eta\frac{\partial u}{\partial r} + \dot{\sigma} - \frac{j\,\mathrm{u}}{R_s}\right) \tag{11.176}$$

$$\rho w\left(\frac{\mathrm{d}u}{\mathrm{d}t}\right)_{\mathcal{S}} + \left(\frac{\mathrm{d}P}{\mathrm{d}t}\right)_{\mathcal{S}} = \rho a^2\left(\eta\frac{1}{\rho}\frac{\mathrm{D}\rho}{\mathrm{D}t} + \dot{\sigma} - \frac{w^2}{a^2}\frac{j\,\mathrm{u}}{R_s}\right) \tag{11.177}$$

$$\rho w\left(\frac{\mathrm{d}u}{\mathrm{d}t}\right)_{\mathcal{S}} + \left(\frac{\mathrm{d}P}{\mathrm{d}t}\right)_{\mathcal{S}} = \rho a^2\left(\eta\frac{1}{\rho a^2}\frac{\mathrm{D}P}{\mathrm{D}t} + \frac{w^2}{a^2}\dot{\sigma} - \frac{w^2}{a^2}\frac{j\,\mathrm{u}}{R_s}\right) \tag{11.178}$$

Using the thermodynamic transformations and shock jump conditions, the left-hand side can be written in terms of the derivatives on the Hugoniot and the shock acceleration

$$\rho w\left(\frac{\mathrm{d}u}{\mathrm{d}t}\right)_{\mathcal{S}} + \left(\frac{\mathrm{d}P}{\mathrm{d}t}\right)_{\mathcal{S}} = \left[1 + \rho_1 U\left(\frac{\mathrm{d}u}{\mathrm{d}P}\right)_{\mathcal{H}}\right]\left(\frac{\mathrm{d}P}{\mathrm{d}U}\right)_{\mathcal{H}}\frac{\mathrm{d}U}{\mathrm{d}t} \tag{11.179}$$

The coefficient mutiplying shock acceleration can written in terms of a nondimensional function f

$$f = \frac{1}{\rho_1 a_1}\left\{\left[1 + \rho_1 U\left(\frac{\mathrm{d}u}{\mathrm{d}P}\right)_{\mathcal{H}}\right]\left(\frac{\mathrm{d}P}{\mathrm{d}U}\right)_{\mathcal{H}}\right\}, \tag{11.180}$$

and the left-hand side of (11.178) can be written as

$$\rho_1 U\left(\frac{\mathrm{d}u}{\mathrm{d}t}\right)_{\mathcal{S}} + \left(\frac{\mathrm{d}P}{\mathrm{d}t}\right)_{\mathcal{S}} = \rho_1 a_1 f\frac{\mathrm{d}U}{\mathrm{d}t}\,. \tag{11.181}$$

For a perfect gas, the function f can be given analytically in terms of shock Mach number $M_s = U/a_1$

$$f = \frac{4}{\gamma+1}\left[\frac{3}{2}M_s + \frac{1}{2M_s}\right] \tag{11.182}$$

Expressing the unsteady contributions in terms of shock acceleration, the the substantial derivative of pressure at the shock front can be expressed as

$$\eta\frac{\mathrm{D}P}{\mathrm{D}t} = \underbrace{-\,\rho w^2\dot{\sigma}}_{\text{chemical}} \quad \underbrace{+\rho w^2\frac{\mathrm{u}\,j}{R_s}}_{\text{curvature}} \quad \underbrace{+\rho_1 a_1 f\frac{\mathrm{d}U}{\mathrm{d}t}}_{\text{unsteady}}\,. \tag{11.183}$$

(11.184)

The chemical term represents the exchange of energy between molecular process and the flow. This contribution is identical to that obtained in the previous analyses of reaction zones behind steady shock waves. The curvature term is more properly described as a transverse divergence contribution and can be generalized as discussed below. The unsteady terms are all proportional to the shock acceleration $\mathrm{d}U/\mathrm{d}t$. The sign and magnitude of each term depends on the specific details of chemistry and shock wave configuration. The main distinctions are between exothermic $\dot{\sigma} < 0$ and endothermic $\dot{\sigma} > 0$ reactions at the shock front, diverging ($R_s > 0$) and converging ($R_s < 0$) shock waves, accelerating ($\mathrm{d}U/\mathrm{d}t > 0$) and decelerating ($\mathrm{d}U/\mathrm{d}t < 0$) shocks.

