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The Zeldovich spontaneous reaction wave propagation concept in the fast/modest heating limits

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Quantitative mathematical models describe planar, spontaneous, reaction wave propagation (Zeldovich, *Combust. Flame*, vol. 39, 1980, pp. 211–214) in a finite hot spot volume of reactive gas. The results describe the complete thermomechanical response of the gas to a one-step, high-activation-energy exothermic reaction initiated by a tiny initial temperature non-uniformity in a gas at rest with uniform pressure. Initially, the complete conservation equations, including all transport terms, are non-dimensionalized to identify parameters that quantify the impact of viscosity, conduction and diffusion. The results demonstrate unequivocally that transport terms are tiny relative to all other terms in the equations, given the relevant time and length scales. The asymptotic analyses, based on the reactive Euler equations, describe both induction and post-induction period models for a fast heat release rate (induction time scale short compared to the acoustic time of the spot), as well as a modest heat release rate (induction time scale equivalent to the acoustic time). Analytical results are obtained for the fast heating rate problem and emphasize the physics of near constant-volume heating during the induction period. Weak hot spot expansion is the source of fluid expelled from the original finite volume and is a 'piston-effect' source of acoustic mechanical disturbances beyond the spot. The post-induction period is characterized by the explosive appearance of an ephemeral, spatially uniform high-temperature, high-pressure spot embedded in a cold, low-pressure environment. In analogy with a shock tube the subsequent expansion process occurs on the acoustic time scale of the spot and will be the source of shocks propagating beyond the spot. The modest heating rate induction period is characterized by weakly compressible phenomena that can be described by a novel system of linear wave equations for the temperature, pressure and induced velocity perturbations driven by nonlinear chemical heating, which provides physical insights difficult to obtain from the more familiar 'Clarke equation'. When the heating rate is modest, reaction terms in the post-induction period Euler equations exhibit a form of singular behaviour in the high-activation-energy limit, implying the need to use a nonlinear exponential scaling for time and space, developed originally to describe spatially uniform thermal explosions (Kassoy, *Q. J. Mech. Appl. Maths*, vol. 30, 1977, pp. 71–89). Here again the result will be the explosive appearance of an ephemeral spatially uniform high-temperature, high-pressure hot spot. These results demonstrate that an initially weak temperature non-uniformity in a finite hot spot can be the source of acoustic

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Written as a tribute to J. F. Clarke, my late paradigm, mentor and co-author.

and shock wave mechanical disturbances in the gas beyond the spot that may be related to rocket engine instability and engine knock.

Key words: combustion, gas dynamics, Navier–Stokes equations

1. Introduction

Zeldovich *et al.* (1970) are concerned with preferential autoignition sites occurring in reactive gases characterized by a momentary non-uniform temperature distribution varying around a relatively low mean temperature. A transient, Cartesian, one-dimensional model, based on the reactive Euler equations, is developed to describe the evolution of the combustion process from an initially imposed local, negative linear temperature gradient in a hot spot surrounded by a much larger semi-infinite domain at relatively low temperature. After correcting a typo in equation (3.2) of the 1970 manuscript, it is clear that the model is developed for a characteristic chemical heat release time scale similar to the local acoustic time scale, based on the distance a wave can propagate during the heat release process. The objective is to identify the dependence of combustion wave evolution on the amplitude of the linear temperature gradient. They seek to identify critical gradients that facilitate relatively strong shocks that can couple to an adjacent reaction zone leading to detonation formation. Following up on these ideas, Zeldovich (1980) describes an intuitive, qualitative theory for the propagation of a 'spontaneous reaction wave' through a reactive gas, initiated by an imposed temperature inhomogeneity (hot spot gradient) in an initially constant-pressure gas at rest. He argues that the inhomogeneity will initiate a sequence of adiabatic thermal explosions that propagate down an imposed negative temperature gradient due to the sensitivity of the local induction time to the temperature at each point, with the result that a reaction front can be identified and tracked. He considers '... the extreme case of large space lengths and small gradients so that one may neglect interaction between adjacent volumes of reacting substance (so that)... in each particle of the substance thermal explosion occurs independently'. In other words, he postulates a continuous sequence of perfectly constant-volume thermal explosions. Zeldovich contrasts this type of propagating chemical reaction wave to traditional transport-dominated flames, high-speed deflagration and detonation waves. It is implicit in such a process that the localized energy addition cannot induce gas motion or any form of gas dynamic disturbance, limitations recognized subsequently by many researchers (Short 1995, 1997; Kapila *et al.* 2002; Seitenzahl *et al.* 2009; Kassoy 2010, 2014*a*,*b*). The qualitative theory lacks a quantitative mathematical model for the evolution of the reaction wave, including relevant time and length scales, the characteristic gradient magnitude, as well as the characteristic chemical power and the energy deposition. Subsequently, Zeldovich *et al.* (1988) used numerical solutions based on the Euler equations to study the effect of initial concentration and temperature gradients on the generation of pressure waves, with the objective of explaining detonation initiation. The model and interpretation of the numerical data recognizes the importance of the thermomechanical response of the gas to thermal energy deposition. The authors state '... that spontaneous generation of shock and detonation waves may occur in conditions close to self-ignition of the reactive mixture', results that '... may provide insight into the onset of nonlinear combustion instability in various technical systems' (e.g. rocket engines and knock

in internal combustion engines are mentioned). The authors cite numerous related technical papers by themselves, their colleagues and others addressing the detonation initiation and evolution problem.

Makviladze & Rogatykh (1991) formulate a mathematical model for reaction initiation and evolution in a localized hot spot, with an imposed negative linear temperature gradient, initially at constant pressure with zero speed. The model is based on the planar, reactive, non-stationary Euler equations, with one-step Arrhenius kinetics used to produce transient, spatially distributed heat release. The non-dimensional space and time variables are chosen to facilitate a characteristic time scale for heat release (the induction time of a thermal explosion) comparable to the acoustic time scale (wave passage time) in the spot. Significant non-dimensional parameters are identified in the conservation equations, boundary and initial conditions and then used in a succession of numerical solutions to determine solution dependence on the parameter values. The authors identify a criterion for '... dangerously explosive regimes...,' in terms of the non-dimensional temperature gradient parameter λ, equation (16) in their text. An *ad hoc* assumption of zero speed is used to define a reduced equation set describing constant-density, adiabatic heat addition to the gas. The analytical solution is used to describe the spatially dependent time for maximum heat release rate. This model for the Zeldovich spontaneous reaction wave is characterized by a thermal explosion propagating down the negative gradient at a specific speed. The temperature reaches the adiabatic explosion value just behind the propagating front, with a concomitant high-pressure value (pressure rises with temperature in a constant-density heat addition process. Kassoy (2010, 2014*a*,*b*) has explained the physical consquences of relatively rapid heat addition with near inertial confinement.) Numerical solutions of the full equations are used to discuss the relationship between a propagating spontaneous 'chemical' reaction wave and familiar propagating gas dynamic waves (shocks and detonations). The authors note that an induction period with relatively small changes in dependent variables is followed by a full-scale explosion on a substantially shorter 'excitation' time scale (Gu, Emerson & Bradley 2003) during which most the heat release and fuel consumption occurs. It is this relatively rapid heat addition process that occurs in a nearly inertially confined gas volume, as described in the cited Kassoy references above.

During the 1980s and extending to the present, there has been extraordinary interest in using asymptotic and/or computational methods to resolve reaction initiation phenomena, and/or gas dynamic consequences arising from either inhomogeneous initial conditions or thermal energy deposition into a gas volume. A non-exhaustive selection of these studies is cited in brevity below, primarily to inform the interested reader of the modelling diversity. More detailed information can be obtained from the publication introduction sections and their bibliographies.

Sileem, Kassoy & Hayashi (1991) use numerical methods to study planar detonation initiation following thermal energy deposition into a reactive gas volume adjacent to a planar boundary. Clarke, Kassoy & Riley (1984*a*,*b*) describe a related modelling effort where a hot planar boundary is an energy source that heats the adjacent inert gas by conduction, causing localized gas expansion. The induced motion (... 'piston effect'...) is the source of a shock wave propagating into the adjacent cold environment.

Jackson, Kapila & Stewart (1989) study the evolution of a high-activation-energy ($\varepsilon \to 0$) chemical reaction within a finite slot when the chemical time scale for the induction period is identical to the acoustic time scale. A traditional thermal explosion formulation facilitates a quantitative description of the thermomechanical response of

the gas to transient, spatially resolved, chemical heat addition, initiated by an $O(\varepsilon)$ negative temperature gradient in the slot. The describing equations are essentially those for linear acoustics driven by a nonlinear reaction term and are equivalent to 'Clarke's equation' (Clarke 1978). Numerical solutions of the system show that the induction-period temperature and pressure perturbations become unbounded in the vicinity of the $O(\varepsilon)$ temperature maximum in the initial condition and at a finite thermal explosion time, t_e. The failure of the numerical method as $t \to t_e$ is interpreted to mean that a familiar thermal explosion logarithmic singularity characterizes the runaway process. The authors then use coordinate expansion asymptotics to describe the spatially multiscale evolution of the hot spot. The solution development is confined to the vicinity of the $O(\varepsilon)$ initial temperature maximum. A post-induction period analysis employs nonlinear rescaling of the time and space, the former developed originally by Kassoy (1977), to describe the full-scale explosion in the vicinity of the original $O(\varepsilon)$ temperature maximum. The results show that the reactant is totally consumed on exponentially short time and space scales while the spatially uniform temperature rises to the adiabatic explosion value in an essentially constant-volume process, with a concomitant increase in pressure and almost no induced fluid speed. The post-induction theory is also confined to a very thin region adjacent to the original temperature maximum.

