Numerical Simulation of Pulse Detonation Engine Phenomena

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Abstract

This paper describes one- and two-dimensional numerical simulations, with simplified as well as full reaction kinetics, of a single cycle pulse detonation engine (PDE). The present studies explore the ignition energies associated with the initiation of a detonation in the PDE tube, and quantify reactive flow phenomena, performance parameters, and noise generation associated with full and simplified kinetics simulations of the PDE. Comparison of these parameters is made with available experimental data. The present simulations demonstrate the ability to predict PDE reactive flow phenomena and associated performance and noise characteristics, and hence have promise as a predictive tool for the evolution of future PDE designs.

Introduction

The Pulse Detonation Wave Engine (often called the Pulse Detonation Engine or PDE) is a constant volume engine concept which allows periodic ignition, propagation, and transmission of detonation waves within a detonation tube, with associated reflections of expansion and compression waves which can act in periodic fashion to produce thrust [1, 2]. Because the PDE concept holds promise for high thrust density in a relatively simple, compact device, a number of groups have been exploring PDEs for propulsion applications [2–9]. Performance parameters commonly used to characterize the pulse detonation engine include the impulse, I, typically defined in terms of the temporal integral of the pressure at the closed thrust wall over a cycle of operation, the specific impulse, I_{sp}, which scales the product of the impulse and the tube area by the initial weight of reactant gases in the PDE tube, and the fuel-based specific impulse, $I_{sp,f}$, which further scales the I_{sp} by the fuel mass fraction initially present within the tube.

Overviews of past and ongoing numerical simulations of PDEs are described in recent articles by Kailasanath [2, 6, 7]. Recent simulations have focused on various flow and geometrical features of the PDE, including the effects of nozzles placed downstream of the detonation tube [3, 5, 10] and the effects of multiple adjacent PDE tubes [9, 11]. Other studies have explored the effect of thermally initiated detonations in PDEs and other tube systems via the deflagration-to-detonation transition (DDT) [12–16].

Prior computational studies by our group pertaining to detonation phenomena in general [17] and the pulse detonation engine in particular [18] involve both one- and two-dimensional simulations with single step reaction kinetics, employing essentially non-oscillatory or ENO schemes [19, 20] for spatial integration. The studies suggest that useful performance and noise related estimates may be obtained even from one-dimensional computations of the pulse detonation wave engine with simplified reaction kinetics. The present study focused on using these high order numerical schemes to study the behavior of the pulse detonation engine, using simplified as well as complex reaction kinetics. The work focuses on the influence of the PDE's flow and reaction characteristics on performance parameters as well as noise generation by the PDE.

Problem Formulation and Numerical Methodology

The reactive Euler equations were solved in both one and two spatial dimensions in the present study. Single step reaction kinetics for the $CH_4 - O_2$, $H_2 - O_2$, and H_2-air reactions [9, 18] were explored, as well as full reaction kinetics for mixtures of $H_2 - O_2$, $H_2 - O_2 - Ar$, and $H_2 - O_2 - N_2$ (representing H_2-air). The latter mechanism contained 23 elementary reactions involving N = 11 species and was part of the CHEMKIN II library [21]. Only straight PDE tubes

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were explored; a parallel study is examining the influence of nozzle extensions [22]. In the 1D simulations, the computational domain consisted primarily of the detonation tube or tube and nozzle (containing at least 600 grid points), with only a few grid points extending beyond the tube end in order to capture the external pressure. In the 2D simulations, the air external to the detonation tube was assumed to be uniformly at atmospheric pressure, and the computational domain extended well downstream of the end of the tube, in general at least one and one half tube lengths downstream and at least two tube diameters away from the detonation tube in the dimension perpendicular to the axial dimension.

