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A Fundamental Mathematical Theory in the Dynamics of Combustion Processes

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This research project has emphasized the formulation of rational mathematical models for transient and steady combustion processes. In particular thermal explosions, detonation wave initiation and high speed combustion waves have been examined. In each case the describing mathematical system is analyzed using both formal and constructive techniques. The former are employed to consider issues of existence and uniqueness, solution bounds and general trajectory properties. Constructive solution development is based on a combination of asymptotic and numerical methods. This hybrid approach to the study of combustion problems has permitted us to develop both a rigorous and quanitative under-standing of complex, initial-boundary value problems. This report contains a summary description of each of the 15 papers contributed by the research group. Keywords;

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1. Introduction

The dynamic effects of combustion arise from the thermomechanical response of a compressible medium to localized heat addition. Thermal expansion of a fluid element, caused by a rapidly rising temperature, induces wave-phenomena into the surrounding material. One may observe acoustic fields, weak or strong shock waves, depending upon the time scale of heat addition. The interaction between the chemical processes and the induced gasdynamic phenomena are essential to an understanding of ignition, explosion, high speed deflagrations, detonations, and transition of flames to detonations. These topics are integral to the study of accidental explosions, premature ignition of explosives, blast damage caused by large fires and internal combustion engine knock, to name a few examples.

During the 3–year period of our research program, dealing with the dynamics of combustion, we have focused on the following areas:

(1) Source theory for shock wave generation in inert and reactive compressible gas mixtures including detonation wave initiation.

(2) Evolution of an autoignited thermal explosion in a confined reactive, compressible gas beyond the induction period.

(3) High speed steady combustion waves with complex chemical kinetics.

The studies in (1) and (2) are fundamentally transient in character and closely related in terms of conceptual development. They comprise an organized effort to model the basic physical processes occurring in dynamical combustion events. Initial-boundary value problems are formulated for each system. Solutions describe the transient response of the system, and permit one to predict which type of combustion process evolves on relatively long time scales. For example, interest is focused on the factors that lead to flame initiation accompanied by acoustics in a given configuration, in contrast to those associated with the generation of a detonation wave in the same system.

The study of high speed combustion waves in (3) emphasizes the interaction of complex chemical kinetics with a steady compressible flow. Chain branching and termination, as well as high temperature dissociation and recombination are incorporated in the modeling in order to emulate processes in H_2-O_2 and hydrocarbon systems.

Mathematical modeling is based on the general describing equations for a reactive, com-

pressible mixture of perfect gases including transport effects. Formal methods of analysis are used to study solution properties including uniqueness, long-time evolution, sensitivity to essential parameters and bounds. Limit processes, derived from perturbation analysis, are used to construct rational approximations to the complete equations, for various parameter values. Solutions, constructed in terms of asymptotic expansions appropriate for problems exhibiting disparate time and length scales, describe the complete time-history of spatially distributed processes. This approach to dynamical combustion problems complements the complete computational treatment of the full equations. It provides general parameter dependence of solutions and "benchmarks" to be used for testing complex code reliability. The latter issue is of importance because the discretized form of the mixed parabolic–hyperbolic systems, describing dynamical combustion, can generate a variety of extraneous nonphysical phenomena which are difficult to detect solely by numerical testing.

Progress in each of the three specified research areas is described below. More detailed information is available in the summary descriptions given in Section 2 or in the publications themselves listed in Section 3.

Major accomplishments of our detonation wave initiation work include:

(a) development of a robust implicit Navier–Stokes solver capable of providing reliable solutions for reactive, compressible flows with transport effects.

(b) characterization of initiation of detonation in a reactive gas by boundary power deposition.

(c) development of a robust MacCormak scheme for the reactive Euler equations and solution generation for volumetric power deposition initiation of reactive gasdynamics.

(d) in preparation for studying reactive wave initiation in compressing gases, mathematical methods have been developed to study the dynamic compression of a gas in a cylinder.

Major accomplishments in our work on thermal explosions include:

(a) a unified theoretical formulation for diffusive and nondiffusive thermal explosions.

(b) an exact solution for a class of nondiffusive thermal explosion IBV problems, which inccludes examples of global rather than pointwise blow-up.

(c) a mathematical model for reaction transients in a gas with dissociation–recombination chemical kinetics.

(d) a precise description of where thermal explosions are located for gaseous reactive–diffusive

ignition models showing that global blow-up can occur for certain types of reactions.

(e) a description of how the thermal explosion singularity evolves for rigid reactive–diffusive models.

Major accomplishments in the study of high speed steady combustion waves include:

(a) the modeling of initiation of hig speed reaction waves in a compressible reactive gas with transport effects.

(b) the discovery that non-Chapman–Jouguet conditions exist in high speed reaction zones when the chemistry leads to reductions in the mixture mole number as the reaction evolves.

