THE ROYAL SOCIETY

Remarks on diffusionless combustion

By John F. Clarke[1] and Nikolaos Nikiforakis[2]

[1]*Department of Aerospace Science, College of Aeronautics, Cranfield University, Cranfield MK43 0AL, UK*

[2]*Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Silver Street, Cambridge CB3 9EW, UK*

Classical studies of the dynamics of compressible media incorporate the possibility of exothermic actions in the field via the use of model combustion waves treated as discontinuous, and hence quasi-steady, phenomena. The latter are familiar under their broad titles of plane detonation waves, which travel at supersonic speeds, and deflagrations, which travel subsonically. Such deflagrations are not like conventional premixed flames insofar as laminar heat conduction and mass diffusion have no part to play in them; it is convenient to categorize these combustion waves as diffusionless.

With the inclusion of adiabatic shock waves and contact discontinuities, a whole range of formally unsteady phenomena can be analysed with the aid of these discontinuous combustion-wave models. Such skeletal theoretical ideas can be instructive, but they do suffer from a serious difficulty since they do not relate speeds of propagation of the combustion waves to the local environments that they inhabit, and it is necessary to call on empirical evidence to close the theory.

The present paper shows that these difficulties can be overcome by adopting an asymptotic parameter-perturbation approach to the construction of a self-contained rational theory of diffusionless combustion. It is demonstrated that asymptotic ideas are intrinsic to the classical studies of gas dynamics. Then logical pursuit of asymptotic thinking helps to consolidate the theory into a complete and consistent form, banishes the need for empiricism and sheds light on the physics of compressible reacting flows. The latter is exemplified here with an examination of the ephemeral character of weak detonations and their role in the birth of strong detonation waves.

Keywords: compressible reactive flow; detonation initiation; asymptotic theory; numerical simulations; unsteady diffusionless combustion

1. Introduction

The notation used here writes u^* for gas velocity, a^* for sound speed (which is, of course, of the same order as a mean molecular speed), ν^* for kinematic viscosity (roughly equal to a^{*2} times a mean molecular binary-collision interval), L^* for a suitable length-scale and t^*_{chem} for a chemical time-scale; all of these quantities are intended to typify conditions in all, or certainly significant parts, of a field. In general terms, a chemically active flow is characterized by the set of dimensionless numbers $M = (u^*/a^*)$, $Re = (u^*L^*/\nu^*)$ and $\mathcal{D} = (L^*/u^*t^*_{\mathrm{chem}})$, which signify local values of Mach number, Reynolds number and Damköhler number, respectively.

$\mathcal{D}$ will evidently be of the order of unity if chemical reactions are to have a significant effect on the flow and vice versa. The implication is that $L^* \sim u^*t^*_{\mathrm{chem}}$,

which means that $Re \sim (M^2 t^*_{\rm chem})/(\nu^* a^{*-2})$. The product $(\nu^* a^{*-2})$ is of the order of the time between binary molecular collisions in the gas, so that the order of magnitude of $t^*_{\rm chem}$ for a simple Arrhenius-type reaction can be written in the form $(\nu^* a^{*-2}) \exp(E^*_{\rm A}/R^* T^*_0)$, where $E^*_{\rm A}$ is equal to the activation energy for the reaction, T^*_0 is a suitable typical local temperature, and R^* is the universal gas constant; it follows that $Re \sim M^2 \exp(E^*_{\rm A}/R^* T^*_0)$. Since $E^*_{\rm A}/R^* T^*_0$ is usually a large number, it is clear that Re will be large too unless M^2 is very small.

The theories of Zeldovich and Frank-Kamanetski (ZFK, for short; see, for example, Zeldovich *et al.* (1985)) showed that the Mach number of propagation of a plane laminar premixed flame contains a factor $\exp(-E^*_{\rm A}/2R^* T^*_0)$, where T^*_0 is chosen to be the temperature behind the flame; as a consequence, the Reynolds numbers associated with these flames are of order unity. Since these ZFK flames necessarily involve diffusive effects, modest values of Re are to be expected. However, for any combustion waves whose propagation Mach numbers are in an order class of quantities that are larger than M for a laminar flame it is clear that their associated Reynolds numbers will be large, diffusion can properly be ignored and the set of Euler relations will provide an adequate basis on which to model such 'fast' flames.

The remainder of the paper is laid out as follows. The conservation equations are listed in § 2, together with information about equations of state and chemical reaction rates that is sufficient for the purposes of this article; the remainder of this section is taken up with discussions of activation-energy limits in § 2 *a*, discontinuous solutions of the Euler equations in § 2 *b* and continuous solutions viewed from various standpoints in § 2 *c* (i),(ii). The conservation equations are transformed to Lagrangian coordinates in § 3 and are then used, in primitive variable form, to discuss behaviour in induction domains in § 3 *a*, especially the development of singularity paths and their identification with quasi-steady weak detonations in § 3 *b*. Asymptotic matching of such weak detonation waves to fields in essentially unsteady induction domains is described in § 3 *c*, as are the consequences for early-time-evolution of events in compressible chemically active media. Comparisons between the general asymptotic-analytic solutions and an example of an accurate numerical solution of the full Euler equations for an illustrative problem are made in § 4; results are summarized and conclusions drawn in the final section.

2. Euler equations for a one-dimensional unsteady field

For the present, confine attention to a single spatial dimension, such as one may find in an ideal model of behaviour in a tube. An integral form of the Euler equations can now be written as

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{x_{\rm l}}^{x_{\rm r}} \boldsymbol{U} \, \mathrm{d}x = -\boldsymbol{F}_{\rm r} + \boldsymbol{F}_{\rm l} + \int_{x_{\rm l}}^{x_{\rm r}} \boldsymbol{R} \, \mathrm{d}x, \tag{2.1}$$

where the interval $x_{\rm l} \leqslant x \leqslant x_{\rm r}$ defines a fixed control volume and the surface that surrounds it. Using the notation p, ρ $(= 1/v)$, T, c, u, a, e to denote dimensionless values of pressure, density (specific volume), absolute temperature, mass fraction of a reactant species, gas velocity, local sound speed, and internal (or intrinsic) energy, respectively,† the vectors of dimensionless conserved quantities $\boldsymbol{U}$, fluxes (in the