As in [18], the present study used the Weighted Essentially Non-Oscillatory (WENO) method [23], a derivative of the ENO method [19, 20] for spatial interpolation of the system of governing equations. The WENO scheme was fifth order accurate in smooth regions and third order accurate in the vicinity of discontinuities. To avoid entropy-violating expansion shocks near sonic points, where characteristic velocities change sign, high order dissipation was added in the present study via the Local Lax Friedrichs (LLF) scheme [24], which adds extra numerical viscosity throughout the computational domain at each time step. The ENO/WENO schemes were tested on a variety of problems, including shock tubes with open ends, analogous to the exit of the PDE [18], and that of the classical one-dimensional, overdriven, pulsating detonation [17]. For the single step kinetics simulations, the third order total variation diminishing (TVD) Runge-Kutta method was used for time discretization. For full kinetics simulations, the method of operator splitting [25] was used, whereby the system of governing equations (including $N-1$ species equations) was split into two separate equations, one which only included the advection-diffusion terms (solved via WENO) and one which only included the reaction rate source terms. A stiff ODE solver, DVODE (a variation of VODE [26]) was employed for the solution of the rate equations; thermodynamic parameters and rate constants were obtained via the CHEMKIN II subroutine [21].

A computational "spark" adjacent to the thrust wall was used to initiate the detonation at the start of the PDE cycle. This narrow, high pressure, high temperature region (3 grid cells in width) was able to initiate a propagating shock and ignite the reactants; the flame front then caught up with the shock, forming a detonation. As suggested by prior studies [12–14], however, such thermal initiation of detonation depends very strongly on the initial rate of deposition of energy in the reactants. This concept was explored in the present studies by altering the initial temperature and pressure in the computational "spark" to be able to determine minimum input energy densities leading to detonation initiation.

In addition to the standard performance parameters used to characterize the PDE (I, I_{sp}, and $I_{sp,f}$), the sound pressure level (SPL) at various locations within and external to the detonation tube was also computed. As done previously [18], these noise levels were estimated by examining the Fourier transform of the time-dependent pressure measured at various locations within the computational domain. The SPL was then computed based on peak pressures in the Fourier spectrum. In most cases these peaks occurred at the PDE cycle frequency.

Results

An example of the temporal evolution of the 2D pressure field within and exterior to a straight PDE tube, over a single cycle, is shown in Figure 1, for the case of of a single step methane-oxygen reaction. Here the initiation and propagation of the detonation wave through the tube (Figures 1ab and the exit of the shock from the tube and reflection of the expansion fan from the exhaust back into the tube (Figures 1cd) are clear. As the detonation exited from the open end of the PDE tube, a vortical structure coincident with the shock was formed and propagated downstream, simultaneous to the propagation of a reflected expansion wave back into the tube. The waveforms created in this simulation became relatively smooth and unidimensional, even with increased grid resolution. The single step kinetics simulations were separately able to produce cellular detonation structures when specific conditions for 2D overdriven detonations were explored computationally [27]. Our prior studies [18] demonstrate that a 1D simulation of this same PDE tube quantitatively yields a very similar pressure field evolution to that of the 2D simulation, even without inclusion of a 1D pressure relaxation length.

Time-series pressure data at specific locations could be used to estimate the noise generated at various points in the flowfield over a single PDE cycle. Estimates of the sound pressure level using both 1D and 2D simulations of the straight PDE tube with

a single step $CH_4 - O_2$ reaction are shown, for example, in Table 1. Since the 1D simulations only resolved the flow within the PDE tube, comparisons were made only for interior and tube exit noise levels; noise levels did decay significantly beyond the tub end, yet the SPL values were still quite high. In all locations for this case we observed the peak in pressure to appear close to the frequency associated with the period of the PDE cycle, roughly 330 Hz.

Location	2D SPL	1D SPL
Thrust Wall	212 dB	212 dB
Mid-tube	211 dB	211 dB
Tube end	202 dB	203 dB
1L past tube end	173 dB	–

Table 1. Computed sound pressure level (SPL) at various locations within the tube (thrust wall, center of tube, and tube end) and 1 tube length L beyond the tube end. Results are computed from both 2D and 1D simulations of the $CH_4 - O_2$ reaction.

Consistent with the evolution of the pressure field and the performance parameters [18] the noise levels were nearly the same for 1D as for 2D simulations. Similar findings were obtained for other single step reaction mechanisms in comparing 1D and 2D simulations. The magnitudes of the noise levels in the present computations were close to those quantified in PDE experiments [28, 29].