2. Research Activities: A Summary

During the 34–month lifetime of the research project described in this Final Report the participants published 15 articles in peer-judged journals covering the fields of combustion science, fluid mechanics and applied mathematics. In addition two additional manuscripts have been submitted for publication. The principle investigators and their students have given a total of nearly 50 technical presentations at colloquia, meetings, seminars and short courses. Both Profs. Bebernes and Kassoy held NATO Cooperative Research Grants during the grant period that fostered international cooperation with research colleagues abroad.

Outreach activites of Prof. J. Bebernes include:

1. Invited talk, EQUADIFF 6, Czechoslovak Academy of Sciences, Brno, August 1985.
2. Invited talk, Instituto di Matematica Applicata, Universitá di Padova, Padova, January 1986.
3. Visiting Professor, University of Wyoming, January–June 1986.
4. Invited Lecturer, 3 Lectures, Department of Mathematics, Univ. of Utah, November 1986.
5. Awarded Faculty Fellowship, 1986–87, University of Colorado.
6. Invited Lecture, Nonlinear Workshop, BYU, Provo, Utah, March 1987.
7. Invited Lecture, Dept. of Mathematics, BYU, Provo, Utah, March 1987.
8. Invited Lecture, Dept. of Mathematics, Utah State, March 1987.
9. Talk, NATO Advanced Research Workshop on Mathematical Modeling in Combustion, Lyon, France, April 1987.
10. Invited Lecturer, Institut Mathématique, Université Catholique de Louvain, Belgium, April–May, 1987.
11. Keynote Lecturer, Belgian Mathematical Society, Hasselt, Belgium, May 1987.
12. Invited Lecture, Departmento de Matemáticas, Universidad Complutense de Madrid, Spain, May 1987.

13. Invited Lecture, Joint USA/Japan Workshop on Mathematical Combustion, Juneau, Alaska, August 1987.

14. Invited Talk, Mathematics Dept., Colorado State Univ., Fort Collins, November 1987.

15. Invited Lecture, Dept. of Mathematics, Univ. of Pittsburgh, Pittsburgh, March 1987.

16. Invited Lecturer, Special Year on Reaction–Diffusion, Dept. of Mathematics, Heriot–Watt Univ., Edinburgh, Scotland, May 1988.

17. Invited Lecture, Dept. of Phys. Chemical, Univ. Leeds, Leeds, England, May 1988.

Outreach activities of Prof. D. R. Kassoy include:

1. "Mathematical Methods for Combustion Modeling": A series of 12 lectures. Department of Aeronautical Engineering, University of Nagoya, Nagoya, Japan, 6/10–20/85.

2. "Unified Theory of Low and High Speed Flames," University of Tokyo, Dept. of Reaction Chemistry, 6/24/85.

3. Saitoma University, Mechanical Engineering Department, Tokyo, Japan, 6/25/85.

4. "Unified Theory of Low and High Speel Flames," and "Unified Chain-Branching & Thermal Explosion Theory," Tsukuba University, Engineering Mechanics Institute, Japan, 6/26/85.

5. "Detonation Wave Initiation by Rapid Energy Deposition at a Confining Boundary," 10th International Colloquium on Dynamics of Explosions and Reactive Systems, 8/?/85.

6. "The Status of Thermal Explosion Singularity Modeling," International Workshop on Mathematics in Combustion, 8/12/85.

7. "Compression of a Confined Inert Gas by a Piston," American Physical Society, Fluid Dynamics Division, Tucson, Arizona, 11/24/85.

8. "Compression of an Inert Gas in a Cylinder by a Piston," University of East Anglia, Norwich, England, 11/29/85; and Cranfield Institute of Technology, Cranfield, England, 12/4/85.

9. "Detonation Wave Initiation by Rapid Energy Deposition at a Confining Boundary," 4th Army Conference on Applied Mathematics and Computing, Ithaca, New York, May 28–30, 1986.

10. "Detonation Wave Initiation," International Workshop on Mathematics in Combustion, Garmisch–Parten–Kirchen, Germany, August 9–11, 1986.

11. "Subsonic High Speed Reaction Zone Structure for Variable Mole Chemistry," Western States Combustion Institute Meeting, Tucson, Arizona, October 27–29, 1986.

12. "Compression of a Confined Inert Gas by a Piston," Fluid Dynamics Division of the American Physical Society, November 23–25, 1986.

13. "Structure of a Planar High Speed Reaction Zone," Fluid Dynamics Divison of the American Physical Society, November 23–25, 1986.

14. "Initiation of Gasdynamics by Intense Power Deposition," Computational Mathematics Group, C.U.–Denver, 2/17/87.

15. "Detonation Wave Initiation by Energy Deposition at a Boundary," invited presentation, Minisymposium I, SIAM Conference on Numerical Combusion, San Francisco, 3/10/87.