† Definitions are as follows, with a superscript * denoting a dimensional value and a subscript zero indicating that the value applies to a chosen reference condition: $f \equiv f^*/f^*_0$ $(f = p, \rho, T, c, a)$; $u \equiv u^*/a^*_0$, $e \equiv e^*/a^{*2}_0$, $t \equiv t^*/t^*_0$, $x \equiv x^*/a^*_0 t^*_0$.

x-direction only) $\boldsymbol{F}$ and sources $\boldsymbol{R}$ are, respectively,

$$\boldsymbol{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho E \\ \rho c \end{pmatrix}, \quad \boldsymbol{F} = \begin{pmatrix} \rho u \\ \rho u^2 + \gamma^{-1} p \\ \rho u(E + \gamma^{-1} p v) \\ \rho c u \end{pmatrix}, \quad \boldsymbol{R} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -\rho \mathcal{R} \end{pmatrix}, \tag{2.2}$$

with

$$E \equiv e(p, v, c) + \tfrac{1}{2}u^2, \quad \mathcal{R} \equiv (t_0^* \mathcal{P}^*) c \exp(-1/\epsilon T), \quad \epsilon \equiv R^* T_0^* / E_{\mathrm{A}}^*. \tag{2.3}$$

The dimensional quantities $\mathcal{P}^*, R^*, E_{\mathrm{A}}^*$ are, respectively, a pre-exponential factor (the factor $\mathcal{P}^*$ is a measure of binary collision rates in the gas, which means that, in the present case, it is of order $a^{*2}\nu^{*-1}$ (cf. remarks in § 1)), the gas constant and the activation energy. It can be seen that we propose to use the simplest Arrhenius-type chemical reaction in the present study; it will be quite adequate for our needs. Likewise it is sufficient for present purposes to use the simplest thermal and caloric equations of state that, in dimensionless variables, are

$$pv = T, \quad (\gamma - 1)e = \frac{pv}{\gamma} + cQ, \quad Q = \frac{c_0^* Q^*}{C_{\mathrm{p}}^* T_0^*}, \tag{2.4}$$

where Q^* is the chemical energy of unit mass of reactant, C_{p}^* is specific heat at constant pressure and γ is the ratio of specific heats.

There is advantage in selecting a value for t_0^* that is equal to the value of the induction time at constant pressure in the reference state (validation of this interpretation of t_0^* can be found in § 3 *a* (i)); thus we choose

$$t_0^* \equiv (\mathcal{P}^* Q)^{-1} \epsilon \exp(\epsilon^{-1}), \tag{2.5}$$

so that

$$Q\mathcal{R} = c\epsilon \exp(\epsilon^{-1}(1 - T^{-1})) \equiv \Omega. \tag{2.6}$$

(*a*) *Large activation-energy limits*

When E_{A}^* is large compared with the rough measure of thermal energy $R^* T_0^*$, the number ϵ is small; formally, $\epsilon \ll 1$, and the reaction-rate quantity Ω in (2.6) takes on the following values when $\epsilon \to 0$ (assume that c is greater than zero and bounded):

$$\text{when } T = 1 + O(\epsilon), \quad \Omega = O(\epsilon), \tag{2.7}$$

$$\text{when } T = (1 - a)^{-1}, \quad a \in (0, 1), \quad \Omega = O(\epsilon \exp(a/\epsilon)). \tag{2.8}$$

In the limit, when ϵ is equal to zero,

$$T = 1, \quad \Omega = 0, \tag{2.9}$$

$$T = (1 - a)^{-1}, \quad a \in (0, 1), \quad \Omega \to \infty. \tag{2.10}$$

Thus, under these conditions, and arbitrarily close to the reference state, chemical activity is negligible but, when the temperature rises even a little from its reference value, chemical activity becomes infinitely intense. A rational interpretation of the physics implicit in these facts is that the field consists of patches of frozen chemical activity, separated by limitingly thin (discontinuous) regions across which chemical reactions go to some kind of completion.

(*b*) *Discontinuities*

Discontinuous solutions of the Euler equations exist, but they must obey the conservation rules laid down in (2.1). With the discontinuity assumed to lie along a general time-dependent path $x_{\rm p}(t)$ in the interval $x_{\rm l} \leqslant x_{\rm p}(t) \leqslant x_{\rm r}$, and using the notation $[f]$ to signify a jump in the value of f across a discontinuity, it can be shown, using (2.1), that

$$-S[\boldsymbol{U}] = -[\boldsymbol{F}] + [\boldsymbol{R}], \quad \text{where } S \equiv {\rm d}x_{\rm p}/{\rm d}t. \tag{2.11}$$

For physical reasons the chemical source term $\mathcal{R}$ in (2.2) must remain bounded, and it is clear that $[\boldsymbol{R}]$ is zero in reality. However, it can be useful to imagine a limiting case, for which the chemical source term $\mathcal{R}$ in (2.2) is unbounded, within an infinitesimal neighbourhood of $x_{\rm p}(t)$, in such a way that the last integral in (2.1) produces a finite non-zero contribution to the species conservation relation across the discontinuity. (For a classical view of this situation consult Shchelkin & Troshin (1963).) The magnitude of this contribution is not fixed by any physical law but, limited only by the broadest of physical necessities, may be chosen freely; note related remarks about reactant consumption in the third paragraph in § 2 *c* (ii). Clearly such situations are implicit in the limit of zero ϵ in § 2 *a*, specifically in (2.10).

The velocity of the gas relative to the discontinuity will be denoted by the symbol U, where

$$U \equiv S - u, \tag{2.12}$$

whence the first row in (2.11) shows that

$$[\rho U] = 0 \Rightarrow \rho U = \mathcal{W}, \tag{2.13}$$

where $\mathcal{W}$ is the mass flux through the discontinuity.

If $\mathcal{W}$ is zero, the discontinuity (a contact surface) is moving with the speed of the fluid; the fourth-row equation in (2.11) is satisfied by any value $[c]$ that makes physical sense; the remaining relations in (2.11) require $[p], [u] = 0$, but $[e]$ and $[v]$, like $[c]$, are unrestricted.

