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INTERIM SCIENTIFIC REPORT IN THE

PROGRAM OF RESEARCH ON THE

FORMATION AND PROPAGATION MECHANISMS OF DIVERGING GASEOUS DETONATION WAVES

Sponsored by the Energetics Division,
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13. ABSTRACT

The unconfined gaseous detonation wave problem can be summarized in terms of three phenomenological aspects: initiation, global propagation and evolution of structure. The initiation aspect concerns the study of the mechanisms and immediate consequences of rapid energy transfer from a spatially localized source into a highly explosive gaseous medium. On the basis of source power density considerations we have successfully achieved correlation of a broad range of experimental results and we are currently extending our studies into the realm of ultra-short (picosecond laser spark) duration ignition. The global propagation and evolution of structure are determined by the local nonlinear coupling between chemical kinetics and hydrodynamics in the transient expanding flow field immediately behind the leading shock front. Experimentally, we are continuing our detailed measurements of thermodynamic states and chemical species concentrations in the reaction zone. Theoretically, we are attempting to include in our modelling the general case of varying degrees of coupling to advance over the weak coupling situation that has been treated heretofore.

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FORMATION AND PROPAGATION MECHANISMS OF DIVERGING GASEOUS DETONATION WAVES

This report is an assessment of progress of ongoing research and a summary of anticipated directions for future studies as of May 1, 1971 in the program sponsored by the Energetics Division of USAFOSR under Grant AFOSR-69-1752B.

1. Introduction

The resolution of the unconfined gaseous detonation wave problem essentially involves achieving an understanding of the three fundamental phenomenological aspects inherent in the existence of such waves, namely their initiation, global propagation and evolution of structure. The first aspect, i.e., the genesis or the formation and early history of unconfined detonation waves, constitutes one phase of our research efforts in this program. Specifically, it concerns a study of the mechanisms and immediate consequences of rapid energy transfer from a spatially localized source into a highly explosive gaseous medium. The second phase of our research program deals with the phenomena consequent to initiation, i.e., what happens at late time away from the immediate vicinity of the source. Here it is the local non-linear coupling between chemical kinetics and hydrodynamics in a transient expanding flow field immediately behind the leading shock wave that determines the global dynamics and characteristic structure of the expanding reactive front. Specifically, the investigation of the non-linear coupling problem

involves the detailed assessment of the thermodynamic states and chemical species concentrations in the reaction zone.

The following sections deal in turn with the progress to date and current directions in these two phases of our investigation. Some of the listed References are anotated with an asterisk and these represent publications that have emanated or are being processed for print directly as a result of this AFOSR sponsored program.

2. Initiation

For the initiation problem, over the years it has been observed experimentally [1-5] that in a given explosive gaseous mixture the direct creation of a diverging detonation wave is not determined solely by the properties of the explosive medium (such as, for example, the chemical energy release per unit mass, Q) but that it also depends on the nature and properties of the initiation source. For example, the earliest experimental studies [6-13] showed that for a particular class of igniter the instantaneous generation of a diverging detonation wave requires an impulsive deposition of a finite and critical amount of energy at the source. Thus from these studies there evolved what appeared to be a controlling initiation parameter, namely E_0, the quantity of energy deposited at the source, whose value determined the existence or non-existence of a diverging detonation for the particular igniter used in a given explosive gaseous medium. However, efforts to correlate results between different researchers on the basis of their observed values of critical initiation energy

led to discrepencies which varied by three to four orders of magnitude. It soon became evident, especially on the basis of our quantitative measurements presented at the 14th International Combustion Symposium, Utah [2], that initiation energy, E_0, alone is not a universal controlling independent initiation parameter, but that discharge or energy deposition time Δt as well as the source volume Δv are relevant as well.

Consequently, as a result of these experiments, the average power density, i.e., (the total source energy)/(the deposition time) x (the source volume) = $E_0/\Delta t \Delta v$, has been introduced as a physically more meaningful initiation parameter. Indeed, it was observed that for the particular case of stoichiometric acetylene-oxygen mixture at an initial pressure of 30 torr, the critical energies for direct initiation vary from 0.6 joules for the laser spark to 450 joules for slow electrical discharges, yet the power density remains essentially the same at 3×10^{17} watts/m^3. Thus for a given explosive, there is a variation of critical energy for different initiators whereas the power density apparently remains invariant.

However, a paradox emerges here, since according to physical reasoning the power density alone cannot be a universally meaningful parameter since it admits the possibility of zero critical energy in the limit when the discharge time or the source volume or both are arbitrarily reduced without limit. Physical reasoning indicates that there should still exist a definite minimum quantity of energy for direct initiation even in the limit of infinite power density since it must simply take just so many energetic molecules to start off the initiation process.

It is this aspect of ultrashort deposition times and miniscule source volumes in the initiation process that is currently receiving particular attention, both theoretical and experimental, in our laboratory. Theoretically we are modelling the source to include not only the source energy E_0 but the discharge time Δt and the source volume Δv as well. The initiation parameters E_0, Δt and Δv are modelled theoretically by a spherical piston which expands impulsively from zero radius at $t = 0$, deposits a fixed quantity of energy into the flow field at a source and at a rate predetermined by the trajectory of the piston. This theoretical work constitutes a part of a Ph.D. program undertaken by Mr. W.H. Kyong in our group. For the experimental phase of the work we are attempting to achieve collaboration with the Physics Division of the National Research Council of Canada to investigate ignition of spherical detonations by ultrashort (picosecond) laser sparks obtained by judicious switching-out and amplification of a single laser pulse from a train of pulses in a mode-locked neodymium laser system. In our paper [14], "The Laser Spark for GasKinetic Studies", accepted for presentation at the 8th International Shock Tube Symposium, London, we discuss the efficacy of the picosecond laser spark as it applies to detonation and transient chemical kinetic studies.