16. "Modeling the Early Phases of Planar Detonation Wave Initiation," 2nd ASME–JSME Thermal Engineering Joint Conference, Honolulu, 3/24/87.

17. "High Speed Reactioan Zone Structure for Variable Mole Chemistry," Mathematical Sciences Institute, Cornell University, Ithaca, 5/4/87.

18. "High Speed Reaction Zone Structure for Variable Mole Chemistry," 11th International Colloquium on Dynamics of Explosions and Reactive Systems, Warsaw, Poland, 8/5/87.

19. "Detonation Wave Initiation and Related Ignition Phenomena," 8th International Workshop on Mathematics in Combustion, Warsaw, Poland, 8/4/87.

20. "Studies Related to Planar Detonation Initiation and Straucture" and "Formulation of Diffusive and Nondiffusive Thermal Explosion Theory," JOint "USA/Japan Seminar on Mathematical Modeling in Combustion Science, Alaska, 8/81/87 and 8/19/87.

21. "Diffusive and Nondiffusive Thermal Explosions," Mathematics Department, University of Colorado, 9/3/87.

22. "Detonation Wave Initiation by Power Deposition: Numerics and Asymptotics," SIAM 35th Anniversary Meeting, 10/13/87.

23. "A Unified Formulation for Diffusive and Nondiffusive Thermal Explosions, University of California at San Diego, 4/20/88; and University of Southern California, 4/22/88.

3. Publications

Summaries of each of the published and submitted articles follow:

J. Bebernes, D. Eberly, and W. Fulks, "Solution profiles for some simple combustion models," *Nonlinear Analysis: Theory, Methods and Applications*, 10 (1986), 217–228.

Using phase space techniques, the solution shapes for the Gelfand problem $-\Delta u = \delta e^u$ and the perturbed Gelfand problem $-\Delta u = \delta \exp\left(\frac{u}{1+\epsilon u}\right)$, $\delta > 0$, $\epsilon > 0$ are analyzed. Both of these models play a fundamental role in the mathematical theory of thermal explosions for finite rigid and gaseous systems. For rigid systems the physical processes are determined by a pointwise balance between chemical heat addition and heat loss by conduction. During the inductive period, with a duration measured by the conduction time scale of the bounding container, the heat released by the chemical reaction is redistributed by thermal conduction. As the temperature of the container increases, the reaction rate grows dramatically. Eventually the characteristic time for heat release becomes significantly smaller than the conduction time in a well-defined hot spot embedded in the system. Then the heat released is used almost entirely to increase the hot spot temperature. Both the models studied detect this hot spot development in a very precise manner. For example, for a ball $B_1 \subset \mathbb{R}^3$, the minimal solution of the Gelfand problem is bell-shaped, that is, exhibits the hot spot, for a range of parameter values δ, $\bar{\delta} < \delta < \delta^*$. When $0 < \delta < \bar{\delta}$, the physically significant minimal solution is concave down while all other solutions are bell-shaped. Here δ^* is the Frank–Kamenetskii critical value and $\bar{\delta}$ is a uniquely determined parameter value.

J. Bebernes, "Solid Fuel Combustion–Some Mathematical Problems", *Rocky Mountain J. Math.*, 16 (1986), 417–433.

The initiation of a combustion process involves a myriad of complex physical phenomena which are fascinating to observe and challenging to describe in quantitative terms. In general one is concerned with the time-history of a spatially varying process occurring in a deformable material in which there is a strong interaction between chemical heat release, diffusive effects associated with the transport properties, bulk material motion as well as several types of propagating wave phenomena. Mathematical models capable of describing these combustion systems incorporate not only familiar reaction–diffusion effects associated with rigid materials, but those arising from material compressibility as well. For a combustible gas, the complete reactive Navier–Stokes equations are required to describe the phenomena involved.

In this paper, we shall focus on the *initiation and evolution of thermal explosion processes* in rigid materials. In this situation the physical processes are determined by a pointwise balance between chemical heat addition and heat loss by conduction.

J. Bebernes and D. Kassoy, "Solution profiles and thermal runaway," *Lecture in Applied Mathematics*, 24 (1986), 217–228.

This is an expository description of how thermal runaway occurs for the induction period *model of a high activation energy thermal explosion* in a bounded container. Assuming a slab geometry, the temperature perturbation $\theta(x,t)$ (solution of (*) $\theta_t = \Delta\theta + \delta e^\theta$) blows up at a single point $x = 0$ as $t \to T$ and $\theta(x,t) \to \theta_e(x)$ for $0 < x \le 1$. In principle $\theta_e(x)$ is found from an initial value numerical solution of (*). Assuming $\theta_e(x)$ as a known quantity, a final value theory for this problem is described. This allows one to predict the shape of the temperature $\theta(x,t)$ in a neighborhood of the singularity.

J. F. Clarke, D. R. Kassoy and N. Riley, "On the direct initiation of a plane detonation wave," *Proc. Royal Soc. London* A408 (1986), 129–148.