The consequences of spatial inhomogeneities in pressure, temperature, concentration and speed, on the evolution of a reaction process at relatively modest activation energy are predicted by Short (1995, 1997). He provides a thorough review of the literature available in that period. A high-activation-energy theory (based on the familiar small parameter $\epsilon = R'T_0'/E' \ll O(1)$) is formulated to describe the initiation of a chemical process by $O(\epsilon)$ spatial inhomogeneities in the initial values of the dependent variables, leading ultimately to the appearance of a detonation. His models describe chemical heat deposition into a volume of reactive gas, characterized by dimension l_R', when the induction time scale of the thermal explosion, denoted by t_R', is compared to the acoustic time scale $t_a' = \ell_R'/c_0'$, where c_0' is the characteristic speed of sound. He considers models for the time-scale ratio $\mu = t_R'/t_a' = 1$ and also $\mu \ll O(1)$ ('long-wavelength analysis'). The former describes a weakly compressible response of the gas to minor heat addition during the induction period of a thermal explosion. In contrast, the latter corresponds to nearly constant-volume heat addition. Short recognizes the limitations of the Zeldovich concept cited above and develops an asymptotic analysis for variable density corrections to the lowest-order constant-volume solution valid for $\mu = 0$.

High-activation-energy asymptotics are used by Short (1996) to quantify the spatially homogeneous evolution of thermodynamic variables in a compressible atmosphere containing initial disturbances in velocity and pressure. The induced gas motion (either expansion or compression) influences the thermal process in a fundamental way. Large expansion rates prevent thermal runaway from occurring. Conditions leading to the appearance of a thermal explosion are defined.

In contrast to the self-initiation phenomena in the references above (small-amplitude initial disturbances), direct initiation of gaseous detonations is the subject of a paper by Eckett, Quirk & Shepherd (2000). A spherical blast wave, generated by the rapid deposition of a large amount of thermal energy into a small volume of reactive gas, ignites a chemical reaction in a reactive gas through which it propagates. (Traditional blast wave theory is based on an unphysical idealization; instantaneous deposition

of energy into a point.) The study seeks to determine blast wave properties (critical energy) that lead to a sustained spherical detonation, associated with the 'competition between heat release, wavefront curvature and unsteadiness.'

Vasquez-Espi' & Liñan (2001) model the initiation of a high-activation-energy chemical reaction in a reactive gas following 'instantaneous' spatially resolved thermal energy deposition to create a well-defined hot, high-pressure spot (it is assumed that the energy addition occurs at constant volume and that '... there is no time for the generation of motion...', thus neglecting the thermomechanical response of the gas to energy addition.) The problem formulation is developed for reaction time scales of the order of the local acoustic time, $\mu = O(1)$. The acoustically linearized reactive Euler equations with a nonlinear chemical energy term found by Clarke (1978) are derived. Highly resolved numerical methods are used to ascertain a critical value of the 'Dahmköhler number,' $(1/\mu)$. Beyond the critical value, a well-defined ignition process occurs because the local chemical power addition is large enough to overcome the cooling effect of local gas expansion.

Kapila *et al.* (2002) develop a model for detonation formation arising from an existing tiny linear temperature gradient in a semi-infinite domain. The compressible non-dimensional equations are valid when the characteristic thermal energy deposition time (really the thermal explosion induction time) is similar in magnitude to the local acoustic time. Familiar high-activation-energy thermal explosion theory is employed to study the impact of asymptotically small gradients on induction-period history. The analysis leads to a recognition that the post-induction period time scale will be exponentially short compared to the local acoustic time. The asymptotic methodology enables a cause–effect understanding of the physics of shock formation that is difficult to obtain from numerical experiments alone. 'Accurate and well-resolved numerical computations are (used) to determine the mode of detonation formation as a function of the size of the initial gradient.' Solutions are obtained for a wide range of temperature gradients to demonstrate the diversity of evolutions to detonation. The authors recognize that '... Zeldovich ideas, while extremely instructive, are limited in accuracy...' due to the lack of gas dynamic response of the gas to spatially distributed transient heat deposition.

Gu *et al.* (2003) use computational solutions to the reactive compressible flow equations, including all transport terms to study the sensitivity of reaction front propagation to small linear temperature gradients imposed on a spherical hot spot. Detailed kinetic schemes for stoichiometric H_2–CO–air and H_2–air mixtures are used to describe the autoignition process. Initially, the temperature rises significantly throughout the spot in a nearly spatially homogeneous process, with a slight temperature maximum evolving at the origin, far larger than the maximum associated with the initial tiny gradient. A rapid reaction process follows in the vicinity of the maximum, leading to a localized hot spot. A reaction wave then spreads quickly across the spot, creating a region of very high temperature. Subsequently, the entire spot explodes and all fuel is consumed on the relatively short 'excitation time scale,' t'_e. A non-dimensional parameter, ξ, related to the magnitude of the initial linear temperature gradient is used to discriminate between five different modes of reaction front propagation. (The parameter ξ is in fact the inverse of the reaction wave propagation Mach number.) The authors note the importance of a second parameter, the ratio (t'_a/t'_e), where t'_a is the acoustic time scale of the spot. The transient reaction process is distinct from that in a traditional thermal explosion (Kassoy 1977). The latter is described in terms of a relatively long induction time, where little fuel is

consumed and only small temperature changes occur, followed by an extremely rapid full explosion where the temperature rises to the adiabatic explosion value as all the fuel is consumed.

Kurdyumov, Sanchez & Linan (2003) extend the aforementioned CKR model for a planar compact heat source to cylindrical and spherical geometries. Conduction heat transfer from the source to the adjacent gas raises the temperature of a volume with characteristic length scale r_h' on an energy deposition time scale t_d', where the latter is compared to the characteristic acoustic and conduction time scales of the volume, $t_a' = r_h'/a_0'$ (a_0' is the characteristic speed of sound at the initial temperature T_0') and $t_c' = r_h'^2/\kappa_0'$ (κ_0' is the characteristic thermal diffusivity), respectively. A continuum gas theory requires that the ratio of the acoustic time to the conduction time, equivalent to the Knudsen number: $Kn = (\alpha_0'/a_0'\ r_h') \ll O(1)$. The compact heat source, a spark, hot wire or laser shot delivers a specified amount of energy E_j' during the deposition time scale, which heats the volume such that $\rho_0' C_p' T_0'\ r_n'^{j+1} \sim E_j'$ ($j = 0, 1, 2$ for planar, cylindrical and spherical geometries, respectively) defines the dimension r_h'. C_p' is the characteristic specific heat at constant pressure. When $t_d' = t_a'$, energy from the source to the gas volume raises the local temperature $O(T_0')$ in a nearly isobaric process, with the density decrease inversely proportional to the temperature increase. Gas expelled from the heated volume acts as a piston to drive mechanical disturbances into the unheated gas. The thermomechanical analysis is carried out for a wide range of deposition time scales: ($t_d'/t_a' \ll O(1)$, rapid heating), ($t_d'/t_a' = O(1)$, modest heating), ($t_d'/t_a' \gg O(1)$, slow heating). The mechanical consequences of each ratio are articulated in the Conclusion section of the cited reference.

High-fidelity computational simulations based on the compressible reactive Navier–Stokes equations, including transport terms, with hydrogen chemistry for the kinetics are carried out to simulate phenomena that may occur in an HCCI engine (Sankaran *et al.* 2005). A turbulent flow field in a high-pressure gas with an uncorrelated turbulent temperature field is imposed as an initial condition. The field consists of individual hot spots with relatively small temperature inhomogeneities being strained and dissipated by the turbulence. The results identify a first ignition site and subsequent combustion elsewhere in the field. The authors note the impact of localized gas compression on the heat budget of autoigniting hot spots. Ignition development is found to be sensitive to '... temperature distribution statistics'. Two regimes of ignition are identified: '... spontaneous propagation and deflagration...'. '... a criterion based on the propagation speeds (of the waves) is proposed to distinguish between the two... regimes.' However, cause–effect relations cannot be determined from the computational dataset.

Spontaneous initiation of detonation in astrophysical objects (white dwarfs) is the subject of a computational modelling effort by Seitenzahl *et al.* (2009). The dimensional reactive Euler equations are solved for appropriate astrophysical thermodynamic conditions and thermonuclear reaction kinetics to determine whether a hot spot of fixed size with an initial temperature inhomogeneity can be the source of a detonation. In particular, the authors seek to determine '... the smallest size for a heated region that still leads to detonation...'. Several different initial spatial temperature distributions are incorporated in the modelling. The differing gradients in induction times (Zeldovich model) play a major role in outcome, although the authors recognize that '... Zeldovich's spontaneous wave concept... ignores nonlinear gas dynamic evolution...'. The use of dimensional equations prevents the reader from identifying non-dimensional parameters that characterize the reactive gas dynamics.