3. Non-linear Coupling

The second aspect of our program concerns the local non-linear coupling between chemical kinetics and hydrodynamics under transient conditions. Such coupling determines not only the

dynamics of late time propagation of diverging reactive fronts but also their character and structure. Experimentally we have documented [1, 2, 5, 15, 16] rather thoroughly the propagation histories and characteristic structure of diverging reactive fronts under varying degrees of coupling. These correspond to three propagation regimes for diverging reactive fronts, namely, the deflagrative, the transitional and the detonative regimes. On the basis of extensive experimental evidence [1-5], it is now universally accepted that the deflagrative, transitional and detonative regimes for spherical waves correspond to sub-critical, critical and supercritical values of initiation energy. Sub-critical initiation energy invariably leads to separation of the reaction front from the shock wave, i.e., to decay of an initially overdriven detonation to a spherical deflagration wave. For the supercritical values of initiation energy the initially overdriven detonation decays continuously to a multiheaded detonation wave reaching an average velocity of propagation corresponding approximately to the theoretical C-J value. When the source energy equals the critical value, the overdriven detonation at first decays and decoupling of the shock and reaction fronts occurs. Then for a period of time the shock and reaction fronts propagate as a "quasi-steady" complex at a constant sub C-J velocity. During this quasi-steady period instabilities develop and the reaction front takes on the turbulent structure. These instabilities lead to localised explosions which occur suddenly and randomly at isolated spots in the reaction zone forming "detonation bubbles" which then grow and completely engulf the shock sphere, terminating the

quasi-steady regime and resulting in a highly asymmetrical multiheaded detonation wave.

Clearly the most intriguing and important of these experimental observations is the one pertaining to critical initiation energy. Here all at once it embodies the two distinctive propagation modes of spherical reacting fronts characterized initially by a smooth decoupled spherical front followed ultimately by a highly irregular multiheaded detonation front. Of particular interest is the peculiar nature of transition from one to the other via the quasi-steady regime and the development of detonation bubbles therein. Here then is a phenomenon which in the absence of all confinement and other extraneous effects and purely by the local interplay of hydrodynamics and chemical kinetics of heat release has provided the first distinct traces of the evolution of a detonative structure from a featureless decaying shock-flame complex.

These then are the sort of things that have been observed experimentally. Such experimental observations are not only intriguing but they have contributed considerably in putting the phenomenological aspects of detonative combustion in a clearer perspective. Potentially they may yet prove pivotal in achieving a significant breakthrough in the understanding of gaseous detonative combustion. However, experiments alone have not been sufficient so far in unravelling the inherent mechanisms responsible for the particular dynamics and phenomenological behavior observed. In other words, whereas the character and behavior of spherical reacting fronts are by now well documented over a broad range of conditions, they are by no means well understood.

Our current efforts are concentrated in attempting to reproduce theoretically the sort of dynamics and phenomenological behavior that has been observed experimentally. If such theoretical modelling proves successful the experimentally observed behavior can then be explained in terms of the physical model that was used in the theoretical formulation of non-linear coupling as it applies to chemical reactions in an expanding flow field.

The first recent step in the theoretical modelling process, taking into account varying degrees of coupling, has been the phenomenological theory of Bach and Lee [2], first reported at the 23rd APS Fluid Dynamics Meeting in Charlottesville, Virginia and subsequently summarized in our 13th International Combustion Symposium paper. In this case, the coupling between the shock and the reaction front is modelled by the so-called effective energy function which depends on the local shock strength and the shock radius band on the induction zone thickness. As it pertains to the motion of the detonation front, the model manages to recover all the essential experimentally observed features. However, the model is limited in that it ignores the influence of the chemical reactions on the hydrodynamic flow structure and that it retains the reactive shock discontinuity assumption.

The strong coupling problem, in principle, can only be achieved by the numerical approach. Kadan [17] and Taki and Fujiwara [18], applying the conventional characteristic method and the finite difference approach respectively, provided some description of the problem in the overdriven regimes of the shock motion. However, some predictions are doubtful in spite of the fact that the detailed kinetics of the chemical reaction processes have

been considered in the hydrodynamic flow field. The failure of such calculations is a direct result of the absence of transient chemical kinetic data, a lack of which is plaguing contemporary efforts in detonation research. What is really needed is transient chemical kinetic data. We have proposed in our paper [14] in the 8th International Shock Tube Symposium, London, to exploit the blast wave from a picosecond laser spark to this end.

In our ongoing theoretical treatment of the non-linear coupling problem (which constitutes a part of a Ph.D. program undertaken by Mr. W.H. Kyong in our group), we adopt a simplified chemical kinetics model rather than the detailed reaction processes (since the applicability of quasi-steady chemical kinetics is quite dubious and the total absence of transient chemical kinetic data is as of now overwhelming). Hartree's characteristic method is used for numerical calculations. The main body of the theoretical effort can be divided into two parts. The first part deals with the parametric study of direct initiation and the asymptotic motion of diverging detonations under the limiting condition of strong coupling. The second part relates to the determination of the critical initiation energy and the theoretical description of the propagation regimes corresponding to various degrees of coupling. The results of these studies will progressively be appearing in print as soon as a sufficient degree of completion is achieved in each aspect of the problem.

Finally, attention must be drawn to the invited review paper by Lee [19] which will be presented at the 3rd International Colloquium on Gas Dynamics and Reactive Systems, Marseille. The

substance of the paper emanates from the overall long term AFOSR support for our efforts at McGill University over the last five years or so.

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