It is assumed that energy is transferred at a rapid rate through a plane wall into a spatially uniform and initially stagnant combustible gas mixture. This action generates a shock wave, just as it does in an inert mixture, and also switches on a significant rate of chemical reaction. The Navier-Stokes equations for plane unsteady flow are integrated numerically in order to reveal

the subsequent history of event. Four principal time domains are identified, namely 'early', 'transitional', 'formation', and 'ZND/. The first contains a conduction-dominated explosion and formation of a shock wave; in the second interval the shock wave is reponsible for the acceleration of chemical activity, which becomes intense during the 'formation' period. Finally a wave whose structure is in essence that of a ZND detonation wave emerges.

<u>J. Bebernes, A. Bressan, and D. Eberly</u>, "An asymptotic description of blow-up," *Indiana Univ. J. Math.* 36 (1987), 295–305.

The purpose of this paper is to give a precise description of the asymptotic behavior of a radially symmetric solution $u(x,t)$ of

$$(I) \qquad\qquad u_t - \Delta u = e^u$$

in a neighborhood of the blow-up point as t approaches the finite blow-up time $T < \infty$ provided $x \in B_R \equiv \{x : |x| < R\} \subset I\!\!R^n$ and $n = 1$ or 2. Giga and Kohn recently characterized the asymptotic behavior of the solution $u(x,t)$ of

$$(II) \qquad\qquad u_t - \Delta u = u^p, \qquad \Omega \subset I\!\!R^n$$

near a blow-up singularity assuming a suitable upper bound on the rate of blow-up, provided $n = 1, 2$ or $n \geq 3$ and $p \leq \frac{n+2}{n-1}$. For $\Omega = B_1 \subset I\!\!R^n$, in light of recent *a priori* bounds established by Freedman and McLeod, this implies that the solution $u(x,t)$ of (H) with suitable initial and boundary conditions satisfies

$$(T - t)^\beta u(|x|,t) \to \beta^\beta \quad \text{as} \quad t \to T^-$$

provided $0 \leq |z| \leq C(T - t)^{1/2}$ for some C and $\beta = \frac{1}{p-1}$.

For (I) we prove that the solution $u(x,t)$ satisfies

$$u(x,t) - \ell n \frac{1}{T - t} \to 0$$

uniformly on $0 \leq |x| \leq C(T - t)^{1/2}$, $C > 0$, as $t \to T^-$.

Equation (I) is the ignition period model for the thermal explosion of a nondeformable material of finite extent undergoing a single-step exothermic reaction. This model neglects

the consumption of fuel and describes the temperature u at any time and at any point in the bounded container. For $R > 0$ sufficiently small, the temperature $u(x,t)$ becomes unbounded in the L^∞-sense as t approaches a finite blow-up time T and the blow-up occurs at a single point, the center of the ball B_R.

Our main result gives a precise description of how the blow-up asymptotically behaves. The proof is valid only in dimensions 1 and 2. The real difficulty in understanding the blow-up for (I) lies in determining the nonincreasing globally Lipschitz continuous solutions of the associated steady-state equation

$$(K) \qquad\qquad y'' + \left(\frac{n-1}{\eta} - \frac{\eta}{2}\right) y' + e^y - 1 = 0$$

on $[0, \infty)$ where $y'(0) = 0$, $y(0) = \alpha \geq 0$. For $n = 1$ Bebernes and Troy proved that the only such solution is $y \equiv 0$.

Kassoy–Poland and Kapila in earlier papers derived (K) from an asymptotic final time analysis of (I) and predicted on the basis of numerical calculations the existence of a solution of (K) which satisfies the asymptotic condition $y(\eta) \sim -2\ell n\eta + K_o$ as $\eta \to \infty$. This implies the existence of a globally Lipschitz continuous solution of (K). Our result shows that, for $n = 1$ and 2, their final time analysis is incomplete. More precisely, we remark that: i) their derivation of the asymptotic condition is incorrect, and ii) the space variable in the inner expansion $\eta = x/\sqrt{T-t}$ is stretched too much so that no information concerning the spatial behavior of the solution is retained in the limit. This leaves open the problem of finding a different rescaling of the space coordinates for which in the limit a non-constant behavior of solutions can still be observed.

