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This grant to supported the salary Mark Short as a Research Associate to work with D. S. -Stewart, for a period of up to three years and one month of Prof. Eliot Fried's salary, plus travel of Short and various supported graduate students, and miscellaneous fund. In the Fall of 1998, Mark Short became an Assistant Professor in the Department of Theoretical and Applied Mechanics and the funds in this grant were used (with permission) to support Prof. Short's summer salary, and provide funds for support of a graduate student to work with Short and or Stewart. The research of the carried out by this grant was on the I) analytical theory of detonation stability and II) development of new models for description of the mechanical ignition of condensed explosives. The research directly and indirectly supported a separate effort at UIUC on the engineering design of explosive systems, specifically condensed phase explosives and the use of related numerical technologies. This other grant is funded by USAFRL Wright/Laboratory Amarment Directorate (D. S. Stewart PI). The main research findings are represented in a series of papers on detonation stability and dynamics by Short and Stewart and the development of a new continuum mechanical model for condensed energetic materials that uses phase-field theory by Ruderman/Stewart and Fried. A description of all the main papers, where the papers appeared is included in thc main body of the report.

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Final Report

Analytical Investigations on Detonation Theory and Mechanical Ignition of Explosives

AFOSR Grant No. F49620-96-1-0260
Dr. Arje Nachman, Program Manager
Physical Mathematics and Applied Analysis
Directorate of Mathematical and Computer Sciences
United States Air Force Office of Scientific Research

6/1/96 - 9/30/99

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Abstract

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The main research findings are represented in a series of papers on detonation stability and dynamics by Short and Stewart and the development of a new continuum mechanical model for condensed energetic materials that uses phase-field theory by Ruderman/Stewart and Fried. A description of all the main papers and where they appeared is included in the main body of the report.

Introduction

This document is a final report for AFOSR Grant No. F49620-96-1-0260, Air Force Office of Scientific Research, Physical Mathematics and Applied Analysis, Dr. Arje Nachman, program manager. D. SCOTT STEWART, Principal Investigator (PI) in the Department of Theoretical and Applied Mechanics (TAM), carried out the work at the University of Illinois at Urbana-Champaign (UIUC). Herein the PI's group will be referred to as UIUC. The report is split into sections as follows.

Section 1. is a brief summary of the stated goals and objectives as represented in the original proposal.

Section 2. Includes the authors, titles, citation and abstracts of the papers written on this grant.

Section 3. is summary of supported personnel, published archival papers and Ph.D. theses.

Section 1. Summary of goals and objectives in the original proposal

Goals of the proposal

Substantial progress was made towards accomplishment of two of the stated goals in the original proposal:

• Completion of an analytically-based theory of detonation stability and evolution. Short/Stewart

• Analytic investigations and solutions to models of mechanical ignition of condensed explosive materials. Ruderman/Stewart/Fried

A third stated goal, to develop regularization theory derived from the modern interface theories of continuum mechanics applied to the self-propagating fronts, was not pursued in depth.

Section 2. Archival papers and Ph.D. theses

Below we list important papers written (in chronological order) that cite AFOSR funding. The abstract of each paper is reproduced here below the paper entry to summarize the research findings.

Published papers

1. Short, M. & Stewart, D.S. (1997) Low-frequency two-dimensional linear instability of plane detonation. J. Fluid Mech., 340, 249--295.

Abstract: An analytical dispersion relation describing the linear stability of a plane detonation wave to low-frequency two-dimensional disturbances with arbitrary wavenumbers is derived using a normal mode approach and a combination of high activation energy and Newtonian limit asymptotics, where the ratio of specific heats tends to one. The reaction chemistry is characterized by one-step Arrhenius kinetics. The analysis assumes large activation energy in the plane steady-state detonation wave and a characteristic linear disturbance wavelength, which is longer than the fire-zone thickness. Newtonian limit asymptotics are employed to obtain a complete analytical description of the disturbance behavior in the induction zone of the detonation wave. The analytical dispersion relation that is derived depends on the activation energy and exhibits favorable agreement with numerical solutions of the full linear stability problem for low-frequency one- and two-dimensional disturbances, even when the activation energy is only moderate. Moreover, the dispersion relation retains vitally important characteristics of the full problem such as the one-dimensional stability of the detonation wave to low-frequency disturbances for decreasing activation energies or increasing overdrives. When two-dimensional oscillatory disturbances are considered, the analytical dispersion relation predicts a monotonic increase in the disturbances growth rate with increasing wavenumber, until a maximum growth rate is reached at a finite wavenumber. Subsequently the growth rate decays with further increases in wavenumber until the detonation becomes stable to the two-dimensional disturbance. In addition, through a new detailed analysis of the behavior of the perturbations near the fire front, the present analysis is found to be equally valid for detonation waves traveling at the Chapman-Jouguet velocity and for detonation waves which are overdriven. It is found that in contrast to the standard imposition of a radiation or piston condition on acoustic disturbances in the equilibrium zone for overdriven waves, a compatibility condition on the perturbation jump conditions across the fire zone must be satisfied for detonation waves propagating at the Chapman-Jouguet detonation velocity. An insight into the physical mechanisms of the one- and two-dimensional linear instability is also gained, and is found to involve an intricate coupling of acoustic and entropy wave propagation within the detonation wave.