The interpretation of the curvature term is facilitated by referring to the quasi-steady flow discussion of Section 11.10, which gave the relationship of stream tube area A change immediately behind the front to the shock radius R_s. In the shock-fixed coordinate system, this correspondence is

$$\frac{j\,\mathrm{u}}{R_s} = w\frac{1}{A}\frac{\mathrm{d}A}{\mathrm{d}x} \tag{11.185}$$

In an unsteady flow, there are no well-defined stream tubes so it is more appropriate to refer to the curvature term as being associaed with the transverse component of flow divergence. The kinematics of fluid motions links the flow divergence to the density or volume rate of change through the continuity equation

$$\frac{1}{\rho}\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\frac{1}{v}\frac{\mathrm{D}v}{\mathrm{D}t} = -\nabla\cdot\mathbf{u} \tag{11.186}$$

The divergence can be divided into components parallel and transverse to the path line. In cartesian coordinates, the divergence is

$$\nabla\cdot\mathbf{u} = \underbrace{\frac{\partial u}{\partial x}}_{\text{parallel to path}} + \underbrace{\frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}}_{\text{transverse to path}} \tag{11.187}$$

In radially symmetric coordinates attached to the shock front (see Sec. 11.10), the transverse component is

$$\underbrace{\nabla\cdot\mathbf{u}}_{\text{transverse to path}} = \frac{j\,\mathrm{u}}{R_s - x}\,. \tag{11.188}$$

Nonuniform Curvature

Rabie and Wackerle (1978) derived a generalization of the one-dimensional model (11.178) to (almost) arbitrary shock shapes by considering the differential geometry of the front and generalizing the curvature term at the shock front to be

$$\frac{j}{R_s} \to \kappa\,, \tag{11.189}$$

where κ is twice the mean curvature of the shock front, which can be defined in terms of the surface shape

$$\kappa = -\nabla\cdot\hat{\mathbf{n}}\,. \tag{11.190}$$

where $\hat{\mathbf{n}}$ is the unit normal to the shock surface in the oriented in the direction of shock propagation. An alternative representation is in terms of the principal radii of curvature of the surface, $R_{s,1}$ and $R_{s,2}$

$$\kappa = \frac{1}{R_{s,1}} + \frac{1}{R_{s,2}}\,. \tag{11.191}$$

This generalization (Eq. 35 of Rabie and Wackerle, 1978)

$$\rho w\left(\frac{\mathrm{d}u}{\mathrm{d}t}\right)_{\mathcal{S}} + \left(\frac{\mathrm{d}P}{\mathrm{d}t}\right)_{\mathcal{S}} = \eta\frac{\mathrm{D}P}{\mathrm{D}t} + \rho w^2\dot{\sigma} - \rho w^2\mathrm{u}\kappa$$

only makes sense when streamlines are not significantly curved within the reaction zone. When the streamlines behind the shock are significantly curved, a different approach is needed with transformation to shock conformal coordinates and the recognition that curvature of the shock may generate significant vorticity in the downstream flow even for uniform upstream flows. For example, in a steady, planar flow, the vorticity immediately downstream of the shock is

$$\nabla \times \mathbf{u} = U\kappa \cos\beta \left(1 - \frac{\rho_1}{\rho_2}\right)^2 \frac{\rho_2}{\rho_1}$$