J. Bebernes and W. Troy, "Nonexistence for the Kassoy problem," *SIAM J. of Math. Analysis*, 18 (1987), 1157–1162.

When blow-up or thermal runaway occurs in finite time for the thermal explosion of a nondeformable material, the developing hot spot becomes unbounded at a single point of the container if it is radially symmetric. These supercritical processes which are characterized by the appearance of this singularity at a finite time T have been considered earlier by Kassoy–Poland and Kapila. Using computational methods for symmetric slab, cylindrical, and spherical geometries, they predict that $\theta(x,t)$ becomes unbounded at the symmetry point $x = 0$ at time

T. Elsewhere $\theta(x,t) \to \theta_e(x)$, $x \in \Omega$, $x \neq 0$, as $t \to T$. By applying a final-value asymptotic analysis at T, they predict the character of the singularity function $\theta_3(x)$. This prediction is based on the existence of a nontrivial solution of $y'' = \frac{x}{2}y' + e^y - 1 = 0$, $y'(0) = 0$, and $y(x) \sim -2\ell nx + c$ as $x \to \infty$. By using connectedness and shooting technique arguments, we prove that no such solution can exist. This means a more detailed analysis of the blow-up singularity is required and this has been done in subsequent papers.

J. Bebernes and W. Troy, "Existence for the modified Kassoy problem," *Proc. Royal Soc. Edinburgh*, 106A (1987), 131–136.

In this paper, the differential equation

$$(1) \qquad\qquad y'' - \frac{x}{2}y' + e^y - 1 = 0$$

with

$$(2) \qquad\qquad y(0) = \alpha, \qquad y'(0) = \beta$$

is considered. Solutions to (1)–(2) are sought which have the asymptotic property $y(x, \alpha, \beta) \sim -2\ell nx + K_\alpha$ as $x \to \infty$. We prove that there exists $\bar{\alpha} > 0$ such that for each $0 \leq \alpha \leq \bar{\alpha}$, there is at least one $\beta(\alpha) < 0$ such that (1)–(2) has a solution $y(x, \alpha, \beta)$ with the desired asymptotic property.

J. Bebernes, A. Bressan, and A. Lacey, "Total blow-up versus single point blow-up," *J. Differential Equations*, 73 (1988), 30–44.

Traditional thermal explosion theory is used to describe reaction initiation in condensed explosives and is limited formally to nondeformable materials. Kassoy and Poland significantly extended this theory to develop an ignition model for a reactive gas in a bounded container in order to describe the induction period. During this induction period there is a spatially homogeneous pressure rise in the system which causes a compressive heating effect in the constant volume container. Mathematically this compressibility of the gas is expressed by means of an integral term in the induction model for the temperature perturbation $\theta(x,t)$. This model is given by

$$(D) \qquad\qquad \theta_t - \Delta\theta = \delta e^\theta + \frac{\gamma - 1}{\gamma} \cdot \frac{1}{\mathrm{vol}\,\Omega} \int_\Omega \theta_t(x,t)dx$$

and (D)

Bebernes and Bressan analyzed earlier ignition model (D) for a compressible gas and proved: For any $\delta > 0$ and any $\gamma \geq 1$, (D) has a unique classical solution $\theta(x, t)$ on $\Omega \times [0, T)$ where $\Omega \subset I\!\!R^n$ is a bounded container and $T < +\infty$ or $T = +\infty$. In the latter case, $\theta(x, t)$ blows up as t approaches T. If $\delta > \delta_{FK}$, the Frank–Kamenetski critical value, then $T < \infty$ and blow-up or thermal runaway occurs in finite time.

In this paper, a description of where blow-up occurs in the given container Ω is given for the more general problem

$$u_t - \Delta u = f(u) + g(t)$$

(G)
$$u(\ ,0) = \phi(x), \quad x \in \Omega$$

$$u(x, t) = 0, \qquad x \in \partial\Omega, \quad t > 0.$$

If Ω is a ball of radius R in $I\!\!R^n$ and blow-up occurs at finite time T, then:

I) If $\int_0^T g(T)dt = +\infty$, then blow-up occurs everywhere.

II) If $\int_0^T g(t)dt < +\infty$ and $f(u) = e^u$ or $f(u) = (u + \lambda)^p$, $\lambda \geq 0$, $p > 1$, then blow-up occurs only at $x = 0$.

III) If $g(t) = \frac{K}{\text{vol}\,\Omega} \int_\Omega u_t(x, t)dx$, $K < 1$, and $f(u) = (u + \lambda)^p$, $\lambda \geq 0$, $1 < p < 1 + 2/n$, then blow-up occurs everywhere.

IV) If $g(t) = \frac{K}{\text{vol}\,\Omega} \int_\Omega u_t(x, t)dx$, $K < 1$, and $f(u) = e^u$, then blow-up occurs at a single point.

V) If $g(t) = \frac{K}{\text{vol}\,\Omega} \int_\Omega u_t(x, t)dx$ and $f(u) = (u + \lambda)^p$, $\lambda \geq 0$, $p > 1 + 2/n$, then blow-up occurs only at $x = 0$ provided $K < 1$ is sufficiently small.

J. Bebernes and D. Eberly, "A description of self-similar blow-up for dimensions $n \geq 3$," *Annales de l'Institut Henri Poincaré–Analyse non linéaire*, 5 (1988), 1–21.