2. Short, M. (1997) A parabolic linear evolution equation for cellular detonation instability. *Combust. Theory Modell.* 1, 313--346.

Abstract: Using the combined limits of a large activation energy and a ratio of specific heats close to unity, a dispersion relation has recently been derived which governs the stability of a steady Chapman-Jouguet detonation wave to two-dimensional linear disturbances. The analysis considers instability evolution time scales that are long on the time scale of fluid particle passage through the main reaction layer. In the following, a simplified polynomial form of the dispersion relation is derived under an appropriate choice of a distinguished limit between an instability evolution time scale that is long on the time scale of particle passage through the induction zone and a transverse disturbance wavelength that is long compared to the hydrodynamic thickness of the induction zone. A third order in time, sixth order in space, parabolic linear evolution equation is derived which governs the initial dynamics of cellular detonation formation. The linear dispersion relation is shown to have the properties of a most unstable wavenumber, leading to a theoretical prediction of the initial detonation cell spacing and a wavenumber above which all disturbances decay, eliminating the growth of small-wavelength perturbations. The role played by the curvature of the detonation front in the dynamics of the cellular instability is also highlighted.

3. Buckmaster, J. D., Short, M. and Stewart, D. S. The use of activation energy asymptotics in detonation theory, with Comment on 'Multidimensional stability analysis of overdriven gaseous detonation; [*Phys. Fluids* **9**, 3764 (1997)]. *Physics of Fluids* **10**, 3027-3030.

Abstract. A powerful defense is given for the use of activation energy asymptotics in opposition to erroneous and misleading work carried out by Clavin and Williams.

4. Short, M. & Stewart, D.S. Cellular detonation stability: A normal mode linear analysis. *Journal of Fluid Mechanics*, **368**, 229-262 (1998).

Abstract: A detailed investigation of the hydrodynamic stability of a steady, one-dimensional detonation to transverse linear disturbances in an ideal gas undergoing an irreversible, unimolecular reaction with an Arrhenius rate constant is conducted via a normal-mode analysis. The method of solution is an iterative shooting method, which integrates between the detonation shock and reaction equilibrium point. Variations in the disturbance growth rates and frequencies with transverse wavenumber, together with two-dimensional neutral stability curves and boundaries for all unstable low- and high-frequency modes are obtained for varying detonation bifurcation parameters. These include the detonation overdrive, chemical heat release and reaction activation energy. Spatial perturbation eigenfunction behavior and phase and group velocities are also obtained for selected sets of unstable modes. Results are presented for both Chapman-Jouguet and overdriven detonation velocities. Comparisons between the earlier pointwise determination of stability and interpolated neutral stability boundaries obtained by Erpenbeck are made. Possible physical mechanisms which govern the wavenumber selection underlying the initial onset of either regular or irregular cell patterns are also discussed.

5. Short, M. and Stewart, D. S. The multi-dimensional stability of weak heat release detonations. *J. Fluid Mech., s382*, 109-135 (1999).

Abstract. The stability of an overdriven planar detonation wave is examined for a one-step Arrhenius reaction model with an order one post-shock temperature-scaled activation energy in the limit of a small post-shock temperature-scaled heat release. The ratio of specific heats, is taken to be close to one. Under these assumptions, which cover a wide range of realistic physical situations, the steady detonation structure can be evaluated explicitly, with the reactant mass fraction described by an exponentially decaying function. The analytical representation of the steady structure allows a normal-mode description of the stability behaviour to be obtained via a two-term asymptotic expansion in the heat-release. The resulting dispersion relation predicts that

for a finite overdrive the detonation is always stable to two-dimensional disturbances. For large overdrives, the identification of regimes of stability or instability is found to depend on a choice of distinguished limit between the heat release and the detonation propagation Mach number. Regimes of instability are found to be characterised by the presence of a single unstable oscillatory mode over a finite range of wavenumbers.