Many of the results can be understood in terms of the thermomechanical response of a compressible gas to transient, spatially resolved thermal energy addition (Clarke *et al.* 1984*a*; Kassoy 2010).

Poludnenko, Gardiner & Oran (2011) focuses on turbulent flames interacting with a turbulent flow field as a source of detonation initiation, with application to unconfined systems (e.g. gas cloud explosions, supernovae). Results are obtained from a DNS based on the compressible flow equations with one-step Arrhenius kinetics, including transport effects. A planar turbulent flame interacts with a previously created turbulent flow field. The flame is observed to accelerate during a runaway process to supersonic propagation speeds under specifically defined physical conditions. '... burning is controlled by flame propagation and not by autoignition... (precluding) the formation of global spontaneous reaction waves'. Unlike most of the previously cited studies, specific hot spot properties are not required. A semiquantitative (order-of-magnitude) steady state analysis for spontaneous runaway is presented, based on thermal power deposition on the local acoustic time scale with the result that a Chapman–Jouguet deflagration propagation speed is predicted. '... the spontaneous DDT mechanism... does not place any ... constraints on equation of state, reaction model or ... flame properties.'

LES methods are used by Kulkarni, Zellhuber & Polifke (2013) to determine the impact of turbulence on autoignition in a non-premixed hydrogen–air system. The objective is to determine physical processes (mixing) that enable autoignition to occur in isolated volumes (hot spots) of fuel–air mixture. Results are presented for autoignition lengths with respect to turbulent flow properties.

The relationship between super-knock and autoignition of pre-ignition kernels in supercharged spark-ignition engines is the topic of research described in Peters, Kerschgens & Paczko (2013). A new theory of turbulence, developed by the first author, is used to describe the stochastic properties of likely small-scale temperature inhomogeneities as they might appear during phases of cylinder compression. Three-dimensional DNS simulations of homogeneous isotropic turbulence are used to obtain the necessary statistical information. The basic premise is that some of the hot spots are sites for the Zeldovich-gradient-determined spontaneous reaction wave propagation to be initiated. A 'resonance' between the acoustic waves generated by the thermomechanical response of the gas to localized transient, spatially resolved thermal energy deposition, and the spreading reaction wave is the source of a detonation (the super-knock).

Kassoy's (2010) thermomechanical model employs systematic asymptotic methods to predict the consequences of spatially resolved, transient thermal energy deposition into a volume of inert gas. In contrast to the compact initial source approach, a generalized thermal source term with explicitly defined properties is used in the energy equation to represent a spark, laser shot, heated electric wire or chemical heat addition. The model quantifies both the thermodynamics and fluid mechanical responses of the gas to volumetric energy deposition on a time scale short compared to the acoustic time of the volume. The analysis leads to a non-intuitive result: nearly constant-volume heat addition prevails when the energy deposited is less than a specific critical value. The internal expansion Mach number is subsonic. Gas expelled from the volume acts as a piston to drive mechanical disturbances into the unheated environment. Beyond the critical value of energy deposition, the heat addition process is fully compressible, characterized by an $O(1)$ internal gas expansion Mach number and a large expelled gas Mach number responsible for a blast wave propagating into the adjacent environment. This finite source, heated on a finite time scale, replaces

the classical blast wave model of instantaneous energy addition into a point (e.g. Taylor 1946, 1950). The thermomechanical modelling has been extended to a reactive gas with a high-activation-energy reaction by Kassoy (2014*a*) and to a wide range of heat deposition time scales (Kassoy 2014*b*). The latter model quantifies the nearly isobaric response of an inert gas to energy deposition on a time scale long compared to the acoustic time of the volume. Each of these asymptotic models quantifies the role of viscous, conductive and mass diffusion in the thermomechanical response.

Radulescu, Sharpe & Bradley (2013) provide an extensive review of a parameter, used to '... characterize the detonability and explosion hazard of reactive media'. Theory and experiment suggest that hot spot ignition and the subsequent appearance of strong shock waves is uniquely related to the parameter magnitude. The thermomechanical response to localized, spatially distributed heat addition transients can be predicted if the parameter is known.

The current paper presents a systematic and rational asymptotic formulation for autoignition within a finite volume of reactive gas with an instantaneous spatially non-uniform temperature distribution, T', varying around a mean temperature T'_0. This configuration may occur in a non-uniform mixture of reactive gas where some volumes of the gas are warmer than the mean and others are colder, leading to a preferred ignition site. The reaction initiation process is driven by an imposed dimensional temperature gradient, measured by $\Delta T'/\ell' \ll O(T'_0)/\ell'$, which characterizes the local gradient and where ℓ' is the length scale of the temperature inhomogeneity. A primary objective is integrate the thermomechanical response of the gas into the Zeldovich model (1980) for both fast and modest rates of chemical energy addition (both quantified in §§ 2.1 and 3) in a rational manner in order to identify physical conditions compatible with constant-volume heat addition physics implicit in his model. The analysis, related to Short's work (1995, 1997) and that of Jackson *et al.* (1989) and Kapila *et al.* (2002), should enable the reader to gain a fundamental and quantitative physical understanding of how autoignition driven initially by a small temperature gradient generates a propagating, spatially distributed, high-activation-energy thermal explosion, also known as a spontaneous reaction wave, including induced fluid motion and the generation of mechanical waves (acoustics, shocks and blast waves).

2. Mathematical model

The mathematical model is formulated by using asymptotic techniques described by Clarke & Kassoy (1984) as well as Kassoy (2010, 2014*a*,*b*). It quantifies the multifaceted heat transfer phenomena evolving from an imposed inhomogeneous temperature distribution like that in figure 1. The primary objectives are to establish the physical conditions that must exist for a spontaneous reaction wave to propagate down the negative gradient and for the Euler equations to be an appropriate model.

2.1. *Generalized thermomechanical analysis*

The analysis begins with the complete planar dimensional (primes′) conservation equations for a perfect gas including all transport terms and a generalized thermal source term in the energy equation that may represent external energy addition from a spark or laser shot, or from an exothermic chemical reaction. These equations are chosen to emphasize the thermomechanical physics of gaseous systems with imposed energy addition. An important objective is to identify non-dimensional parameters

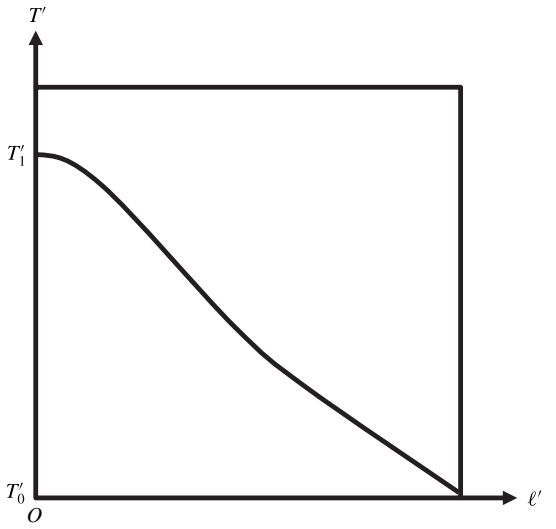

FIGURE 1. A spatially non-uniform initial temperature distribution $T_i'(x)$ varying around a mean value T_0', where the former is larger than the latter for $0 \leqslant x \leqslant \ell'$ and less beyond ℓ' on a similar length scale.

modulating the transport terms in order to justify the use of the reactive Euler equations in a subsequent study of reactive gas autoignition and thermomechanics.

$$\rho'_{t'} + (\rho' u')_{x'} = 0 \tag{2.1}$$

$$\rho'(u'_{t'} + u' u'_{x'}) = -p'_{x'} + V' \tag{2.2}$$

$$\rho' C'_v (T'_{t'} + u' T'_{x'}) = -p' u'_{x'} + C' + \rho' \dot{Q}'_s + D' \tag{2.3}$$

$$p' = \rho' R' T' \tag{2.4}$$

$$Y_{t'} + u' Y_{x'} = \frac{\dot{Q}'_s}{q'_R} + \mathscr{D}', \tag{2.5}$$

where V', C', D' and $\mathscr{D}'$ represent familiar planar viscous, conduction, dissipation and mass diffusion operators, respectively. The thermal power heat source is defined by

$$\dot{Q}'_s = \frac{q'_R}{t'_s} \dot{Q}_s, \tag{2.6}$$

where q'_R is the heat of reaction per unit mass, t'_s is the source heat addition time scale and $\dot{Q}_s$ is the non-dimensional heat source.