The condition $\mathcal{W} \neq 0$ ensures that there is a flow of gas through the discontinuity. The first three rows of (2.11) are not affected by the choice of $\mathcal{R}$ in $[\boldsymbol{R}]$, which only influences the final row in (2.11). The first three rows in (2.11) can be manipulated to give relationships between p and v that are recognizable as the Rayleigh-line and Hugoniot-curve relations, respectively, as follows:†

$$\mathcal{L}_{\rm i}(p, v; \mathcal{W}) = \gamma^{-1}(p - p_{\rm i}) + \mathcal{W}^2(v - v_{\rm i}) = 0, \tag{2.14}$$

$$\mathcal{H}_{\rm i}(p, v; c) = e(p, v; c) - e(p_{\rm i}, v_{\rm i}; c_{\rm i}) + \tfrac{1}{2}\gamma^{-1}(p + p_{\rm i})(v - v_{\rm i}) = 0. \tag{2.15}$$

† It is appropriate to remark at this point on the notation for the identification of Rayleigh lines and Hugoniot curves. Thus, a symbol $f_{\rm i}$, ($f = p, v, c, \ldots$, etc.), will indicate that the quantity f relates to an *inflow* to the discontinuity; more will be said about the identification of inflows in subsequent sections. The notation $\mathcal{L}_{\rm i}(p, v; \mathcal{W})$, or $\mathcal{L}_{\rm i}(\mathcal{W})$ for short, indicates that the Rayleigh line is a locus of p versus v that passes through point $(p_{\rm i}, v_{\rm i})$ on the (p, v)-plane, and is parametrized by the mass flux $\mathcal{W}$ through the wave. When there is no need to be specific about the role of $\mathcal{W}$ this notation can be shortened to $\mathcal{L}_{\rm i}$. $\mathcal{H}_{\rm i}(p, v; c)$ identifies a family of curves on the (p, v)-plane that is parametrized by the value of c. One member of this family passes through an inflow point $(p_{\rm i}, v_{\rm i})$ and is identified by the inflow value for c, namely $c_{\rm i}$. Other members of the family are located by specifying a value for $c \neq c_{\rm i}$. The notation can often be shortened to $\mathcal{H}_{\rm i}(c)$ without ambiguity.

Intersections of $\mathcal{L}_{\rm i}(\mathcal{W})$ and $\mathcal{H}_{\rm i}(c)$ define pairs of values of p and v versus c, for a given $\mathcal{W}$, that satisfy the necessities of the conservation laws. The particular pair relationships derived from (2.14) and (2.15) with c equal to $c_{\rm i}$ describe discontinuous changes that occur without change in the value of c from its inflow value of $c_{\rm i}$; such phenomena are often referred to as (chemically) frozen shock waves.

When $c < c_{\rm i}$ the pair-values that satisfy (2.14) and (2.15) describe inflow to and outflow from combustion waves modelled as discontinuities in the Euler field. These discontinuous waves are key components in the classical studies of combustion gas dynamics that have been referred to above. Since they are consistent with the limiting behaviour of Ω defined in (2.10), one can see that a link exists between classical combustion waves and the asymptotic deconstruction of fields that they occupy.

(*c*) *Continuous combustion waves*

Continuous parts of the Euler field are described by differential forms of the conservation relations (2.1), namely

$$\frac{\partial \boldsymbol{U}}{\partial t} + \frac{\partial \boldsymbol{F}}{\partial x} = \boldsymbol{R}. \tag{2.16}$$

It is often more revealing to view events in a field from some standpoint other than the Cartesian frame that is prescribed by coordinates x and t. This is particularly true in the present case when one makes a path, say $\mathrm{P} : t = t_{\rm p}(x)$, traced out by some distinctive feature of a system, the basis of a new coordinate system.

Thus, defining new independent variables (τ, χ) as follows:

$$\tau = t_{\rm p}(x) - t, \quad \chi = x, \tag{2.17}$$

and transforming (2.16) to the new system, gives

$$-\frac{\partial \boldsymbol{U}}{\partial \tau} + \frac{1}{S}\frac{\partial \boldsymbol{F}}{\partial \tau} + \frac{\partial \boldsymbol{F}}{\partial \chi} = \boldsymbol{R}, \tag{2.18}$$

where S, defined in (2.11), is the speed of a point on the path.

Solutions of (2.18) can provide a structure between points of inflow to and outflow from a continuous combustion wave that follows a path $t_{\rm p}(x)$; if the first approximation to such a wave is modelled as a discontinuity one would use $x_{\rm p}(t)$ (cf. (2.11)) to define P; an example of such a structure is given in the next section.

(i) *Steady combustion waves*

Suppose that $(\partial \boldsymbol{F}/\partial \chi)$ in (2.18) vanishes in a significant neighbourhood of path P, which means that conditions in that neighbourhood are what is usually referred to as steady and $\mathrm{P} : x = St$ with S constant. Then some of the equations in (2.18) can be integrated and reduced to the set of algebraic relations

$$-S\{\boldsymbol{U}_3\} = \{\boldsymbol{F}_3\}, \quad \{f\} \equiv f - f_{\rm i}, \quad f = u, p, v, \tag{2.19}$$

where the *continuous* differences $\{\boldsymbol{U}_3\}$ and $\{\boldsymbol{F}_3\}$ include only the first three rows of $\boldsymbol{U}$ and $\boldsymbol{F}$, and $f_{\rm i}$ defines evaluation at some suitable inlet condition (cf. footnote in § 2 *b*).

Evidently (2.19) mimics (2.11), but with the jumps $[f]$ in the latter replaced by continuous differences, written as $\{f\}$. One can take over definitions and results (2.12), (2.13), (2.14) and (2.15), and use them to control the hypothesized locally steady-state changes. This means, in particular, that one will know p and v as functions of c along the Rayleigh line defined by the value of $\mathcal{W}$.

However, the arbitrary discontinuous jump in c described in § 2 *b* is no longer acceptable; remembering that $\boldsymbol{F}_\chi$ must be zero in the present situation, the statement about jumps in c must be replaced by the partial differential equation in the fourth row of (2.18). Solutions of this equation in conjunction with (2.19), which will be *exact* solutions of the Euler equations, will give c, u, p, v as functions of τ; in other words, these solutions will provide a history of a fluid particle as it travels through the continuous structure of a steady-state combustion wave. The discontinuous models of combustion waves given in § 2 *b* merely connect conditions at inflow and at outflow from a wave; by contrast, solutions of (2.19) and the partial differential equation in the fourth row of (2.18) provide a continuous chemically induced structure that connects these specific points of inflow and outflow. Implications of these facts for asymptotic treatment of diffusionless systems will be outlined in § 3.