6. Short, M. and Kapila, A. K. Blow-up in semi-linear parabolic equations with weak diffusion. *Combust. Theory Modelling*, **2**, 283-291 (1998).

Abstract. Finite time blow-up in the semilinear reactive-diffusive parabolic equation is examined in the limit of weak diffusion for a Cauchy initial value problem with which possesses a smooth global maximum. An asymptotic description of the evolution is obtained from the initial time through blow-up using singular perturbation techniques. Near blow-up, an exact self-similar focusing identical to that previously associated with non-diffusive thermal runaway, is shown to be appropriate. However, in an exponentially small layer close to the blow-up time, the focusing structure must be modified to ensure a uniformly valid solution. This modification uncovers the asymptotically self-similar focusing structure previously recognized for blow-up. In contrast to previous studies, however, the structure arises here as a natural consequence of removing the non-uniformity in the expansions which occur exponentially close to blow-up when the effects of diffusion have to be reinstated. Identical weak-diffusion limit asymptotics can be applied to a variety of semilinear or quasilinear parabolic equations that exhibit finite

time blow-up in order to reveal the associated focusing structure.

7. Stewart, D. S. The Shock Dynamics of Multi-dimensional detonation and gas-phase detonations, *Proc. Of 27th Symp. (International) on Combustion, pp 2189-2205, (1998)*

Abstract. Detonations are comprised of broad detonation shocks supported by thin reaction zones. Approximations based on weak shock curvature measured on the inverse reaction zone scale, and quasi-steady flow, measured on the particle passage time through the reaction zone can be used to simplify the mathematical description of detonations that are governed the gasdynamic equations for a reacting flow. When the detonation reaction zone contains a sonic locus it is possible to derive intrinsic (coordinate independent) partial differential equations for the lead detonation shock's motion in terms of the normal detonation shock velocity, the shock curvature and higher normal time derivatives. We refer to this collection of theory and supporting experimental results as Detonation Shock Dynamics after Whitham's Geometrical Shock Dynamics. The reduced detonation dynamics is based on the concept of a eigenvalue (sonic) detonation, an idea that goes back to the original investigations in the 1940's. We present a review of the theoretical and experimental developments and attempt to update Fickett and Davis' discussion of work prior to 1980. We give examples of the theory and applications which include: i) weakly-curved, quasi-steady, near-CJ detonatioo ii) critical detonation curvature iii) quasi-steady extinction and ignition (and low velocity detonation) iv) shock acceleration effects and v) cellular and pulsating detonation in gases. We also review the engineering method of Detonation Shock Dynamics as it is applied to explosive systems.

8. Stewart, D. S. and Yao, J., The normal detonation shock-velocity curvaure relationship for materials with nonideal equation of state and multiple turning points, *Combustion and Flame,* 113, 224-235 (1998)

Abstract. We present a model and simple to implement numerical procedure that obtains the normal detonation shock velocity curvature relationships for an explosive material with non-ideal equation of state and an arbitrary reaction rate law. In addition we illustrate numerically (for a non-ideal equation of state) and analytically (for an ideal equation of state with a large activation energy rate law) that for sufficient rate-state -sensitive explosives, the response curve can have two turning points such that the curve has a Z-shape. The top branch of the Z response curve has been previously been associated with detonation extinction at a critical curvature. The bottom branch can be possibly associated with low velocity detonation and rapid change from low order detonation to high order.

9. Short, M., Kapila, A. K. and Quirk, J. J. The hydrodynamic mechanisms of pulsating detonation wave instability. *Phil. Trans. Roy. Soc. Lond. A*, **357**, 3621-3638 (1999).