The initial conditions, defined by

$$t' = 0, \quad 0 \leqslant x' \leqslant \ell': \quad (T', \ p', \ \rho') = (T'_i(x'), p'_0, \ p'_0 / R' T'_i(x')), \tag{2.7a}$$

$$u' = 0, \quad Y = 1, \tag{2.7b}$$

describe a gas at constant pressure (p'_0), at rest ($u' = 0$), with imposed temperature and density inhomogeneities. The initial conditions at $x' = 0$ and ℓ' are defined by

$$x' = 0, \quad T'_i(0) = T'_1 > T'_0 \tag{2.8a}$$

$$x' = \ell', \quad T'_i(\ell') = T'_0 \tag{2.8b}$$

as shown in figure 1. The boundary at ℓ' is open, allowing fluid to be expelled into a cold fluid beyond.

The details of the initial gradient $\mathrm{d}T_i'/\mathrm{d}x'(t'=0,x')$ are left undefined so long as the gradient is negative for $0<x'<\ell'$ and $T_i'<T_0'$ in some domain beyond $x'=\ell'$. Non-dimensional variables are defined by:

$$(T,p,\rho)=(T'/T_0',\ p'/p_0',\ \rho'/\rho_0') \tag{2.9a}$$

$$u=u'/a_0' \tag{2.9b}$$

$$x=x'/\ell' \tag{2.9c}$$

$$t=t'/t_s', \tag{2.9d}$$

where a_0' is the characteristic speed of sound at T_0'. When used in (2.1)–(2.9), the non-dimensional equations take the form

$$\rho_t+\mu(\rho u)_x=0 \quad \mu=t_s'/t_A' \tag{2.10}$$

$$\rho[u_t+\mu u u_x]=-\mu\frac{p_x}{\gamma}+t_s'/t_v'V \tag{2.11}$$

$$\rho[T_t+\mu u T_x]=-(\gamma-1)\mu p u_x+(t_s'/t_{CD}')C+(q_R'/e_0')\rho\dot{Q}_s+(\gamma)(\gamma-1)(t_s/t_v')D \tag{2.12}$$

$$p=\rho T \tag{2.13}$$

$$[Y_t+\mu u Y_x]=-\dot{Q}_s+(t_s'/t_{DIFF}')\mathscr{D}, \tag{2.14}$$

where the characteristic acoustic, viscous, conduction and mass diffusion time scales are defined by

$$t_A'=\ell'/a_0', \quad t_v'=\ell'^2/\nu_0', \quad t_{CD}'=\ell'^2/\alpha_0', \quad t_{DIFF}'=\ell'^2/D_m', \tag{2.15a–d}$$

respectively, where ν_0', α_0', D_m' are the characteristic kinematic viscosity, thermal diffusivity and the mass diffusivity, respectively.

The non-dimensional initial conditions are

$$t=0; \quad (T,p,\rho)=(T_i(x),1,1/T_i(x)) \tag{2.16a}$$

$$u=0, \quad Y=1, \tag{2.16b,c}$$

where $T_i(x)=T_i'(x')/T_0'$. The initial condition in (2.8a) can be written in non-dimensional terms as

$$x=0, \quad T=1+\tau, \quad \tau=\frac{T_1'-T_0'}{T_0'}, \tag{2.17}$$

where the parameter τ quantifies the temperature difference across the gradient.

The viscous, conductive and diffusive transport terms in (2.11), (2.12) and (2.14) are modulated by the time scale ratios t_s'/t_v', t_s'/t_{CD}' and t_s'/t_{DIFF}', respectively. These ratios can be rewritten as $(t_s'/t_A')(t_A'/t_v')$, $(t_s'/t_A')(t_A'/t_{CD}')$ and $(t_s'/t_A')(t_A'/t_{DIFF}')$. Given the definitions in (2.15), the ratios of the acoustic time to each of the viscous, conductive and diffusion time scales are proportional to the Knudsen number $Kn=\nu_0'/a_0'\ell'$, which must be very small in a continuum gas. Except for exceptionally large ratios t_s'/t_A', all transport terms are suppressed in (2.11), (2.12) and (2.14) in the limit $Kn\to 0$. In particular, when $t_s'=t_A'$, the full nonlinear compressible Euler equations for a source-driven ($\dot{Q}_s$) system are recovered in the limit $Kn\to 0$. The thermomechanically

induced Mach number, $M = u'/a' = a'_0 u/a'_0 a = O(1)$. However, it must be stated that, for sufficiently large values of τ, the combination $(t'_s/t'_{CD})C$ could be $O(1)$, thus accounting for a very large heat flux due to an asymptotically large τ. This is not a likely physical scenario. In the absence of transport physics, traditional flame propagation cannot occur, leaving only the possibility of spontaneous reaction waves, or what Kassoy & Clarke (1985) called 'fast flames', and reactive gas dynamic waves.

The limit $\mu \to 0$ is studied initially with the objective of developing a transparent understanding of the physics of the evolving system when the heat addition process is relatively fast. This corresponds to what many authors refer to as 'instantaneous' heat addition. A second advantage is that a fully analytical solution can be obtained. In order to include a pressure-gradient-driven flow field in the limit, (2.11) implies that the speed must be rescaled as

$$u = \mu U \tag{2.18}$$

so that the associated induced Mach number

$$M = \frac{u'}{a'} = \frac{u'/a'_0}{a'/a'_0} \equiv \frac{u}{a} = O(\mu) \ll 1, \quad a = O(1) \tag{2.19}$$

is subsonic. It follows from (2.11) and (2.16) that the momentum equation takes the form

$$\rho[U_t + \mu U U_x] = -\frac{p_x}{\gamma} + \mu Kn \widetilde{V}, \tag{2.20}$$

where $Kn \to 0$ in the limit and $\widetilde{V}$ is the rescaled non-dimensional viscous term. If (2.18) is used in (2.10), it follows that the density must be rescaled by

$$\rho = 1/T_i(x) + \mu^2 R, \tag{2.21}$$

with the result that in the limit $\mu \to 0$, (2.10) becomes

$$R_t + (\rho U)_x = 0. \tag{2.22a}$$

Then the energy equation (2.12) is transformed to

$$\rho[T_t + \mu^2 U T_x] = -(\gamma - 1)\mu^2 p U_x + (t'_s/t'_{CD})C + \gamma(\gamma - 1)(t'_s/t'_v)\mu^2 D + q_R \rho \dot{Q}_s, \tag{2.22b}$$

$$q_R = q'_R/e'_0, \tag{2.22c}$$

where q'_R is a heat of reaction with units J kg^{-1} and e'_0 is the initial internal energy with the same units. The species equation is

$$Y_t + \mu^2 U Y_x = -\dot{Q}_s + (t'_s/t'_{DIFF})\mathscr{D}, \tag{2.23}$$

and the state equation becomes

$$p = \left[\frac{1}{T_i(x)} + \mu^2 R\right] T. \tag{2.24}$$

The asymptotically reduced describing equations, initial and boundary conditions are

$$R_t + (U/T_i(x))_x = 0 \tag{2.25}$$

$$U_t = -\frac{p_x}{\gamma} T_i(x) \tag{2.26}$$

$$p = T/T_i(x) \tag{2.27}$$

$$T_t = q_R \dot{Q}_s \tag{2.28}$$

$$Y_t = -\dot{Q}_s \tag{2.29}$$

$$t = 0; \quad (T, p, \rho) = \left(T_i(x), 1, \frac{1}{T_i(x)} \right), \quad u = 0, \quad Y = 1, \tag{2.30}$$

where $T_i(0) = 1 + \tau$ and $T_i(1) = 1$. It is implicit in the analysis that the non-dimensional parameters q_R and τ, defined in (2.22*c*) and (2.17), respectively, are $O(1)$ quantities. Asymptotically large heat of reaction or temperature differences would imply the need for rescaling of T, p and U. Kassoy (2010) has considered heat addition large compared to the initial internal energy, which has a non-intuitive consequence on the thermomechanics.

The physical interpretation of the reduced equation system (2.26)–(2.31) enables a fundamental understanding of the thermomechanical consequences of 'fast' heating, $\mu = o(1)$. Equation (2.28) describes constant-volume heating from the source. The rising temperature is accompanied by rising pressure, defined in (2.27). The induced speed, described by (2.26), demonstrates that regardless of how fast energy deposition occurs, $(\mu \to 0)$, there will be a mechanical response as long as a temperature–pressure gradient exists. The weak density change is given by (2.25) in the context of (2.21). Similar equations appear in Kassoy (2010, 2014*a*,*b*). Fully analytical solutions for (2.26)–(2.30) subject to the initial conditions in (2.31) follow,

$$T = T_i(x) + q_R \int_0^t \dot{Q}_s(x, \widehat{t})\, \mathrm{d}\widehat{t} \tag{2.31}$$

$$p = 1 + q_R \int_0^t \frac{\dot{Q}_s(x, \widehat{t})}{T_i(x)}\, \mathrm{d}\widehat{t} \tag{2.32}$$

$$U = -\frac{T_i(x)}{\gamma} q_R \int_0^t \mathrm{d}\widehat{t} \int_0^{\widehat{t}} \left(\frac{\dot{Q}_s(x, \widetilde{t})}{T_i(x)} \right)_x \mathrm{d}\widetilde{t} \tag{2.33}$$

$$R = -\int_0^t \left(\frac{U}{T_i(x)} \right)_x \mathrm{d}\widehat{t} \tag{2.34}$$

$$y = 1 - \int_0^t \dot{Q}_s\, \mathrm{d}\widehat{t}. \tag{2.35}$$

The solutions are valid for arbitrary spatial distributions of $\dot{Q}_s$ and $T_i(x)$, whether symmetric or non-symmetric relative to $x = 0$. The integrals describe the disturbances to the initial state due to the heat addition defined by $\dot{Q}_s$.