The purpose of this paper is to give a precise description of the asymptotic behavior for solutions $u(z, t)$ of

(1)
$$u_t = \Delta u + f(u)$$

which blow-up in finite positive time T. We assume $f(u) = u^p$ $(p > 1)$ or $f(u) = e^u$, and $z \subset B_R = \{z \in I\!\!R^n : |z| < R\}$ where R is sufficiently large to guarantee blow-up.

Giga and Kohn recently characterized the asymptotic behavior of solutions $u(z, t)$ of (1) with $f(u) = u^p$ near a blow-up singularity assuming a suitable upper bound on the rate of blow-up and provided $n = 1, 2$, or $n \geq 3$ and $p \leq \frac{n+2}{n-2}$. For $B_4 \subseteq I\!\!R^n$ using recent *a priori* bounds established by Friedman–McLeod, this implies that solutions $u(z, t)$ of (1) with suitable initial-boundary conditions satisfy

$$(2) \qquad\qquad (T - t)^\beta u(z, t) \to \beta^\beta \quad \text{as} \quad t \to T^-$$

provided $|z| \leq C(T - t)^{1/2}$ for arbitrary $C \geq 0$ and where $\beta = \frac{1}{p-1}$.

For $f(u) = d^u$ and $n = 1$ or 2, Bebernes, Bressan, and Eberly proved that solutions $u(z, t)$ of (1) satisfy

$$(3) \qquad\qquad u(z, t) + \ln(T - t) \to 0 \quad \text{as} \quad t \to T^-$$

provided $|z| \leq C(T - t)^{1/2}$ for arbitrary $C \geq 0$.

The real remaining difficulty in understanding how the single point blow-up occurs for (1) rests on determining the nonincreasing globally Lipschitz continuous solutions of an associated steady-state equation

$$(4) \qquad\qquad y'' + \left(\frac{n-1}{x} - \frac{x}{2} \right) y' + F(y) = 0, \quad 0 < x < \infty$$

where $F(y) = y^p - \beta y$ or $e^y - 1$ for $f(y) = y^p$ or e^y respectively and where $y(0) > 0$ and $y'(0) = 0$.

For $F(y) = y^p - \beta y$ in the cases $n = 1, 2$, or $n \geq 3$ and $p \leq \frac{n}{n-2}$, we give a new proof of a special case of a known result that the only such positive solution of (4) is $y(x) \equiv \beta^\beta$. For $F(y) = e^y - 1$ and $n = 1$, Bebernes and Troy proved that the only such solution is $y(x) \equiv 0$. Eberly gave a much simpler porof showing $y(x) \equiv 0$ is the only solution for the same nonlinearity valid for $n = 1$ and 2.

For $3 \leq n \leq 9$, Troy and Eberly proved that (4) has infinitely many nonincreasing globally Lipschitz continuous solutions on $[0, \infty)$ for $F(y) = e^y - 1$. Troy proved a similar multiplicity result for (4) with $F(y) = y^p - \beta y$ for $3 \leq n \leq 9$ and $p > \frac{n+2}{n-2}$.

This multiple existence of solutions complicates the stability analysis required to precisely describe the evolution of the time-dependent solutions $u(z, t)$ of (1) near the blow-up singularity.

In this paper we extend the results of Giga–Kohn and Bebernes–Bressan–Eberly to the dimensions $n \geq 3$ by proving that, in spite of the multiple existence of solutions of (4), the asymptotic formulas (2) and (3) remain the same as in dimensions 1 and 2. The key to unraveling these problems is a precise understanding of the behavior of the nonconstant solutions relative to a singular solution of (4) given by

$$(5) \qquad\qquad S_e(x) = \ln \frac{2(n-2)}{x^2}$$

for $f(u) = e^u$ and $n \geq 3$, and

$$(6) \qquad\qquad S_p(x) = \left\{ -4\beta \left[\beta + \frac{1}{2}(2-n) \right] / x^2 \right\}$$

for $f(u) = u^p$ and $\beta + \frac{1}{2}(2-n) < 0$, $n \geq 3$. This will be accomplished by counting how many times the graphs of a nonconstant self-similar solution crosses that of the singular solution.

M. A. Birkan, C. K. Law and D. R. Kassoy, "Transient decomposition–recombination dynamics of dissociating and ioninzing gases," *Proc. Royal Soc. London* A418 (1988), 331–343.

A generic gas AB, initially at a relatively high temperature, undergoes a spatially homogeneous, constant-volume decomposition–recombination reaction represented by $AB + M \rightleftarrows A + B + M$. The complete time-history of this variable temperature reaction is calculated by employing high activation energy asymptotic analysis developed originally for thermal explosion problems. The evolution of the reaction is described in terms of an initiation period with small changes in the mixture temperature and composition, a longer major decomposition period during which most of the conversion of AB to A and B occurs, and an extended final period during which recombination becomes important as the system relaxes to the equilibrium state. Explicit timescales are derived for each of the distinct reaction processes. The analytically derived solution agrees quantitatively with the numerical solution and qualitatively with experimental results.