The full kinetics simulations of the reactant-filled, straight PDE tube allowed a more detailed examination of the detonation ignition and propagation process to be made, in addition to more quantitative comparisons with experimental data. Figure 2 displays the evolution of the 2D pressure field associated with the PDE tube and its surroundings, for a full $H_2 - O_2$ reaction. As seen in Figure 1 for the case with simplified kinetics, the propagation of the detonation out of the tube resulted in the propagation of a vortical structure coincident with the shock and simultaneous reflection of an expansion fan back into the tube. Increased complexity in the wave structures (as compared with that for simplified reaction kinetics) was observed in Figure 2 for the complex kinetics simulation, especially in the propagating shock/vortex structure downstream of the tube exit. High frequency oscillations in pressure, species, and other parameters were observed at various locations within and external to the PDE tube in the complex kinetics cases, similar to those observed in experimental studies [4]. Estimates of PDE specific impulse from the single step as well as the full kinetics simulations were quite close to each other; for the case of the $H_2 - O_2$ reaction, both were on the order of 240 sec, as will be discussed below.

The influence of the initial pressure and temperature (and resulting energy deposition) on initiation of a detonation wave was studied here using the full kinetics simulations. Figure 3 shows the centerline pressure distribution for a 1D, full kinetics simulation of an $H_2 - O_2 - Ar$ mixture, for different initial temperatures and pressures in the 3 grid cell-wide "spark" adjacent to the thrust wall. Critical combinations of temperature and pressure were observed to be necessary for the classical ZND detonation structure to evolve; if the initial energy deposition was too small, a weak shock front did not ignite the mixture and thus did not transition to a detonation, as seen by the solid lines in Figures 3ab. As expected, the critical input energies for ignition of a detonation were found to be different for these different reactions. In the case of $H_2 - O_2 - N_2$, a critical energy deposition per unit area of about $5 \times 10^5\ erg/cm^2$ was required for detonation, whereas for the case of $H_2 - O_2 - Ar$, this critical value rose to about $8.5 \times 10^5\ erg/cm^2$.

The full kinetics simulations also allowed quantitative comparisons to be made between performance parameters from the present simulations and those obtained by experiment (for a single cycle PDE) or analysis. Table 4 below shows the current estimations of I_{sp} for the 2D PDE for $H_2 - O_2$ and $H_2 - O_2 - N_2$ (hydrogen-air) reactions, as compared with the analysis and experiments described in Wintenberger [30] and the studies of Zitoun [31] and Schauer [32].

Study	I_{sp}, H_2-air	I_{sp}, $H_2 - O_2$
Present	128.5 s	240 s
Wintenberger[30]	123.7 s	173 s
CIT expts.[30]	–	200 s
Zitoun expts.[31]	149 s	226 s
Schauer expts.[32]	113 s	–

Table 4. Comparison of specific impulse for single cycle PDE between the present simulations and corresponding experiments and modeling efforts, as noted.

While the present simulations appeared quantitatively to replicate the experimentally observed performance parameters reasonably well, detailed comparisons of the pressure field evolution and noise es-

timates require further examination and are the subject of continued studies.

Conclusions

High resolution numerical simulations of pulse detonation engine phenomena revealed useful information that may be used in future PDE designs. Simulations of PDE evolution with full chemical kinetics suggested that specific minimum energy densities were required to enable the initiation of a detonation, and hence to sustain the PDE cycle. It was further observed that full kinetics simulations were able to capture quantitatively the physical phenomena and corresponding performance parameters for the PDE. Future studies will continue with this quantitative comparison as well as noise generation issues relevant to the PDE.