The reader should recognize that the results are valid for any source $\dot{Q}_s$. The formal analytical solutions in (2.32)–(2.36) provide insights into the dependence of variables on the non-dimensional heat of reaction, q_R, and the non-dimensional heat source distribution in space and time, $\dot{Q}_s(x, t)$, as well as on the initial temperature distribution $T_i(x)$. In addition, (2.34) can be used to identify the speed of the fluid expelled from the hot spot at $x = 1$, where $T_i = 1$. Given the small Mach number in (2.18), the thermomechanical disturbances, in the unheated gas, $x > 1$, will be weak acoustic waves (Kevorkian & Cole 1968).

The solutions in (2.31)–(2.35) can be simplified considerably for an asymptotically small linear negative temperature gradient represented by

$$T_i(x) = 1 - \alpha x \cdots, \quad \alpha = o(1), \tag{2.36}$$

so that the variables depend only on the heat source distribution $Q_s(x, t)$ in a first approximation. This perspective will be useful in the subsequent study of an Arrhenius, high-activation-energy reaction as the source of thermal energy addition.

When the energy addition time scale is longer, $\mu = O(1)$, (2.10)–(2.14) are essentially the compressible Euler equations with a heat source, $q'_R/e'_0 = O(1)$. The transport terms remain suppressed. These equations describe a fully compressible thermomechanical process evolving from the transient, spatially resolved energy addition on the time scale t'_s (see § 5). In this case wave propagation within the hot spot occurs on the same time scale as the energy addition, thus facilitating the compressible (variable density) response. The equation structure implies unequivocally that all thermodynamic variables undergo $O(1)$ changes, in contradistinction to the fast heating limit process, and that the induced Mach number,

$$M = u'/a' = u/a = u/(T)^{1/2} = O(1). \tag{2.37}$$

The Mach number of the fluid expelled from the heat spot is of the same order, and is the source of the 'piston effect' driving strong mechanical disturbances (e.g. shocks) into the unheated cold environment (Kevorkian & Cole 1968). During the heat addition time scale, t'_s, the order of magnitude of fluid motion in the hot spot and beyond is quantified by

$$D' = O(u't'_s) = O(a'_o\ell'/a'_0) = O(\ell') \tag{2.38}$$

while the generated shock wave will move the same order-of-magnitude distance,

$$d'_s = O(a'_0t'_s) = O(\ell'), \quad t'_s/t'_A = O(1). \tag{2.39}$$

This result implies that the expelled fluid will be able to support the shock during the entire heat addition process, $Q_s(x, t) > 0$.

3. Thermomechanical analysis for a reactive gas in the fast heating limit: $\mu \ll 1$

In the following paragraphs an Euler-based analysis is presented for a single-step, high-activation-energy, exothermic reaction in order to include a specific chemical heat source, similar to that in Kassoy (2014*a*). The objective is to address the Zeldovich concept with a rational systematic mathematical model.

The dimensional (primed ($'$)) Euler equations can be written as:

$$\rho'_{t'} + (\rho' u')_{x'} = 0 \tag{3.1a}$$

$$\rho'(u'_{t'} + u'u'_{x'}) = -p'_{x'} \tag{3.1b}$$

$$\rho'(e'_{t'} + u'e'_{x'}) = -p'u'_{x'} + \rho' A' q'_R Y\, \mathrm{e}^{-E'/R'T'} \tag{3.1c}$$

$$Y_{t'} + u'Y_{x'} = -A'Y\, \mathrm{e}^{E'/R'T'}, \tag{3.1d}$$

where ρ', p', T' are the usual thermodynamic variables, u' represents the gas speed induced by energy addition, e' is the internal energy (C'_vT'), where the specific heat is treated as a constant, A' is the pre-exponential (frequency) factor in the Arrhenius rate term, E' is the activation energy, R' is the universal gas constant, q'_R is the heat of reaction and Y is the non-dimensional reactant concentration.

Non-dimensional thermodynamic variables are defined relative to an equilibrium gas state denoted by ρ_0', p_0', T_0': $\rho,\ \ p,\ \ T = (\rho'/\rho_0', p'/p_0',\ \ T'/T_0')$. It follows that $e = e'/e_0'$, where $e_0' = C_v' T_0'$. The gas speed is non-dimensionalized by the equilibrium speed of sound, $(a_0' = \sqrt{\gamma R'\ T_0'})$, $u = u'/a_0'$. The space and time variables are defined by $x = x'/\ell'$ and $t = t'/t_s'$, where ℓ' defines the characteristic length scale of prescribed initial spatial inhomogeneities in the variables, ρ', p', T', Y and $t_s' = \varepsilon \exp(1/\varepsilon)/A'$ (a traditional thermal explosion induction time), where $\varepsilon = R'\ T_0'/E$ is the small activation energy parameter and $q_R = q_R'/e_0'$. Many of these variable definitions differ from those used by Short (1997).

The non-dimensionalized conservation equations take the form:

$$\rho_t + \mu(\rho u)_x = 0 \tag{3.2a}$$

$$\rho(u_t + \mu u u_x) = -\mu p_x/\gamma \tag{3.2b}$$

$$\rho(T_t + \mu u T_x) = -\mu(\gamma - 1) p u_x + A' t_s' q_R \rho Y \,\mathrm{e}^{-1/\varepsilon T} \tag{3.2c}$$

$$Y_t + \mu u Y_x = -A' t_s' Y \,\mathrm{e}^{-1/\varepsilon T}, \tag{3.2d}$$

where $\mu = t_s'/t_A'$ is the ratio of the characteristic thermal explosion induction time to the local acoustic time $t_A' = \ell'/a_0'$. The non-dimensional state equation for a perfect gas:

$$p = \rho T \tag{3.3}$$

completes the mathematical model. The variables in (3.2) and (3.3) are subject to the following initial conditions:

$$t = 0: \quad \rho = \rho_i(x), \quad p = 1, \quad T = T_i(x), \quad u = 0, \quad Y = 1, \quad 0 \leqslant x \leqslant 1, \tag{3.4}$$

corresponding to an initial non-homogeneity in density and temperature on the dimensional length scale ℓ'. This finite model of an initial disturbance is chosen with the explicit objective of identifying the thermomechanical response of the disturbed gas and consequences of the response to the gas external to the disturbed volume.

3.1. *Induction time theory for a spatially dependent thermal explosion*

Following Short (1997), an asymptotic analysis is formulated for a high-activation-energy reaction ($\varepsilon \ll O(1)$) where the induction time is short compared to the acoustic time of the heated volume ($\mu \ll O(1)$), again to obtain a complete analytical solution. The former requires that the thermodynamic variables be defined by the traditional thermal explosion asymptotic expansions, valid in the limit $\varepsilon \to 0$,

$$(\rho,\ \ p,\ \ T) = (1 + \varepsilon(R, P, \varphi) + O(\varepsilon^2)), \tag{3.5}$$

where R, P, φ are spatially variable, time-dependent descriptions of chemically driven perturbations from the initial thermodynamic state: e.g. $t = 0$. $(R, P, \varphi) = (R_i(x), 1, \varphi_i(x))$, where each is non-zero only in $0 \leqslant x \leqslant 1$. The asymptotic expansions in (3.5) imply that the appropriate initial conditions for temperature, pressure and density take the form: $T(0, x) = T_i = 1 + \varepsilon\varphi_i(x)$, $p(0, x) = 1$, $\rho(0, x) = 1 - \varepsilon\varphi_i(x)$.

As a result, the temperature difference parameter in (2.17), $\tau = O(\varepsilon)$, so that an asymptotically small imposed temperature gradient is the driver for the entire evolutionary process to follow. Similarly,

$$Y = 1 - \varepsilon W + O(\varepsilon^2), \tag{3.6}$$

where W is the perturbation in the reactant concentration: at $t = 0$, $W = W_i(x) = 0$ in $0 \leqslant x \leqslant 1$.

