Detonation Initiation on the Microsecond Time Scale: Comparative One and Two Dimensional DDT Results Obtained from Adaptive Wavelet-Collocation Numerical Methods

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1. Introduction

Spatially resolved, thermal power deposition of limited duration into a finite volume of reactive gas is the initiator for planar deflagration to detonation transition (DDT) on the microsecond time scale. Sileem et. al.[1](SKH) and Kassoy et. al.[2,3,](KKNC2,3) use an explicit MacCormack[4] scheme to obtain solutions to the one-dimensional reactive Euler equations with one-step Arrhenius kinetics. SKH conclude that "The one dimensional unsteady mathematical model… appears to provide a physically plausible description of detonation initiation through a transition from deflagration to detonation." However, the high-speed deflagration generated by the initial burst of power supplied by the external source does not itself evolve into a shock-coupled reaction zone. Rather, numerous, localized reaction centers that appear spontaneously are found to be the sources of compression waves that strengthen an initially weak lead shock sufficiently to facilitate closely coupled reaction zones. Localized reaction centers appear when the characteristic reaction time in a volume of reactive mixture is as short as the acoustic time defined by the ratio of the volume dimension to the local speed of sound. In that case momentary, partial inertial confinement is possible and local pressure rises with temperature. Subsequent expansion of the hot, high pressure spot driven by the locally large spatial pressure gradient drives compression waves into the surrounding mixture. Combustion heat release and gasdynamic transients are essential to the formation of the detonation. Oppenheim[5] observed the formation and evolution of reaction centers described as "explosions in the explosion" in a system with transverse wave processes. Compression waves generated by these localized regions of very rapid chemical heat addition were deemed crucial to the DDT process. Others have since observed similar phenomena in multidimensional numerical results[6,7,]. Further development of the SKH approach (KKNC2,3) has focused on solution reliability and a parametric study of solution sensitivity to the magnitude and location of the initial power burst as well as the activation energy of the one step reaction. Results of this work indicate that the transient dynamics of planar DDT evolution are (a) dependent on the magnitude and location of the initial power deposition process, (b) sensitive to the activation energy of the one step Arrhenius reaction, (c) characterized by the spontaneous appearance of several localized hot spots (reaction centers) resulting from conditioning of isolated volumes of reactive mixture by the

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compression wave structure inherent in a reactive gasdynamic environment with thermal power addition from external and chemical sources and (d) likely to lead initially an overdriven detonation which relaxes smoothly to a CJ wave. The amount of overdrive can be quantified by the global heat release rate maximum which occurs when there are multiple reaction zones behind the lead shock. This structure occurs during a period of shock strengthening, when the ignition delay times of sequential fluid particles passing through the shock are significantly shortened as the post shock temperature increases. Less conditioned particles explode farther behind the shock than more conditioned particles that pass the shock subsequently. The global heat release maximum shown in Fig. 1 below, is nearly twice the value of the C.J. heat release for the parameters of the problem, in spite of the fact that the shock Mach number is not nearly large enough to support that large heat release rate with a *single* post shock reaction zone.

2. New Results

The MacCormack scheme[4] used in SKH and KKNC2,3 is known to produce undesirable solution oscillations in the vicinity of large gradients (shocks). In principle, these oscillations are sources of error in the local reaction rate modeled by an Arrhenius exponential term. Recently developed numerical methods are capable of more accurate solution representation when large gradients are present. An adaptive wavelet-collocation method (AWCM) developed originally by Vasilyev and co-workers[8-11] for solving the Navier-Stokes equations in multiple dimensions has been extended recently by Regele and Vasilyev[12] for solving hyperbolic equation systems like the reactive Euler equations that describe thermally initiated DDT processes. The efficiency of the adaptive wavelet-collocation solver is combined with the simplicity of a flux-limited type approach to explicitly add localized artificial viscosity near shocks. A series of inert compressible flow problems with known solutions are used as test cases to successfully validate the effectiveness of the AWCM method.