where β is the shock angle. For a straight but oblique detonation wave in a steady, uniform flow, $\nabla \times \mathbf{u} = 0$, and the reaction zone equations are equivalent (Shepherd, 1994) to the usual steady flow ZND equations. Approximate extensions of the reaction zone models to curved detonation waves and applications to initiation of detonation waves by projectiles are given by Kaneshige (1999) and Hung and Shepherd (2005), Hung (2003). The general case of a two- and three-dimensional steady flow following a curved shock is treated exactly by **?** (See also Hornung and Kaneshige, 1998) who provides detailed derivations and explores in depth the steady-flow analog of the shock-change equations with extensive applications to hypersonic flow (Hornung, 2010) over blunted shapes.

11.13 Unsteady Reaction Zone Models

The analyses of Eckett et al. (2000) and Arienti and Shepherd (2005) of reaction zones behind decaying blast waves in one and two dimensions examined the dominate balance along streams in the reaction zone and divided contributions into terms representing the effects of chemical reaction (effective heat release), stream tube divergence (curvature), and unsteadiness. The balance equations along a streamline behind a propagating shock appear identical in form to the shock change relations but the terms apply throughout flow, not just at the shock front. For example, (2.6c) of Eckett et al. (2000) describes the evolution of the pressure along a particle path with downstream distance from the shock measured by $x = R_s(t) - r$ and with relative velocity $w = U(t) - \mathrm{u}(r,t)$, $U = \mathrm{d}R_s/\mathrm{d}t$. The equations of motion in the (x,t) coordinates are:

$$\eta \frac{\mathrm{D}P}{\mathrm{D}t} = -\rho w^2 \dot{\sigma} + \frac{j}{R_s - x} \rho w^2 (U - w) + \rho w \frac{\mathrm{d}U}{\mathrm{d}t} - \rho w \frac{\partial w}{\partial t} + \frac{\partial P}{\partial t} \,. \qquad (11.192)$$

The corresponding density equation is

$$\eta \frac{\mathrm{D}\rho}{\mathrm{D}t} = -\rho \dot{\sigma} + \frac{1}{a^2} \left[\frac{j}{R_s - x} \rho w^2 (U - w) + \rho w \frac{\mathrm{d}U}{\mathrm{d}t} - \rho w \frac{\partial w}{\partial t} + \frac{\partial P}{\partial t} \right] , \qquad (11.193)$$

and the velocity equation is

$$\eta \frac{\mathrm{D}w}{\mathrm{D}t} = w \dot{\sigma} - \frac{j}{R_s - x} w (U - w) - \left(\frac{w}{a}\right)^2 \frac{\mathrm{d}U}{\mathrm{d}t} + \frac{\partial w}{\partial t} - \frac{w}{\rho a^2} \frac{\partial P}{\partial t} \,, \qquad (11.194)$$

The species evolution equation transforms without any addition terms

$$\frac{\mathrm{D}Y_k}{\mathrm{D}t} = \Omega_k \,. \qquad (11.195)$$

In this coordinate system, the substantial derivative is

$$\frac{\mathrm{D}(\cdot)}{\mathrm{D}t} = \frac{\partial(\cdot)}{\partial t} + w \frac{\partial(\cdot)}{\partial x} \,. \qquad (11.196)$$

At the shock front, $x = 0$, (11.192) identical with (11.178) and this is also the case for the ρ and w evolution equations. Downstream of the front, these equations are an exact transformation of the unsteady, one-dimensional reactive flow equations. However, this system of equations is not closed for a given streamline even if we are given a prescription for the blast wave trajectory $R_s(t)$. The partial derivatives with respect to time of P and w depend on the time variation on adjacent streamlines at a fixed x location, information that can only be reliably found by direct simulation of the entire flow field using the reactive Euler equations. However, this formulation is useful for analyzing direct simulations and serves as motivation for approximate models based estimating the time derivatives.