(ii) *Quasi-steady combustion waves*

The foregoing steady-state solutions can evidently be extended to apply, in an approximate way, to *un*steady fields by replacing the condition $\boldsymbol{F}_\chi \equiv 0$ with the criterion

$$|\boldsymbol{F}_\chi| \ll \frac{1}{|S|}|\boldsymbol{F}_\tau| \Rightarrow \left|\frac{\mathrm{d}t_\mathrm{p}}{\mathrm{d}x} - \left(\frac{\partial t}{\partial x}\right)_{\boldsymbol{F}}\right| \ll \left|\frac{\mathrm{d}t_\mathrm{p}}{\mathrm{d}x}\right|, \tag{2.20}$$

having used (2.17), and given that $\boldsymbol{F}_t = -\boldsymbol{F}_\tau \neq 0$. The quantity $(\partial t/\partial x)$ taken at fixed $\boldsymbol{F}$ defines isolines for each of the elements of $\boldsymbol{F}$. The requirements in the second version of (2.20) may be easier to monitor in computer solutions of the Euler system than those in the first. Combustion waves that satisfy (2.20) will be described as *quasi-steady* waves.

It is interesting to note the hint that waves that satisfy the criterion in (2.20) are unlikely to exist in regions for which $(\mathrm{d}t_\mathrm{p}/\mathrm{d}x) \to 0 \ldots$.

It is a distinct possibility that the quasi-steady waves that satisfy (2.20) may be 'incomplete', which is to say that some reactant will usually have been burnt before it flows into the quasi-steady wave, and the reactant may not then be all burnt before flow emerges from the quasi-steady wave. Clearly any locally quasi-steady behaviour must match smoothly into neighbouring domains of strictly *un*steady behaviour.

The work in § 2 *c* (i) has shown how to construct a locally exact solution for a steady-state wave, sustained by finite-rate chemical activity, and travelling through the system with a mass-flux throughput equal to a constant value of $\mathcal{W}$. The present section shows how to extend these solutions, in an approximate way, to apply when $\mathcal{W}$ is a slowly varying function of t (or τ).

It is important to remember at this point in the analysis that $\mathcal{W}$ *must be chosen, and cannot be calculated.*

3. Primitive variables and equations in Lagrangian form

In pursuit of a rational and self-contained theory for diffusionless combustion we observe that the set of partial differential equations in conservation form, (2.16), can be reorganized into a set of equations for the (dimensionless) primitive variables:

$$\frac{\partial \boldsymbol{V}}{\partial t} + \boldsymbol{\mathcal{A}}\frac{\partial \boldsymbol{V}}{\partial x} = \boldsymbol{S}, \tag{3.1}$$

where

$$\boldsymbol{V} = \begin{pmatrix} v \\ u \\ p/\gamma \\ c \end{pmatrix}, \quad \boldsymbol{\mathcal{A}} = \begin{pmatrix} u & -v & 0 & 0 \\ 0 & u & v & 0 \\ 0 & \rho a^2 & u & 0 \\ 0 & 0 & 0 & u \end{pmatrix}, \quad \boldsymbol{S} = \begin{pmatrix} 0 \\ 0 \\ \rho\Omega \\ -\Omega/Q \end{pmatrix}. \tag{3.2}$$

There is particular merit in the use of Lagrangian coordinates for some of the developments to come in this paper. To this end, note that the mass-weighted dimensionless Lagrangian coordinate ψ will be defined by

$$\psi = \int_{x_0(t)}^{x} \rho(t, s)\,\mathrm{d}s, \tag{3.3}$$

where $x_0(t)$ is the location of a particular fluid particle (e.g. the one on the face of a solid piston whose motion is prescribed). Either by direct derivation or, more simply, via transformation of (3.1), the Lagrangian form of equations for the primitive variables is

$$\frac{\partial \boldsymbol{V}}{\partial t} + \boldsymbol{\mathcal{B}}\frac{\partial \boldsymbol{V}}{\partial \psi} = \boldsymbol{S} \quad \text{with } \boldsymbol{\mathcal{B}} = \rho(\boldsymbol{\mathcal{A}} - u\boldsymbol{\mathcal{I}}) \tag{3.4}$$

with $\boldsymbol{\mathcal{I}}$ denoting the unit tensor.

Note the appearance of the 'time-to-go' variable $\tau = t_{\mathrm{p}}(x) - t$ in § 2 *c*; we can employ the same symbol, redefined here to read as

$$\tau = t_{\mathrm{p}}(\psi) - t, \tag{3.5}$$

for the Lagrangian version of coordinates attached to the path P : $t = t_{\mathrm{p}}(\psi)$, in which case (3.4) reads as

$$-\frac{\partial \boldsymbol{V}}{\partial \tau} + t'_{\mathrm{p}}\boldsymbol{\mathcal{B}}\frac{\partial \boldsymbol{V}}{\partial \tau} + \boldsymbol{\mathcal{B}}\frac{\partial \boldsymbol{V}}{\partial \psi} = \boldsymbol{S}. \tag{3.6}$$

The symbol t'_{p} is defined by

$$t'_{\mathrm{p}} \equiv \frac{\mathrm{d}t_{\mathrm{p}}}{\mathrm{d}\psi} = \frac{1}{\mathcal{W}}, \tag{3.7}$$

where the last result follows from (3.3), the first (mass-conservation) equation in (3.2) and the definitions of S and $\mathcal{W}$ in § 2 *b*.

(*a*) *Induction domains*

Using the terminology of asymptotic singular perturbation methods (e.g. Van Dyke 1975), the situation outlined in § 2 *a*, *b* has a good deal of the character of an *outer solution*. That it does not have *all* of this character is a consequence of the fact that we cannot complete the present outer solution using only rational theory. It has already been remarked, in the final sentence of § 2 *c* (ii), that the speed of, or mass-flux through, discontinuous combustion waves cannot be calculated using a theory that makes $\epsilon = 0$.

This means that one must abandon the conditions defined by (2.9) and (2.10) and use those defined by (2.7) and (2.8) in § 2 *a*. We have already seen something of the influence of non-zero values of ϵ on combustion-wave structure in § 2 *c* and its subsections, but now we must examine the influence of such values on the domains previously regarded as chemically inert (cf. the final paragraph in § 2 *a*).