Initially (3.2*a–d*) take the forms:

$$R_t + (\mu/\varepsilon)(\rho u)_x = 0 \tag{3.7a}$$

$$\rho(u_t + \mu u u_x) = -\mu\varepsilon P_x/\gamma \tag{3.7b}$$

$$\rho(\varphi_t + \mu u \varphi_x) = -(\mu/\varepsilon)(\gamma - 1)pu_x = \rho q_R \mathrm{e}^{\varphi} \tag{3.7c}$$

$$W_t + \mu u W_x = \mathrm{e}^{\varphi}. \tag{3.7d}$$

This mathematical system contains two non-dimensional parameters (μ and ε). The speed and density variables are to be rescaled to obtain a lowest-order reduced mathematical model that couples an explicit mechanical response of the gas to localized spatially distributed transient heating. Gas motion induced by an evolving spatial pressure gradient in (3.7*b*) can be assured in the limit $\varepsilon \to 0$, and $\mu \ll O(1)$ if

$$u = \varepsilon\mu U. \tag{3.8}$$

It follows that (3.7*a–d*) take the forms

$$R_t + \mu^2(\rho U)_x = 0 \tag{3.9a}$$

$$\rho(U_t + \varepsilon\mu^2 U U_x) = -P_x/\gamma \tag{3.9b}$$

$$\rho(\varphi_t + \varepsilon\mu^2 U \varphi_x) = -\mu^2(\gamma - 1)pU_x + \rho q_R \mathrm{e}^{\varphi} \tag{3.9c}$$

$$W_t + \varepsilon\mu^2 U W_x = \mathrm{e}^{\varphi}. \tag{3.9d}$$

Equation (3.9*a*) and the initial conditions imply that, to account for density variation associated with the gas motion, the density perturbation must be rescaled by

$$R = -\varphi_i(x) + \mu^2 \widetilde{R}, \tag{3.10}$$

where $\varphi_i(x)$ represents the initial density distribution compatible with (3.5) and the second term describes a very small change in density. Equation (3.9*a*) takes the form

$$\widetilde{R}_t + (\rho U)_x = 0. \tag{3.11}$$

The equation set composed of (3.9*b–d*) and (3.11) describe a weakly variable density response of a gas to relatively rapid energy deposition, ($\mu \ll O(1)$). The local expansion Mach number is characterized by

$$M = \frac{u'}{a'} = \frac{u}{a} = \frac{u}{\sqrt{T}} = \frac{\varepsilon\mu U}{\sqrt{T}} = O(\varepsilon\mu) = o(1). \tag{3.12}$$

In the limits $\epsilon \to 0$ and $\mu \to 0$ (3.3), (3.5) and (3.9) and (3.11) can be used to define the reduced system of initial value equations and conditions

$$\widetilde{R}_t + U_x = 0, \quad \widetilde{R}(0, x) = 0 \tag{3.13a}$$

$$U_t = -\frac{P_x}{\gamma}, \quad P(0, x) = 0 \tag{3.13b}$$

$$\varphi_t = q_R \mathrm{e}^{\varphi}, \quad \varphi(0, x) = \varphi_i(x) \tag{3.13c}$$

$$P = \varphi - \varphi_i(x) + O(\epsilon, \mu^2) \tag{3.13d}$$

$$W_t = -\mathrm{e}^{\varphi}, \quad W(0, x) = 0. \tag{3.13e}$$

Equation (3.13*c*) describes a constant-volume heat addition process, as envisaged by Zeldovich (1980), for the temperature perturbation φ response to energy addition. The rate of temperature perturbation increase is proportional to the size of q_R, the heat of reaction defined in (2.22*c*). The solution is given by

$$\varphi = \ln \frac{1}{(\mathrm{e}^{-\varphi_i(x)} - q_R t)} = \varphi_i(x) + \ln \frac{1}{(1 - t/t_e(x))}, \tag{3.14}$$

where $\varphi_i(x)$ is an imposed initial (small) temperature disturbance of the type considered by Zeldovich (1980) in his spontaneous wave theory. The temperature perturbation solution in (3.14) appears in Short (1997). It has a classical thermal explosion singularity at a spatially dependent time t_e where

$$t_e(x) = \frac{\mathrm{e}^{-\varphi_i(x)}}{q_R}. \tag{3.15}$$

A simple calculation demonstrates that $(\mathrm{d}\varphi/\mathrm{d}q_R) > O$, as expected from physical perspectives. As noted by numerous authors (Jackson *et al.* 1989; Kapila & Dold 1989; Short 1997), (3.15) implies that the thermal explosion spreads down an imposed negative initial temperature gradient $(\varphi_i'(x) < 0)$, where the bold prime denotes a spatial derivative. The inverse of the thermal explosion propagation speed is found from (2.15) to be

$$\frac{\mathrm{d}t_e}{\mathrm{d}x} = \frac{-\varphi_i'(x)\,\mathrm{e}^{-\varphi_i(x)}}{q_R} \tag{3.16}$$

while a comparison of the dimensional propagation speed relative to the characteristic dimensional speed of sound, a_0', can be obtained from (3.16) as

$$\frac{\mathrm{d}x'/\mathrm{d}t_e'}{a_o'} = -\frac{q_R}{\mu}\frac{\mathrm{e}^{\varphi_i(x)}}{\varphi_i'(x)}, \tag{3.17}$$

showing quantitatively that the thermal explosion moves through the volume of heated gas at a locally supersonic speed, proportional to q_R, when $\mu \ll O(1)$, as noted by Kapila & Dold (1989), Friedman & Herrero (1990), and referred to in Short (1997). The front moves through the volume defined by the characteristic length scale, ℓ', during the induction time period, reaching the edge, $x' = \ell'$, when the dimensional value $t_e' = t_s'/q_R \ll O(t_A')$. Equation (3.17) demonstrates that when the gradient of the initial temperature distribution is zero, the propagation speed is infinite, a non-physical result noted by Short (1997), interpreted to mean that a spatially homogeneous thermal explosion occurs. Jackson *et al.* (1989) have noted that the reaction evolution process differs if at a symmetry point $x = 0$, the gradient is zero or less than zero.

Equation (3.14) demonstrates that an initial temperature inhomogeneity is essential for φ to be spatially dependent. This is crucial to supporting the induced gas motion described by (3.13*b*). The pressure disturbance is equal to the difference between the evolving $\varphi(x, t)$-value and the initial value $\varphi_i(x)$ (see (3.13*d*)). It must be emphasized that, in the absence of an initial small temperature disturbance, the solution in (3.14) shows that the thermal explosion induction period is characterized by a spatially homogeneous thermal temperature, that the spatial pressure gradient is absent and that no local gas motion can occur. Kassoy (2010) has discussed the role of localized gas expansion as an immediate source of mechanical disturbances (Kevorkian & Cole 1968).

x	$\phi_i(x) = 1 - x$	$t_e(x)$
0.01	0.99	0.37
0.25	0.75	0.47
0.5	0.5	0.607
0.75	0.25	0.779
1.0	0	1.0

TABLE 1. The explosion time $t_e(x)$ as a function of location for a linear temperature gradient $\varphi_i(x) = 1 - x$, $x > 0$ with $q_R = 1$.

A Schwab–Zeldovich formulation can be used with (3.13*c*) and (3.13*e*) to show that

$$W = \frac{1}{q_R} \ln \frac{1}{(1 - t/t_e(x))}, \tag{3.18}$$

when $W(0, x) = 0$.

The thermally induced gas speed can be found from the integral of (3.13*b*) ((3.13*d*) and (3.14) are employed):

$$U = -\frac{\varphi_i'(x)}{q_R \gamma} \mathrm{e}^{-\varphi_i(x)} \left[\ln \frac{1}{(1 - t/t_e(x))} - (t/t_e(x)) \right], \tag{3.19}$$

where it is assumed that there is no initial speed disturbance, $U_i(x) = 0$. Equation (3.19) demonstrates that $U > 0$ when $\varphi_i'(x) < 0$, meaning that gas expansion occurs and that the speed is singular when the explosion time t_e is reached at a given location. Equation (3.19) also shows that there is thermally induced low-Mach-number gas motion throughout the heated volume as the reaction wave propagates.

The analytical solutions in (3.14) and (3.19) and the results in tables 1 and 2 enable a complete description of the thermomechanical response of the heated gas. Table 1 lists the value of the explosion time by location x when an initially linear temperature distribution exists, $\varphi_i(x) = 1 - x$ and $q_R = 1$. The results show that a thermal explosion occurs close to $x = 0$ when $t = 0.372$ for $q_R = 1$, and then propagates through the inhomogeneity arriving at $x = 1$ when $t = 1$.

Table 2 lists the induced speed at $x = 0.01$, $x = 0.5$ and the edge of the heated region, $x = 1$, demonstrating that gas is expelled at the non-homogeneity edge ($x = 1$) for all times up to and including $t_e = 0.372$, for the case $\varphi_i'(x) = -1$. Furthermore, (3.19) can be used to show that the gas speed at $x = 1$ will continue to increase for time values up to $t = 1$ when the thermal explosion singularity leads to an unbounded value of the scaled speed U.

Finally (3.13) and (3.19) can be used to find the solution for the weak density change represented by $\widetilde{R}$ in (3.10). The logarithmic dependence in (3.18) and (3.19) is found once again.