Analyzing several cases of direct numerical simulation of decaying, reactive blast waves with a simple chemical reaction models, Eckett et al. (2000) proposed an approximate model of the reaction zone based on examining the magnitude of the terms in (11.192 - 11.195) for path lines leaving the shock near the time when the reaction was quenched due to the decay of the blast wave. For sufficiently large shock wave radii, the dominant balance was found to be between unsteadiness and chemical energy release with lateral (stream tube) expansion playing a minor role. An approximate model was developed using a constant value of the unsteadiness contribution and neglecting the curvature contribution. An asymptotic analysis of this approximate model revealed that there existed a critical magnitude of the unsteadiness that determined when the reaction was quenched. This *critial decay rate* model was applied to the problem of direct initiation of detonations by point energy sources to estimate the magnitude of minimum energy required to establish a self-sustaining detonation. The idea of competition between unsteadiness and chemical energy release has subsequently been applied to other situations such ignition by transient compression events (Shepherd, 2020).

Approximate reaction zone structure equations can be formulated by recognizing that the right-hand side of (11.178) represents the quasi-steady, thin reaction zone model terms and the left-hand side as contribution of the unsteadiness of the shock wave. If approximations for the unsteady and curvature terms can be found, then these reaction zone equations can be integrated to determine the effect of contributions on the reaction zone structure along a particular particle path line downstream of an unsteady shock wave. Consider the pressure (11.192) and density (11.193) equations. These each involve the combination of terms

$$\frac{j}{R_s - x}\rho w^2(U - w) + \rho w \frac{\mathrm{d}U}{\mathrm{d}t} - \rho w \frac{\partial w}{\partial t} + \frac{\partial P}{\partial t}\,. \tag{11.197}$$

At the shock front, these terms are identical to corresponding terms in the shock change equation. The magnitude of the curvature term at the shock front is therefore

$$\frac{j}{R - x}\rho w^2(U - w) = \kappa_s \rho_2 w_2^2 \mathrm{u}_2 \qquad \text{at } x = 0 \text{ and } t = t_0\,, \tag{11.198}$$

where t_o is the instant of time when the fluid element passes through the shock and the subscript 2 indicates the postshock value. The magnitude of the sum of the unsteady terms is

$$\rho w \frac{\mathrm{d}U}{\mathrm{d}t} - \rho w \frac{\partial w}{\partial t} + \frac{\partial P}{\partial t} = \rho_1 a_1^2 f_s \frac{\mathrm{d}M_s}{\mathrm{d}t} \qquad \text{at } x = 0 \text{ and } t = t_0\,. \tag{11.199}$$

We seek models of each of these terms - models that only depend on time or location on a path line in order to integrate (11.192) along the path. The location on a path line is implicitly given by integration of the relative velocity

$$\frac{\mathrm{d}x}{\mathrm{d}t} = w \text{ and } \frac{\mathrm{d}r}{\mathrm{d}t} = U(t) - w(t; t_0) = \mathrm{u}(t; t_0) \tag{11.200}$$

to obtain path lines labeled by the time t_0 when the fluid element crosses the shock front

$$x(t; t_0) = \int_{t_0}^{t} w(t'; t_0)\,\mathrm{d}t' \quad \text{and} \quad r(t; t_0) = \int_{t_0}^{t} \mathrm{u}(t'; t_0)\,\mathrm{d}t' + R_s(t_0)\,. \tag{11.201}$$

Computing density and flow speed on a path line can be accomplished using relationship developed from the exact path line equations

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} = \rho\left[\frac{1}{\rho a^2}\frac{\mathrm{D}P}{\mathrm{D}t} - \dot{\sigma}\right]\,, \tag{11.202}$$

$$\frac{\mathrm{D}w}{\mathrm{D}t} = -\frac{1}{\rho w}\left[\frac{\mathrm{D}P}{\mathrm{D}t} - \frac{\partial P}{\partial t}\right] + \frac{\mathrm{d}U}{\mathrm{d}t}\,, \tag{11.203}$$