In view of (2.7) it is evidently sensible to begin by examining regions of the field in which deviations from a local reference state are small and of order ϵ, including of course the chemical reaction rates; such regions will control the advent of vigorous combustion and will be called induction domains. We propose a formal asymptotic expansion of the dependent variables as follows:

$$f \equiv f_0 + \epsilon f^{(1)}(\psi, t), \quad f = p, \rho(\text{or } v), T, a, u, \tag{3.8}$$

where the f_0 quantities are constants, equal to the value of variable f in the reference state. Then (3.4) simplifies to

$$\frac{\partial \boldsymbol{V}^{(1)}}{\partial t} + \boldsymbol{\mathcal{B}_0}\frac{\partial \boldsymbol{V}^{(1)}}{\partial \psi} = \boldsymbol{S}^{(1)}, \tag{3.9}$$

where

$$\boldsymbol{V}^{(1)} = \begin{pmatrix} v^{(1)} \\ u^{(1)} \\ p^{(1)}/\gamma \\ c^{(1)} \end{pmatrix}, \quad \boldsymbol{\mathcal{B}}_0 = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{S}^{(1)} = \begin{pmatrix} 0 \\ 0 \\ \exp T^{(1)} \\ -Q^{-1}\exp T^{(1)} \end{pmatrix}. \tag{3.10}$$

It is useful to note, from the first of (2.4) and from the fact that $\rho = v^{-1}$, both combined with (3.8), that

$$p^{(1)} + v^{(1)} = T^{(1)} \quad \text{and} \quad \rho^{(1)} = -v^{(1)}. \tag{3.11}$$

(i) *A single equation for* $T^{(1)}$

It is not difficult to see that equations (3.9)–(3.11) can be manipulated to give

$$\frac{1}{\gamma}p^{(1)}_{\psi\psi} + v^{(1)}_{tt} = 0, \tag{3.12}$$

and either

$$T^{(1)}_t - \frac{(\gamma - 1)}{\gamma}p^{(1)}_t = \exp T^{(1)}, \tag{3.13}$$

or

$$T_t^{(1)} + (\gamma - 1)v_t^{(1)} = \gamma \exp T^{(1)}. \tag{3.14}$$

First note that, if pressure is constant ($\Rightarrow p^{(1)} \equiv 0$) and $T^{(1)}(\psi, 0)$ is zero, (3.13) shows that $T^{(1)}$ behaves like $\ln(1-t)$, which validates the idea that the value of t_0^* chosen in (2.5) is indeed the induction time at constant pressure; similarly, when v is constant ($\Rightarrow v^{(1)} \equiv 0$), $T^{(1)}$ behaves like $\ln(1-\gamma t)$ and the dimensional induction time is evidently t_0^*/γ, as is otherwise obvious.

Combining (3.12)–(3.14) shows that

$$\frac{\partial}{\partial t^2}\left(\frac{\partial T^{(1)}}{\partial t} - \gamma \exp T^{(1)}\right) - \frac{\partial}{\partial \psi^2}\left(\frac{\partial T^{(1)}}{\partial t} - \exp T^{(1)}\right) = 0. \tag{3.15}$$

While it is a major objective of the present paper to emphasize the importance of (3.15) in helping to resolve some of the issues relating to the speeds at which diffusionless combustion waves travel, this is not the place to review all the work done by several authors since the equation first appeared (Clarke 1981). Suffice it to say that, as one approaches a locus $t = t_{\mathrm{p}}(\psi)$, it is now well established that solutions of (3.15) 'blow up' like

$$T^{(1)} \to -\ln \tau \quad \text{as } \tau \downarrow 0, \quad \text{where } \tau = t_{\mathrm{p}}(\psi) - t. \tag{3.16}$$

Solving (3.15) for chosen initial and boundary values will give leading-order estimates for temperature perturbations $T - 1$; evidently $t_{\mathrm{p}}(\psi)$ must also be a leading-order estimate of the location of the singularity path. From the fact that solutions of (3.15) are bounded on any particle path (ψ constant) for $t < t_{\mathrm{p}}(\psi)$ it follows (Dold 1989) that $|\mathrm{d}t_{\mathrm{p}}/\mathrm{d}\psi| \equiv |t'_{\mathrm{p}}| < 1$ since the characteristics for (3.15) are families of lines for which $|\partial t/\partial \psi| = 1$.

In other words, the singularity path must travel through the system at supersonic speeds.

The existence and physical significance of such loci, or paths, in the (ψ, t)-plane was first recognized by Dold & Kapila (personal communication in 1989), who called them *singularity paths*. Friedman & Herrero (1990) proved that solutions of (3.15) for bounded initial and boundary-value information must behave like (3.16) locally, and the mathematical existence of singularity paths was established.

A numerical method of solving (3.15), which emphasizes the accurate evaluation of $t_{\mathrm{p}}(\psi)$, has been described by Dold (1989), who also gave some more accurate estimates of the functions $f^{(1)}$ as $\tau \to 0$ than are implied by (3.16). Dold (1989) calculates velocity u rather than specific volume v; but we are more interested in the latter in the present work. In particular, and in the present notation,

$$T^{(1)} = -\ln \tau + \ln \mu + \cdots, \tag{3.17}$$

$$t'^2_{\mathrm{p}} T^{(1)} + (\gamma - t'^2_{\mathrm{p}})v^{(1)} = \gamma a(\psi) + \cdots, \tag{3.18}$$

$$Qc^{(1)} + (1 - t'^2_{\mathrm{p}})\frac{1}{\gamma}p^{(1)} = -b(\psi) + \cdots, \tag{3.19}$$

where $\cdots$ indicates terms that are $O(\tau \ln \tau)$ as $\tau \downarrow 0$, and μ is defined as follows:

$$\mu \equiv \left(\frac{1 - t'^2_{\mathrm{p}}}{\gamma - t'^2_{\mathrm{p}}}\right). \tag{3.20}$$

It is also of particular interest to us here to note the result

$$\frac{1}{\gamma}t_{\mathrm{p}}'^{2}p^{(1)} + v^{(1)} = a(\psi) + \cdots, \tag{3.21}$$

as will be seen in § 3 *c*. The functions $a(\psi)$ and $b(\psi)$ have the same meaning here and in Dold's (1989) paper; they must be found by comparing the foregoing *estimates* for small values of τ with complete solutions of particular initial- and boundary-value problems for (3.15).

In view of the essential nonlinearity of (3.15), complete solutions are usually obtained numerically, although exploitation, initially by Blythe & Crighton (1989),† of the difference $(\gamma - 1)$ as a second small parameter enables derivation of many significant results in analytic/asymptotic forms.

(*b*) *Behaviour near* $t = t_{\mathrm{p}}(\psi)$

The asymptotic limit $\epsilon \to 0$ with (ψ, t) fixed has served to determine early-time behaviour near a reference state but, in view of the breakdown of solutions of (3.15) as $t \to t_{\mathrm{p}}(\psi)$, or $\tau \to 0$, it must now be replaced by a new limit that can take account of the behaviour heralded by the logarithmic character of $T^{(1)}$ in (3.16).