D. R. Kassoy, A. K. Kapila and D. S. Stewart, "A unified formulation for diffusive and nondiffusive thermal explosion theory," *Combustion Science and Technology*, in press (1988).

A mathematical model is developed for the induction period of a parcel of slightly warm reactive gas mixture embedded in a cooler gaseous environment. High activation energy asymp-

totic methods are used to formulate the problem. The important parameters in the nondimensional equations are ratios of characteristic reaction, acoustic and conduction times in the thermally distrubed parcel of dimension ℓ'. The results of the formulation imply that a specified physicochemical system, with a known characteristic chemical time, will experience a traditional diffusively dominated thermal explosion if the dimension ℓ' is sufficiently small. In larger systems transport effects are negligible and the induction period process is dominated by reactive gasdynamic equations. The study provides a unified formulation for the induction period of all thermal reaction problems and specifies the relationship between classical thermal explosion theory for rigid materials and compressible gases and more contemporary efforts to study nondiffusive thermal reactions.

D. R. Kassoy, N. Riley, J. Bebernes and A. Bressan, "The confined nondiffusive thermal explosion with spatially homogeneous pressure variation," *Combustion Science and Technology*, in press (1988).

A solution is developed for a nondiffusive thermal explosion in a reactive gas confined to a bounded container Ω with a characteristic length ℓ'. The process evolves with a spatially homogeneous time-dependent pressure field because the characteristic reaction time t'_R is large compared to the acoustic time ℓ'/C'_0 where C'_0 is the initial sound speed. Exact solutions, in terms of a numerical quadrature are obtained for the induction period temperature, density, and pressure perturbations as well as for the induced velocity field. Traditional single-point thermal runaway singularities are found for temperature and density when the initial temperature disturbance has a single point maximum. In contrast, if the initial maximum is spread over a finite subdomain of Ω, then the thermal runaway occurs everywhere. Asymptotic expansions of the exact solutions are used to provide a complete understanding of the singularities. The perturbation temperature and density singularities have the familiar logarithmic form $-\ln(t'_e - t')$ as the explosion time t'_e is approached. The spatially homogeneous pressure is bounded for single-point explosions but is logarithmically singular when global runaway occurs. Compression heating associated with the unbounded perturbation pressure rise is the physical source of the global thermal runaway.

K. Kirkkopru and D. R. Kassoy, "Induction zone structure of a high-speed deflagration with variable mole chemistry," *The Physics of Fluids*, in press (1988).

The induction zone characteristics of a planar subsonic high-speed reactive flow downstream of a specific origin is investigated theoretically for the global irreversible reaction $F + Ox \rightarrow \nu P$. The equation of state for the reacting gas mixture is more general than that for a constant molecular weight gas. Perturbation methods based on the limit of high activation energy are used to construct the general parameter dependent analytical solutions. The dependence of the ignition delay distance on the kinetic, stoichiometric and flow parameters is discussed in detail. Significantly, it is shown that the maximum ignition delay distance when the chemical heat addition and the origin values of parameters are fixed. The physics and length scales found from the perturbation analysis are used as a guide in generating supporting numerical solutions.

J. Bebernes and D. Eberly, "Characterization of blow-up for a semilinear heat equation with a convection term," *Quarterly J. Mech. Math.*, accepted (1988).

Let $\Omega \subset \mathbb{R}^n$ be a bounded domain with smooth boundary $\partial\Omega$. Consider the initial-boundary value problem

$$
\begin{aligned}
u_t &= \Delta u + f(x,t,u), & (x,t) \in \Omega \times (0,T), \\
u(x,0) &= u_0(x) \geq 0, & x \in \Omega, \\
u(x,t) &= 0, & (x,t) \in \partial\Omega
\end{aligned}
\tag{1}
$$

where $u_0(\partial\Omega) = 0$. Assuming that there is local existence of a classical solution of (1), a recent active area of interest has been to determine and characterize how solutions of (1) cease to exist. For a large class of nonlinearities, solutions cease to exist by becoming unbounded in some norm as a maximal time T is approached. This phenomenon is called *blow-up*.

In particular, the following problems arise naturally when considering the blow-up of solutions and have been considered by various authors for special nonlinearities f.

Problem 1. Find the maximal $T \in (0, \infty]$ for which a classical solution to (1) exists and determine when

a. $T = \infty$ and $u(x,t)$ is finite on $\bar{\Omega} \times [0, \infty]$, or,

b. $T \leq \infty$ and $\| u \| \rightarrow \infty$ as $t \rightarrow T^-$ for some norm.

Problem 2. Describe the set of blow-up points $B \subseteq \Omega$. A point $x_0 \in \Omega$ is a *blow-up point* for (1) if there is a sequence $\{(x_m, t_m)\}_{m=1}^{\infty}$ such that $t_m \to T^-$, $x_m \to x_0$, and $u(x_m, t_m) \to \infty$ as $m \to \infty$.