3.2. *Thermal explosion singularity analysis*

The theory predicts that a thermal explosion propagates down the specified gradient. The singularity occurs close to $x = 0$ when $t_e = 0.372$ for $q_R = 1$. In particular, the expansions in (3.5) and (3.6) fail when $\varepsilon\varphi = O(1)$, $\varepsilon\widetilde{R} = O(1)$ and $\varepsilon W = O(1)$ in the limit $t \to t_e(x)$. It follows from (3.14) that

$$\varepsilon \ln[1/(1 - t/t_e(x))] = O(1) \tag{3.20}$$

t	$U(0.01, t)$	$U(0.5, t)$	$U(1, t)$
0	0	0	0
0.1	0.152	0.006	0.004
0.2	0.41	0.03	0.016
0.3	0.96	0.08	0.041
0.372	∞	0.146	0.066

TABLE 2. The induced fluid speed at locations $x = 0.01$, 0.5 and 1.0 for time values $t \leqslant t_e(0.01) = 0.372$ calculated with $\gamma = 1.4$ and $\varphi_i(x) = 1 - x$, $x > 0$, with $q_R = 1$.

or

$$[t_e(x) - t] = \exp(O(-1/\varepsilon)), \tag{3.21}$$

implying that, when t is exponentially close to $t_e(x)$, a full-scale explosion will occur characterized by $O(1)$ changes in T and Y, as well as $\rho = 1 - \varepsilon\varphi_i(x) + O(\mu^2)$, as all the fuel is consumed and the complete heat of reaction is released. Equation (3.21) demonstrates that the time scale of the full-scale explosion is exponentially short compared to the induction time scale $t = O(1)$. This concept has been used by Kassoy (1977) to describe the full-scale explosion in a spatially homogeneous system by defining a nonlinear time scale transformation:

$$t_e - t = \exp(-s/\varepsilon)[1 + O(\epsilon)], \tag{3.22}$$

where $s > 0$ is the $O(1)$ explosion time variable. (An independent application of this unusual transformation appears in Short (1996).) The application of this unusual scaling to the current spatially distributed system is the subject of § 4. This scaling transformation differs fundamentally from that used by Short (1997) to describe the post-induction period phenomena. In particular, the ε-parameter is absent from the transformation used. As a result, the subsequent analysis cannot describe post-induction physics on the exponentially short time scale defined in (3.22).

It should be noted here that the thermal energy released during the induction period is asymptotically small, $O(\varepsilon)$, because so little reactant is consumed and that the induced non-dimensional kinetic energy,

$$u'^2/e'_o = O(\varepsilon^2\mu^2). \tag{3.23}$$

It should be clear that the initial disturbance in the temperature perturbation $\varphi_i(x)$ considered by Zeldovich (1980) is absolutely essential to describing a meaningful thermomechanical response to localized, spatially resolved, transient energy deposition. Short (1997) has examined the consequences of non-zero initial conditions in the remaining variables.

In summary, a reaction front, represented by a propagating thermal explosion, moves at a supersonic speed across the space $0 < x \leqslant 1$ during a time period, $O(t'_s) \ll t'_A$, much less than the characteristic acoustic time. The front reaches the boundary $x = 1$ at $t = 1$ for the example gradient $\varphi = 1 - x$. Fluid expelled from the boundary throughout the induction time scale period, $U(1, t)$, acts like a piston (Kevorkian & Cole 1968) driving $O(\epsilon\mu)$ acoustic disturbances into the colder gas, $x > 1$.

4. The post-induction time analysis: $\mu \ll 1$

The singularities in the induction-period solutions imply that the variable definitions in (3.5), (3.6), (3.8) and (3.10) fail to be viable when $\epsilon\varphi = O(1)$, $\epsilon U = O(1)$, $\epsilon\widetilde{R} = O(1)$ and $\epsilon W = O(1)$. These solution properties, occurring when $t \to t_e(x)$ as defined in (3.21), imply that the post-induction zone-dependent variables are defined by

$$T, p, \quad \rho = 1 - \epsilon\varphi'(x) + \mu^2\hat{R}, \quad u = \mu V, Y, \tag{4.1}$$

where the nonlinearly rescaled time, s in (3.22), is used along with the related rescaled space scale, X, defined by

$$x = x_F(t) - X\exp(-s/\varepsilon). \tag{4.2}$$

The spatial rescaling defines the distance travelled by the propagating thermal explosion (reaction front) during the exponentially short time scale defined by (3.22), where t_e is replaced by $t_e(x)$ in the current application. Both the length and time scales germane to the physics of the post-induction period are exponentially short with respect to the spot dimension ℓ' and the induction time scale, t'_s, defined in the paragraph above (3.2*a*). When (3.22) and (4.1) are employed in (3.2), and the limit $\varepsilon \to 0$ is taken, the lowest-order result is related closely to that in the analysis of a post-induction period process in a spatially homogeneous system (Kassoy 1977):

$$T = 1/(1-s), \quad p = 1/(1-s), \quad Y = 1 - \frac{sq_R}{(1-s)} \tag{4.3a–c}$$

$$\rho = 1 + O(\mu^2), \quad u = \mu V \tag{4.3d,e}$$

$$T_{MAX} = T_{ADIABATIC} = 1 + q_R, \quad 0 \leqslant s \leqslant s_{MAX} = \frac{q_R}{(1+q_R)} < 1. \tag{4.4a,b}$$

These results describe the consequences of complete reactant consumption and concomitant heat release in an essentially inertially confined, constant-volume heat addition process on a time scale exponentially short compared to the characteristic induction-period time scale t'_s. To lowest order the temperature and pressure are spatially homogeneous in the exponentially thin reaction zone just behind the propagating thermal explosion singularity. The scaled variables can be used to demonstrate that in the reaction zone the characteristic reaction time scale is $t'_R = O(t'_s\,\mathrm{e}^{-s/\varepsilon})$ compared to the local acoustic time scale, $t'_{RA} = 0(t'_A\,\mathrm{e}^{-s/\varepsilon})$ based on the thickness of the reaction zone and characteristic acoustic speed, a result compatible with the inertial confinement mentioned earlier. It is also important to note that the local conduction time scale, based on the width of the reaction zone and a characteristic value of the thermal diffusivity, is small compared to the local reaction time if $\exp(-1)/(\varepsilon) \gg (\mu)(Kn)$, where the latter parameter represents the Knudsen number. As a result the reaction zone is not affected by transport effects relative to the cooler, unburned gas in front of the propagating thermal explosion. In summary, §§ 3 and 4 describe a reaction front, defined by a supersonic, propagating thermal explosion singularity occurring during an induction period in the initially defined hot spot. The front is followed by a relatively thin reaction zone, in which the entire heat of reaction is released on a very short time scale. As a result, the lowest-order temperature rises to the spatially homogeneous adiabatic explosion value just behind the front, along with a concomitant increase in the pressure. The associated change in density is minute, precluding the possibility that the front is a fully formed

shock-reaction zone structure (detonation wave). Rather this spontaneous reaction wave structure (Zeldovich 1980) has its own properties and characteristics. The post-induction period solutions above, evolving on a phenomenally short time scale, show that the propagating thermal explosion leaves behind a spatially homogeneous hot, high-pressure spot, that can expand on the relatively long acoustic time scale, ℓ'/a_0, in analogy with a shock tube process. The $O(1)$ pressure differential, defined by $p_{MAX} = 1 + q_R$, is the source of a strong shock wave in the colder gas beyond $x = 1$.

5. Modest heating rate theory: $\mu = 1$

The modest heating rate models considered by Jackson *et al.* (1989), Short (1997), Vasquez-Espi' & Liñan (2001), among many others, describe the thermal response to chemical heat addition on a time scale identical to the acoustic time of the hot spot. The conservation equations derived and employed for solution development are equivalent to the Clarke equation (1985) describing only the temperature response. It is useful to revisit the models in the context of the Zeldovich problem (1980) to describe a novel set of equations that describe pressure and velocity responses of the gas to the transient, spatially resolved temperature distribution described by the Clarke equation, as well as to display an alternative to the Clarke equation. The foundational equations are those in (3.2) and (3.3) with $\mu = 1$:

$$\rho_t + (\rho u)_x = 0 \tag{5.1a}$$

$$\rho(u_t + uu_x) = -p_x/\gamma \tag{5.1b}$$

$$T_t + uT_x = -(\gamma - 1)Tu_x + A't'_s q_R Y \mathrm{e}^{-1/\varepsilon T} \tag{5.1c}$$

$$Y_t + uY_x = -A't'_s Y \mathrm{e}^{-1/\varepsilon T} \tag{5.1d}$$

$$p = \rho T \tag{5.1e}$$

$$t = 0: \quad p = 1, \quad T = 1 + \varepsilon\varphi_i(x), \quad Y = 1, \quad \rho = 1 - \varepsilon\varphi_i(x), \quad u = 0 \tag{5.1f}$$

subject to the initial conditions in (2.30), where

$$A't'_s = \varepsilon \mathrm{e}^{1/\varepsilon}, \tag{5.2}$$

given the definition of the traditional thermal explosion induction-period time scale, t'_s, in the paragraph just above (3.2). The variable definitions differ from those used in Short (1997). The current choices, beginning with (2.6) and (2.9), are used to derive non-dimensional equations that can be interpreted physically in terms of parameters significant to the physical phenomena.

If a high-activation-energy analysis is used to describe the thermal induction period when $\mu = 1$, the dependent variables are

$$(p, \rho, T) = (1 + \varepsilon(P, R, \varphi) + O(\varepsilon^2)), \quad Y = 1 - \varepsilon W \tag{5.3a,b}$$

$$u = \varepsilon U, \tag{5.3c}$$

where (5.3*c*) is needed to derive a momentum equation capable of describing the thermomechanically induced velocity. In particular, the model is constructed for a hot spot of specific dimension ℓ' and a non-dimensional heat of reaction, q_R, defined relative to the characteristic initial internal energy rather than the enthalpy. Equation (5.2) enables the model equation (5.1*c*) to display explicitly the role of the heat of reaction in the energy dynamics of the problem.