Thus, consider the transformation

$$\tau = \exp(-\sigma/\epsilon) \Longleftrightarrow \sigma = -\epsilon \ln \tau, \tag{3.22}$$

which introduces the new time-like coordinate σ, and then rewrite equations (3.6) in terms of independent variables σ and ψ:

$$(\boldsymbol{\mathcal{I}} - t_{\mathrm{p}}'\boldsymbol{\mathcal{B}})\frac{\partial \boldsymbol{V}}{\partial \sigma} + \epsilon^{-1}\exp(-\sigma/\epsilon)\boldsymbol{\mathcal{B}}\frac{\partial \boldsymbol{V}}{\partial \psi} = \epsilon^{-1}\exp(-\sigma/\epsilon)\boldsymbol{S} \equiv \boldsymbol{\mathcal{S}}. \tag{3.23}$$

Noting the definitions of Ω in (2.6) and $\boldsymbol{S}$ in (3.2) it can be seen that

$$\boldsymbol{\mathcal{S}} = \begin{pmatrix} 0 & 0 & \rho\omega & -\omega/Q \end{pmatrix}^{\top}, \quad \text{where } \omega \equiv c\exp(\epsilon^{-1}(1 - T^{-1} - \sigma)). \tag{3.24}$$

The fourth equation in the set (3.23) is the species equation, namely

$$\frac{\partial c}{\partial \sigma} = -(c/Q)\exp(\epsilon^{-1}(1 - T^{-1} - \sigma)), \tag{3.25}$$

from which it can be seen that $\partial c/\partial\sigma$ is a $O(1)$ quantity in the limit as $\epsilon \to 0$ with (ψ, σ) fixed, provided that

$$1 - T^{-1} - \sigma = \epsilon\mathcal{F} \quad \text{and} \quad \mathcal{F} = O(1). \tag{3.26}$$

When t is sufficiently close to $t_{\mathrm{p}}(\psi)$, σ is positive, and the last term on the left-hand side of (3.23) will be exponentially small compared with the remaining terms in this equation under the new limit $\epsilon \to 0$ with (ψ, σ) fixed. The first asymptotic estimate of behaviour near the singularity path can therefore be found, with exponentially small errors, from solutions of the set of approximate relations

$$\boldsymbol{\mathcal{C}}\frac{\partial \boldsymbol{V}}{\partial \sigma} \simeq \boldsymbol{\mathcal{S}}. \tag{3.27}$$

† More recent work can be found in the thesis by Parkins (1998).

The quantities $\boldsymbol{\mathcal{C}}$ and $\boldsymbol{\mathcal{S}}$ are given by

$$\boldsymbol{\mathcal{C}} \equiv (\boldsymbol{\mathcal{I}} - t'_{\mathrm{p}}\boldsymbol{\mathcal{B}}) = \begin{pmatrix} 1 & t'_{\mathrm{p}} & 0 & 0 \\ 0 & 1 & -t'_{\mathrm{p}} & 0 \\ 0 & -\rho^2 a^2 t'_{\mathrm{p}} & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{\mathcal{S}} = \begin{pmatrix} 0 \\ 0 \\ \rho c \exp \mathcal{F} \\ -Q^{-1} c \exp \mathcal{F} \end{pmatrix}, \tag{3.28}$$

with t'_{p} defined in (3.7). It is easy to see that the continuous solutions described in § 2 *c* (i),(ii) also satisfy (3.27). Given that these continuous solutions can be matched to the induction-domain fields (as will be described in the next subsection) it can be seen that the combustion wave structure near the singularity path is therefore that of a weak detonation, *whose speed is determined by the initial-value and boundary-value problem for* (3.15).

It is at this point that we begin to see that the speeds of propagation of supersonic diffusionless combustion waves will be provided by self-contained analysis, in contrast to the empiricism mentioned at the end of § 2 *c* (i).

(*c*) *Matching induction domain and combustion wave*

We now have some useful information about T in the induction domain, especially from (3.17) near the singularity path in the (ψ, τ)-coordinate system, and about T in the combustion wave, which is also near the singularity path and travelling at the same supersonic speeds, but now the information about T is in terms of coordinates (ψ, σ).

An intermediate time-like coordinate Ξ can be defined via the relations

$$\sigma = -\nu(\epsilon) \ln \Xi, \quad \tau = \Xi^{\nu(\epsilon)/\epsilon}, \quad \text{where } (\epsilon/\nu(\epsilon)) \to 0 \quad \text{as } \epsilon \to 0 \quad \text{and} \quad 0 < \Xi < 1, \tag{3.29}$$

and can then be used to match T in the two adjacent domains. Specifically, we must match $T(\psi, \sigma)$ in the combustion wave, given by (3.26), with $T(\psi, \tau)$ in the induction domain, given by $T = 1 - \epsilon \ln \tau + \epsilon \ln \mu + \cdots$ (cf. (3.17)).

With the proviso that all inflow quantities f_{i} are of the form $1 + o(1)$, it turns out that matching is achieved if

$$\mathcal{F} \sim \ln \mu \tag{3.30}$$

to leading order. There is a requirement in (3.26) for $\mathcal{F}$ to be $O(1)$, so that (3.20) makes it clear that t'_{p}, which must be less than one, cannot be too close to that value. As it happens, this is not an impediment to progress with the present analysis since physical events intervene to disqualify near-sonic singularity-path speeds.

As remarked just below (3.28), it is not difficult to see that the set of equations in (3.27) will lead to results that are the same as the ones discussed in § 2 *c* (i) and, particularly, in § 2 *c* (ii). Therefore, when the combustion wave is quasi-steady, supersonic and located in the neighbourhood of a singularity path, the *structure* of such a wave (a weak detonation) is known although, at this point in the discussion, *inflow conditions* to the wave are not. Note from (3.25) and (3.26) that $\mathcal{F}$ is equal to $\ln(-Qc_\sigma/c)$; with knowledge of the combustion wave structure, especially in the form of p, v and c as elementary functions of T, one can evidently find a value for $\mathcal{F}$ as a function of T at any given ψ. It turns out that $\mathcal{F}$ is indeed equal to $\ln \mu$ to

leading order in the matching region, provided that all of the inlet quantities $f_{\rm i}$ are of the form $1 + o(1)$, and this proviso has already been acknowledged.