The chemical-gasdynamic mechanisms behind the instability and failure of a one-dimensional pulsating detonation wave driven by a three-step chain-branching reaction are revealed by direct numerical simulation. Two types of pulsating instability observed experimentally are explained. The first involves regular oscillations of the detonation front, where the instability is driven by low-frequency, finite-amplitude compression and expansion waves in the chain-branching induction zone between the main reaction layer and the detonation shock. For irregular oscillations of the front, the instability mechanism first involves a decoupling between the shock and main reaction layer. Subsequently, the main reaction layer accelerates, drives a compression wave ahead of it, and undergoes a

transition to detonation. This internal detonation wave overtakes the lead detonation shock, generating a new high-pressure detonation, which rapidly decays. A smaller amplitude pressure oscillation occurs during the decay with a mechanism reminiscent of that observed for the previous regular oscillation, before the detonation and main reaction layer once again decouple and the instability cycle is repeated. For failure scenarios, the shock temperature is observed to drop to the cross-over temperature for the chain-branching reaction, causing the main reaction layer to decouple and retreat indefinitely from the detonation shock.

10. Buckmaster, J. D. and Short, M. Cellular instabilities, sub-limit structures and edge-flames in premixed counterflows. *Combust. Theory Modell.,* **3**, 199-214 (1999).

Abstract: We examine twin premixed flame in a plane counter-flow and uncover a hitherto known domain of cellular instability. This leads us to hypothesize that for small Lewis numbers a two-dimensional (2D) steady solution branch bifurcates from the one-dimensional (1D) solution branch at a neutral stability point located near the strain-induced quenching point. Solutions on the 2D branch are constructed indirectly by solving an initial-value problem in the edge-flame context defined by the multiple-valued bistable 1D solution. Three kinds of solution are found, a single isolated flame string and a pair of interacting flame strings. These structures can exist for values of the strain greater than the 1D quenching value, corresponding to sublimit solutions.

11. Ruderman, G. A., Stewart, D. S. and Fried, E. Modeling the Mechanical Ignition Energetic Materials, *Proceedings of the 11th (International) Symposium on Detonation,* Office of Naval Research, pp 554-561 (2000)

Abstract: A new theory of continuum thermomechanics involving microforces, or forces which drive the evolution of the microstructure in a material, is applied to the modeling of energetic materials, specifically, HMX. Using this theory, a set of partial differential equation are derived in a consistent thermodynamic framework which models HMX as a nonlinearly viscoelastic solid capable of undergoing phase transition to a viscous liquid and ideal gas, as well as a combustion process from unreacted HMX to reacted products. This system was then simplified to a set of one-dimensional model problems, which were solved numerically using advance computation techniques including essentially non-oscillatory (ENO) methods.

12, Ruderman, G. A., A Continuum Thermomechanical Model for Energetic Materials, Ph. D. thesis, University of Illinois, 1998, thesis advisor D. S. Stewart, TAM.

Abstract: Thermomechanical modeling of energetic materials, for example solid rock motor propellants and explosives, is a complex problem due to the large number of behaviors such a material may exhibit. Experiments have shown that these materials are nonliearly viscoelastic, and may also experience plastic flow permanent deformation) ,phases changes (melting and vaporization processes), and combustion. In addition, these phenomena are often strongly coupled, making modeling very difficult. Compounding this difficulty further, reliable experimental data on the properties of these types of materials are quite scarce.

Applying advanced tools of continuum thermomechanics, we have developed a fully three-dimensional framework, which, in the most general form, is able to model all the mentioned behaviors of energetic materials. The concept of a balance of micro-forces, which drives changes in material microstructure, is employed to generate

thermomechanically consistent equations of evolutions for combustion and phase transition.

The model is the simplified to a set of three model problems: the constant-volume thermal explosion, one-dimensional shear loading, and one-dimensional longitudinal loading. These model problems were solved numerically using essentially non-oscillatory and total variation diminishing methods. The solutions reveal extremely rich behavior, including complex wave phenomena, strain localization phenomena, and changes of material phase.

Section 3. Faculty/Research Associates/Student Supported

- Prof. Eliot Fried, TAM, UIUC (1 month summer 1996)

- Dr. Mark Short, Research Associate and Visiting Assistant Prof. (full salary support from 6/96 to 9/98)

- Prof. Mark Short, (1 month summer 1999)

- Dongyao Wang, research assistant. Mr. Wang is now supported on the present AFOSR contract, and is continuing his thesis work in detonation theory.

- Gregory A. Ruderman, research assistant and USFAF Palace Knight. (Ruderman's travel expenses to Eglin AFB, were partially support by this grant). Ruderman graduated in the Fall of 1998, and returned to a position in the Rocket Motor Branch of the Propulsion Directorate and Edwards, AFB, California.