If (5.2) and (5.3) are used in (5.1) and the limit $\varepsilon \to 0$ is taken, the reduced conservation and state equations for the thermodynamic perturbation quantities, the fuel concentration and induced velocity U are given by

$$R_t + U_x = 0 \tag{5.4a}$$

$$U_t = -P_x/\gamma \tag{5.4b}$$

$$\varphi_t = -(\gamma - 1)U_x + q_R \mathrm{e}^{\varphi} \tag{5.4c}$$

$$W_t = \mathrm{e}^{\varphi} \tag{5.4d}$$

$$P = R + \varphi. \tag{5.4e}$$

These equations are subject to the following initial conditions:

$$t = 0; \quad P = 0, \quad \varphi = \varphi_i(x), \quad W = 0, \quad R = -\varphi_i(x), \quad U = 0. \tag{5.5}$$

These Eulerian coordinate equations describe perturbation variable changes due to chemical heat release, modelled by e^{φ}, and the initial temperature disturbance. In the absence of the heat source term, e^{φ}, they describe classical linear acoustical disturbances (Lieuwen 2012) driven by an initial disturbance. Equation (5.4*c*) shows that local gas expansion, $U_x > 0$, retards growth in the temperature disturbance, noted earlier by Short (1996) as well as by Vasquez-Espi' & Liñan (2001), among others. The scaling on u in (5.3*c*) enables a fully integrated thermoacoustic model with the induced speed generated by a pressure gradient in (5.4*b*).

Familiar manipulations with (5.4) enable a pressure–temperature relationship to be derived:

$$P - \left(\frac{\gamma}{\gamma - 1}\right)\varphi = \left(\frac{\gamma}{\gamma - 1}\right)\varphi_i(x) - \frac{q_R}{(\gamma - 1)}\int_0^t \mathrm{e}^{\varphi}\,\mathrm{d}\widehat{t}, \tag{5.6}$$

a result that replaces the standard isentropic relation for an adiabatic system. The integral represents the accumulated effect of chemical heat addition during an interval of time, t. Equation (5.6) can then be used to derive the following set of describing equations:

$$U_{tt} = U_{xx} - \frac{q_R}{\gamma}\mathrm{e}^{\varphi}\varphi_x \tag{5.7a}$$

$$P_{tt} = P_{xx} + q_R \mathrm{e}^{\varphi}\varphi_t \tag{5.7b}$$

$$\varphi_{tt} = \varphi_{xx} + \frac{q_R}{\gamma}\left(\mathrm{e}^{\varphi}\varphi_t - \int_0^t (\mathrm{e}^{\varphi}\varphi_x)_x\,\mathrm{d}\widehat{t} - \varphi_i''(x)\right). \tag{5.7c}$$

Equations (5.7*a*,*b*) describe a thermoacoustic wave propagation process within the hot spot driven by transient, spatially resolved chemical heat release. The integro-differential equation, (5.7*c*), provides a related description for the thermoacoustic response of the hot spot gas to autoignition and is an alternative to the Clarke equation,

$$(\varphi_t - q_R \mathrm{e}^{\varphi})_{tt} = \left(\varphi_t - \frac{q_R}{\gamma}\mathrm{e}^{\varphi}\right)_{xx}. \tag{5.8}$$

The former can be differentiated with respect to t to derive the latter. It is often stated that (5.8) describes the competition between simultaneous constant-volume and constant-pressure heat addition. Equation (5.7) appears to provide a clearer, physically oriented interpretation of the impact of localized heating on the generation of small-amplitude disturbances associated with the common wave equation operator in each equation.

6. Conclusions

A comprehensive, systematic, asymptotic analysis is employed to quantify the evolution of a 'spontaneous reaction wave' propagating within a finite hot spot, defined by an imposed weak temperature non-uniformity embedded in a larger volume of relatively cold reactive gas. One-step, high-activation-energy ($\varepsilon \to 0$) kinetics define the reaction process. Ignition is initiated at the local temperature maximum, only $O(\varepsilon)$ larger than the colder value external to the spot. The reaction spreads down the $O(\varepsilon)$ negative temperature gradient. Classical thermal explosion induction-period analysis for both fast ($\mu \to 0$) and modest ($\mu = 1$) heat release time scales describes a period of $O(\varepsilon)$ reactant consumption, limited energy addition leading to $O(\varepsilon)$ increases in temperature and pressure, and a concomitant weak gas expansion with the hot spot, the source of expelled gas at the surface of the hot spot.

When the induction time scale (characteristic of chemical heat release) is short compared to the acoustic time scale of the hot spot (the limit $\mu \to 0$), a nearly constant-volume process characterizes the thermomechanical response of the gas. An $O(\varepsilon)$ spatial pressure distribution corresponding to the temperature disturbance of the same size is the source of an $O(\varepsilon\mu)$ induced gas seed. Gas expelled through the hot spot surface is the source of weak acoustic compression waves (the 'piston' effect (Kevorkian & Cole 1968)) in the gas external to the spot. A complete analytical solution of the asymptotically reduced equations is possible in the limit ($\varepsilon \to 0$, $\mu \to 0$). Results define the end of the induction period at each x-location when a local thermal explosion singularity occurs at $t_e(x)$. The propagation of the singularity down the asymptotically small negative temperature gradient defines the Zeldovich 'spontaneous reaction wave' properties. The value of $t_e(x)$ increases from the hottest to the coldest locations in the spot and can be inverted to define the supersonic propagation Mach number for the translating singularity.

When the induction time scale is equal to the local acoustic time ($\mu = 1$), the asymptotically reduced equations describe compressible heat addition. The $O(\varepsilon)$ temperature perturbation is described by a physically transparent alternative to the 'Clarke' equation. The $O(\varepsilon)$ pressure and induced speed responses to transient, spatially resolved heat release are described by non-homogeneous linear wave equations. These equations have no obvious analytical solutions, but define clearly the character and properties of the induction-period physics. Numerical results from Clarke's equation are reported by many authors cited in the introduction. They can be interpreted to mean that a classical logarithmic thermal explosion singularity will occur at finite values of time, $t^*(x)$, to be distinguished from the analytically obtained value $t_e(x)$ for the fast heating limit. New results from numerical solutions of (5.7) will be the subject of future work.

The post-induction period analyses offer new opportunities to understand the physics of extremely fast (explosive) reaction processes. In the limit $\mu \to 0$, the nonlinear transformations define exponentially short time and length scales. During and within these two scales, respectively, the reactant is totally consumed as the spatially homogeneous temperature rises to the adiabatic explosion value in a nearly constant-volume process, with a concomitant increase in the spatially homogeneous pressure. In the absence of a pressure gradient, there is no additional change in the fluid speed induced during the induction period. The analytical results are interpreted to mean that the reaction front, located at the thermal explosion singularity, propagates through the hot spot on the induction time scale, leaving behind a spatially uniform ephemeral high-pressure, high-temperature hot spot located in a larger volume of colder, low-pressure gas. In analogy with a shock tube, the spot will begin to expand

on the much longer acoustic time scale, with the result that a strong compression wave moves through the spot itself. In this regard the thermomechanical response of the spot, initiated by a tiny temperature gradient, is the primary source of a subsequent major mechanical disturbances in the gas external to the original spot.

When $\mu = 1$, the high-activation-energy limit $\varepsilon \to 0$ for the post-induction period produces the result that the temperature-dependent part of the reaction term in the energy equation, $\exp((1/\varepsilon)[1 - (1/T)])$, is unbounded in the limit when $T > 1$. This type of singular behaviour implies that the time derivative term in the energy equation must be equally large to obtain physically viable $O(1)$-increases in temperature. These mathematical properties of the describing equations motivate the use of a nonlinear time rescaling, similar to that described earlier, but entirely independent of the logarithmic thermal explosion singularity found in the fast heating limit. It is hypothesized that an 'explosion time', $t^*(x)$, can be defined and used to describe the exponentially short time scale. Here again one can expect essentially constant-volume heating, with pressure and temperature rising together as the adiabatic value is approached. The ephemeral high-temperature, high-pressure spot will relax, with a process similar to that in a shock tube, on the longer acoustic time scale of the spot. It is important to recall that the reaction wave will cross the spot on the acoustic time scale so that the spot expansion process will be initiated during the induction period of the modest heating rate problem. The explicit analysis of the physical process is the subject of current research and will be reported in the future. The present study describes physical phenomena occurring when transient, spatially distributed chemical heat addition takes place in a compressible gas. In particular, the quantitative analysis provides a cause–effect source for mechanical disturbances arising from localized energy addition. Applications to combustion chamber instability and engine knock are of interest. These phenomena can occur in a turbulent reactive flow environment characterized by localized temperature and/or mixture concentration inhomogeneities, which can act as preferential sites for ignition.

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