Matching of p, v and c across intermediate regions between induction domain and combustion wave, and making use of the foregoing information about $f_{\rm i}$, produces a number of relations between inflow conditions, specifically,

$$\frac{1}{\gamma} t'^2_{\rm p}(p_{\rm i} - 1) + (v_{\rm i} - 1) - \epsilon a(\psi) = 0, \tag{3.31}$$

$$t'^2_{\rm p}(T_{\rm i} - 1) + (\gamma - t'^2_{\rm p})(v_{\rm i} - 1) - \epsilon\gamma a(\psi) = 0, \tag{3.32}$$

$$Q(c_{\rm i} - 1) + \frac{1}{\gamma}(1 - t'^2_{\rm p})(p_{\rm i} - 1) + \epsilon b(\psi) = 0. \tag{3.33}$$

Taking note of the relation between $t'_{\rm p}$ and $\mathcal{W}$ in (3.7), (3.31) can now be used with (2.14) to find the following family of Rayleigh lines:

$$\mathcal{L}_{\rm i} = \gamma^{-1}(p - 1) + \mathcal{W}^2(v - 1) - \epsilon\mathcal{W}^2 a(\psi) = 0. \tag{3.34}$$

In the present circumstances these relations describe the family of quasi-steady weak detonations that terminate induction activity. Evidently these supersonic combustion waves are associated with the existence of singularity paths in the induction domain solutions. That not all parts of a singularity path can support quasi-steady wave structures has been hinted at in the text that follows (2.20); the idea is given specific support by the analysis carried out by Jackson *et al.* (1989).

Clearly we have now located a family of diffusionless combustion waves on a (p, v)-diagram using *only* a self-contained rational theory.

It should be emphasized that the asymptotic methods used to acquire the present solutions do not give *values* for inflow quantities $f_{\rm i}$ but *relationships* amongst them. Since conditions in the intermediate regions between induction domain and weak detonation are obtained by *matching*, relationships as opposed to values are no more than one has a right to expect for the $f_{\rm i}$ quantities. A matching process calls for smooth connections between asymptotic solutions in overlapping segments of a field, and is not in any way associated with point values of any of the local variables in the problem.

It should be remarked here that the results in equations (3.31)–(3.34) can be developed to show that Rayleigh lines for supersonic combustion waves, signifying quasi-steady weak detonations, can approach tangency to one of the relevant family of Hugoniot curves, given in (2.15). The implication is that outflow from the weak detonation wave can occur in a Chapman–Jouguet (CJ) condition for which the reactant level is strictly non-zero. Given values of the system parameters, ϵ and γ, these non-zero values of c can be calculated in terms of $\mathcal{W}^2(\psi)$ (or $t'^2_{\rm p}(\psi)$) and the quantities $a(\psi)$ and $b(\psi)$ for any particular particle path. The necessarily unsteady motion that is demanded in the situation just outlined (cf. § 2 *g* in Singh & Clarke (1992), hereafter written as S&C) is therefore taking place in a region of the field for which chemical activity is still intense; this latter fact is crucial to the subsequent birth of a regular detonation wave. Such phenomena were first observed in numerical solutions for specific one-dimensional and two-dimensional flows (cf. S&C and Nikiforakis & Clarke (1996), hereafter written as N&C, respectively), so that it is important to observe that these particular observations are now given more general substance via the analytical results exposed here.

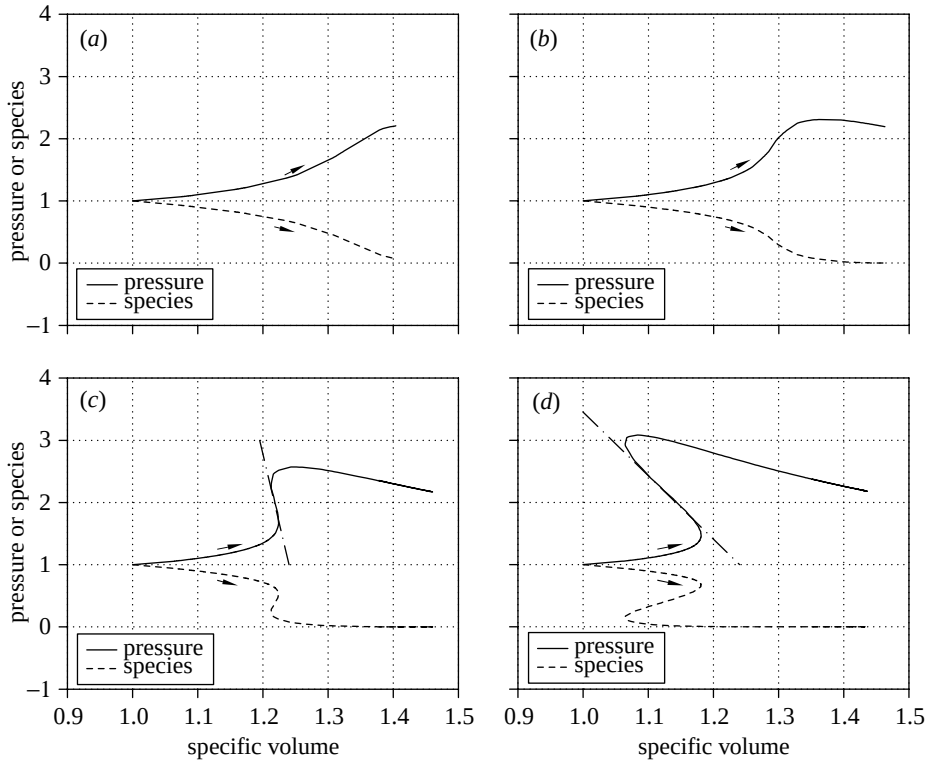

Figure 1. Loci of p versus v, correlated to c versus v, for four particle paths (values of ψ equal to 1.2×10^{-3}, 2.2×10^{-3}, 4.3×10^{-3} and 8.3×10^{-3}, shown in plots (a)–(d), respectively) from a numerical solution of the Euler equations (2.16). Time t increases along each curve as indicated by the arrows.

4. Numerical results

In this section we present solutions of the Euler equations (2.16), which describe continuous parts of the Euler field, for qualitative comparison with the analytical/asymptotic solutions described in § 3 *a–c*. The equations were solved numerically as described in N&C. The particular configuration chosen for our present purpose consists of a precursor shock wave, with a Mach number of 2.2, that is driven by the motion of a piston travelling at constant speed into a semi-infinite domain occupied by combustible gas; $\gamma = 1.4$, $Q = 1.788$ and $\epsilon = 0.0619$.