Problem 3. Describe the asymptotic behavior of $u(x, t)$ as $t \to T^-$. In particular, at a blow-up point x_0, describe how the blow-up singularity evolves with the ultimate goal being to describe the space profile of $u(x, T)$ in the neighborhood of an isolated blow-up point.

Problem 4. For $t > T$, one can determine what happens to the solution $u(x, t)$ of (1) in some "weak solution" sense.

If one considers the more general semilinear parabolic problem

$$u_t = \Delta u + F(x, t, u, \nabla u), \qquad (x, t) \in \Omega \times (0, T)$$

$$u(x, 0) = u_0(x) \geq 0, \qquad x \in \Omega \qquad (2)$$

$$u(x, t) = 0, \qquad (x, t) \in \partial\Omega \times (0, T),$$

then Problems 1 through 4 remain essentially open. For the special case where $F(x, t, u, \nabla u) = |u|^{p-1}u - |\nabla u|^q$ with $p > 1$ and $q > 1$, Chipot and Weissler have given conditions under which solutions blow up in the L_∞-norm in finite time T. In this case, the gradient term has a damping effect working against blow-up, so these results become more delicate to establish. A critical splitting of q given by $\frac{2p}{p+2}$ gives a change in the behavior for this problem. Chipot–Weissler study the case $1 < q \leq \frac{2p}{p+2}$.

In this note we consider a second special case of (2), namely

$$u_t \Delta u + e^u - |\nabla u|^2, \qquad (x, t) \in \Omega \times (0, T),$$

$$u(x, 0) = u_0(x) \geq 0, \qquad x \in \Omega, \qquad (3)$$

$$u(x, t) = 0, \qquad (x, t) \in \partial\Omega \times (0, T).$$

which can be viewed as the limiting case of the critical splitting as $p \to \infty$ in the problem considered by Chipot and Weissler. Becaue of the special form of the nonlinearity, we can give very precise answers to the stated problems 1 through 4.

The keys to our analysis are two simple observations. First, the change of variable $v = 1 - e^u$ transforms IBVP (3) into the equivalent problem

$$v_t = \Delta v + 1, \qquad (x, t) \in \Omega \times (0, T),$$

$$v(x, 0) = v_0(x), \qquad x \in \Omega, \qquad (4)$$

$$v(x, t) = 0, \qquad (x, t) \in \partial\Omega \times (0, T),$$

where $v_0(\partial\omega) = 0$ and $v_0(x) = 1 - \exp(u_0(x)) < 1$. Second, a point $x_0 \in \Omega$ is a blow-up point for (3) with blow-up time T if and only if $v(x_0, T) = 1$ at some first time T. The associated steady-state problem for IBVP (4) is

$$\Delta p + 1 = 0, \quad x \in \Omega,$$
$$p(x) = 0, \qquad x \in \partial\Omega. \tag{5}$$

It is well-known that IBVP (4) and BVP (5) have unique solutions $v(x,t)$ and $p(x)$, respectively. It is also known that $\lim_{t\to\infty} v(x,t) = p(x)$ uniformly for $x \in \bar{\Omega}$.

We first look at the problem of when blow-up occurs. As we have observed, blow-up occurs at $x_0 \in \Omega$ at time T for IBVP (3) if and only if $v(x_0, T) = 1$ at some first time T. Thus, we need only determine conditions which force the solution $v(x,t)$ of (4) to attain the value 1. If we can show that the steady-state solution $p(x)$ of BVP (5) attains the value one for some $x \in \Omega$, then blow-up must occur for IBVP (3).

K. Kirkkopru and D. R. Kassoy, "High-speel reaction zone structure for variable mole chemistry," *SIAM J. Applied Math.*, submitted (1988).

The structure of a high-speed deflagration downstream of a specific origin is investigated theoretically for the global irreversible Arrhenius type reaction $F + Oz \to \nu P$. Attention is focused on the effect of the stoichiometric coefficient value ν on the high-speed reaction zone characteristics. Perturbation and numerical methods are used to find solutions. In the rapid reaction region beyond the induction zone, there is a strong interaction between large chemical heat release and flow compressibility. When the chemical reaction causes a mole reduction ($\nu < 2$) and there is sufficiently large heat release, the flow velocity reaches a maximum and then declines while the temperature increases monotonically throughout the process. Significnatly, it is shown that the flow cannot evolve to the Chapman–Jouguet (C.J.) state where the final local Mach number is unity and the reactant concentration is zero. When the mole number of the evolving flow is constant or increasing ($\nu \geq 2$), the flow velocity always increases and a final C.J. state can develop when the right amount of chemical heat addition is available for a given input Mach number at the origin.

4. Scientific Personnel

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