The current research effort has two primary objectives, First, it is aimed at establishing the effectiveness of the AWCM for solving reactive gasdynamics problems. The planar DDT model described by SKH and KKNC2,3, where the physico-chemical processes and the inherent length and time scales are reasonably well understood, is to be used as a test case. It is anticipated that the results obtained will provide a seminal description of the reactive gasdynamic transients seen in a thermally initiated DDT. The second objective is to model a thermally initiated DDT in two dimensions, including tranverse wave effects like those observed by Oppenheim[5]. This will be done by using a multidimensional version of the AWCM to develop a solution to an initial value problem in a narrow channel, comparable to that in one dimension. (same parameter values) A comparison of the DDT distances predicted by the one- and two-dimensional models for comparable sytems will be made and explained. An ancillary scientific objective is to explain quantitatively why multidimensional quaisisteady detonations propagate at nearly the CJ speed of a planar detonation. The qualitative explanation usually given for this observation is that the total rate of heat release behind the wave front is nearly identical in the one and two-dimensional cases. Figure 1 shows the time history of the nondimensional total heat release rate associated with transient

reactive gasdynamics of an evolving one-dimensional DDT. The plateau shaped curve in the lower left corner represents the time history of the initiating nondimensional thermal power source deposited in a slab shaped region of width1.4mm, located 0.35mm from the boundary surface, during a period of 10 microseconds. The dimensional energy deposition is $1.53X10^7 J/m^3$.

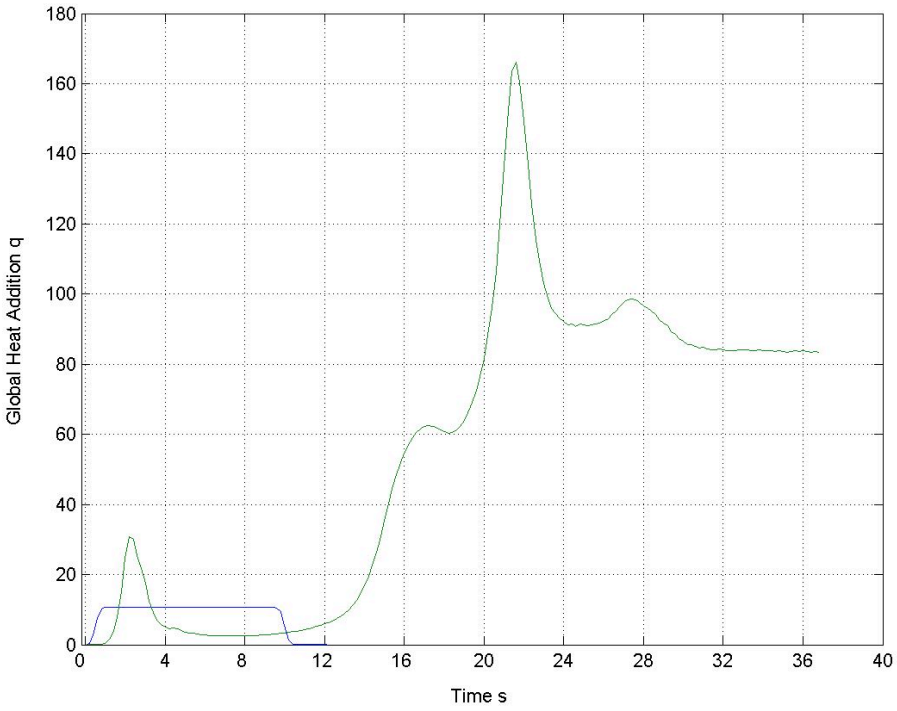

Figure 1. The evolution of the global heat release with time, exhibiting four local maxima and asymptoting to the C.J. value for a steady detonation wave for $z_i = 3$ and $\varepsilon^* = 0.0725$. The mesa-like curve in the lower left hand corner represents the initial power deposition. The absolute maximum global heat release, q = 166.08, occurs at s ≈ 21.6.

The first local maximum is associated with the "explosion" of the reactive mixture in the vicinity of the external source. The second occurs when the first of the local reaction centers appears. The absolute maximum is attributed to a power burst from the appearance of a shock-coupled multiple reaction zones (the overdriven detonation[a.]). The fourth local maximum occurs when previously unburned pockets of reactive mixture located far behind the wave front are finally consumed. It is anticipated that a similar curve for a two dimensional DDT will be constructed by evaluating a spatial integral for the local heat production rate at each time value of interest. Similarities and differences with the results in

[a.] Schauer et. al.[13] observe initially overdriven detonations in pulsed detonation engine spark initiated DDT events.

Fig.1 will be considered and explained in terms of the transverse phenomena occurring behind the wave front. In particular, rapid localized chemical heat addition in two-dimensional reaction centers can be a source of both axial and transverse compression waves, whereas in a planar event only the former are possible. Transverse relief will lead to different energy partitioning than the axially distributed internal and kinetic energy seen in SKH and KKNC2,3.

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