Figure 1 displays only information relevant to the issues raised in the asymptotic analysis, specifically, loci of p and c versus v for four different particle paths, which are close to the surface of the piston and downstream of the precursor shock, where the fields remain continuous for the current configuration. The precursor shock switches on chemical activity in particles of the compressible reacting material as they pass through the shock, as is clear from the reductions in c that begin at post-shock points ($p \sim 1$, $v \sim 1$).

Some general explanations for the kind of pv-behaviour that is encountered in compressible reacting fields with liberation of significant amounts of chemical energy have been given by Clarke (1989, § 6.3). In the present case we note that steady

reductions in c connote the presence of continuing chemical reactions; the associated liberation of energy enables mechanical work to be done on the gas and gives rise to changes in energy density (or pressure) and kinetic energy, which can propagate as dilatational waves through the compressible medium that makes up the system. A fuller analysis of a purely numerical study of behaviour in a similar configuration to the present one can be found in S&C.

The straight (Rayleigh) lines in figure 1c, d effectively coincide with the pv-loci over significant ranges of values of p and v; they signify the presence of significant portions of quasi-steady weak detonations in accordance with the analysis in § 3 b, c. Earlier sections of the loci are predicted by the analysis of induction domains in § 3 a; matching, as described in § 3 c, can be seen in the way that pv-loci and straight lines blend into one another shortly after the first vertical tangents on the pv-loci.

It is interesting to observe from (3.34) that Rayleigh lines $\mathcal{L}_{\rm i}$ intercept $p = 1$ where $v = 1 + \epsilon a(\psi)$; figure 1c, d demonstrates that the functions $a(\psi)$ are positive.

5. Summary and conclusions

The paper first shows that the classical theory of Rayleigh lines and Hugoniot curves, which treats combustion waves in compressible flow as discontinuities, has close connections with asymptotic theories of combustion, in particular in the present case, by exploiting the limit of large activation energies as exemplified by the number ϵ defined in (2.3). In general, classical theory makes use of the limit $\epsilon = 0$, and examines changes that take place from one uniform equilibrium, or metastable equilibrium, state to another across discontinuous shocks, contact surfaces or combustion waves. However, this theory is incomplete as a consequence of the very significant fact that speeds of propagation of combustion waves cannot be calculated as an intrinsic part of such a theory but, if one relaxes the limit on ϵ and considers instead the condition $\epsilon \to 0$, we have seen how some of the methods of analytic/asymptotic singular perturbation theory can be exploited to make theories of high-speed diffusionless combustion internally consistent and complete.

The existence of ϵ as a small parameter in the problem (cf. § 2) encourages study of domains of small perturbation, in particular the so-called induction domain in § 3 a. Here one ultimately observes breakdown of the asymptotic theory, based on use of the limit $\epsilon \to 0$ in the (ψ, t)-frame that describes local induction events. This breakdown, which takes place in the neighbourhood of a singularity path, whose location is predicted by the induction-domain theory, is the herald both of more intense local chemical activity and the need to seek a more suitable coordinate frame in which to analyse its progress. Replacing time t with a new 'fast' time $\sigma \equiv -\epsilon \ln \tau$, and retaining the fluid-particle label ψ, acknowledges that exponentially rapid changes take place within a particle as it approaches the singularity path, as is demanded by the character of the source term $\boldsymbol{\mathcal{R}}$ in the Euler equations.

Using $\lim \epsilon \to 0$ with ψ, σ fixed, § 3 b then shows that the intense chemical activity, experienced as one approaches the singularity path, is governed by those localized forms of Rayleigh lines and Hugoniot curves presented in (2.14) and (2.15). Then § 3 c demonstrates how these quasi-steady structures match into the essentially unsteady induction-domain fields, and finally notes the implications for CJ-like outflows of *unburnt* reactant from the transient family of quasi-steady incomplete (meaning $0 < c < c_{\rm i} < 1$) weak detonations. It is important to remark on the consequent existence

of regions of very-hot very-high-pressure vigorously reacting gas in the essentially unsteady domains that exist behind these incomplete and ephemeral reaction waves.

Numerical evidence (e.g. S&C and N&C) indicates that such regions of vigorously reacting gas can contain the birth of familiar, strong, or even CJ, detonations. This numerical evidence is supported by the asymptotic/analytical studies carried out by Dold & Kapila (1991) (mentioned in § 3 *a* (i)). A subsequent article by Dold (1991), which summarizes theoretical work on initiation up to that time, also takes the discussion into post-weak-detonation periods, as does a more recent paper by Dold *et al.* (1994). *Inter alia*, this latter paper directs attention to differences between the predictions of, on the one hand, numerical methods and, on the other hand, asymptotic techniques, especially in their descriptions of events downstream of weak detonations. These differences could be thought of as more quantitative than qualitative, since all of the same broad features, in essentially the same relationship to one another, are found by either method of solution. However, there are differences, in both location and rapidity of evolution of events leading to the generation of strong detonations, that cannot be ignored. . . .

Numerical methods can produce solutions for values of ϵ that are too large for the present asymptotic theory to be valid, but Dold *et al.* (1994) provide clear evidence that numerical results for smaller and smaller values of ϵ begin more and more to resemble the results derived by using asymptotic/analytic methods. It is the case that numerical methods experience difficulties when $\epsilon \ll 1$, which is where asymptotic methods come into their own. The evidence that these two techniques for the solution of our problems agree in intermediate ranges of ϵ is certainly encouraging, but it is quite clear that further work is called for, especially in view of remarks at the end of the previous paragraph.

The aims of the present paper, as described in the opening summary or abstract, are limited, and it is therefore appropriate to conclude our present discussion at this point. We would like to reiterate the need both for further numerical studies and also for asymptotic/analytical work,† even on the simple one-dimensional unsteady configuration, but especially on events in two- and three-dimensional geometries; and one must not forget the need for more sophisticated chemical-kinetic models, as exemplified in the pioneer paper by Dold & Kapila (1991).

We are grateful to the referees for several comments and suggestions for improvements in our original submission.

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† By continuing to use limits $\epsilon \to 0$, $(\gamma - 1) \to 0$ (as in the work by Blythe & Crighton (1989)), for example, as well as looking for other ways of studying local events by analytical or approximate/analytical means.

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