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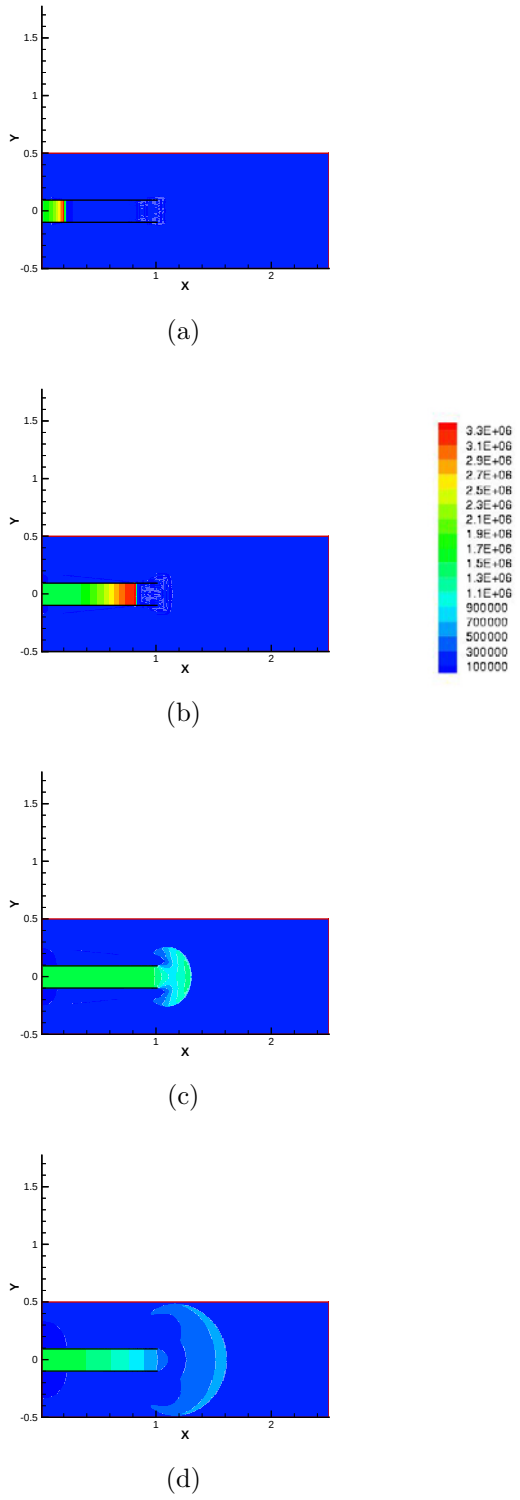
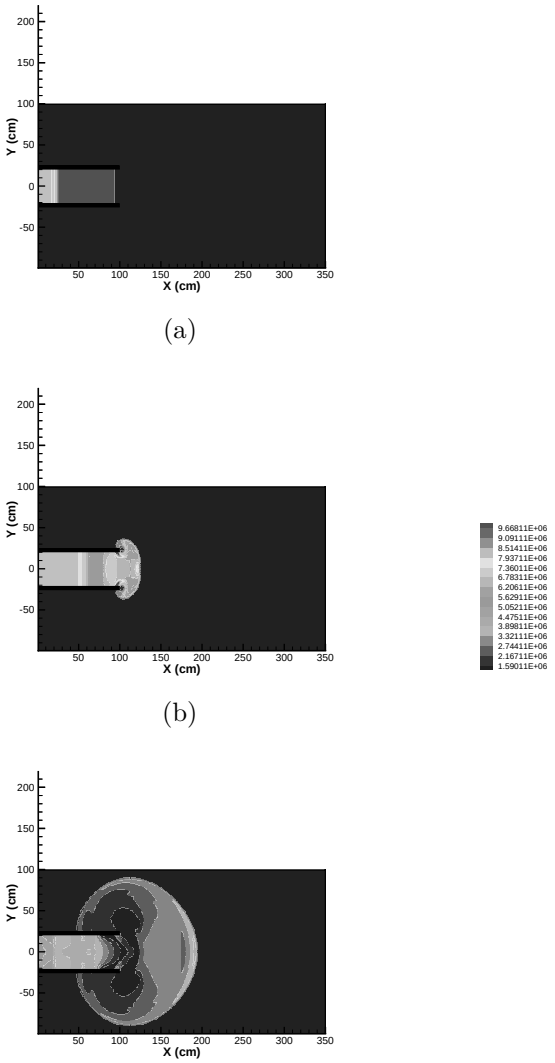


Fig. 1: Temporal evolution of the 2D pressure field for a 2D planar PDE of 1 m length, for a single step $CH_4 - O_2$ reaction, with pressure given in units of Pa. Results are shown at times (a) 0.06 ms, (b) 0.15 ms, (c) 0.49 ms, and (d) 0.76 ms; the full cycle has a period of about 3 ms.

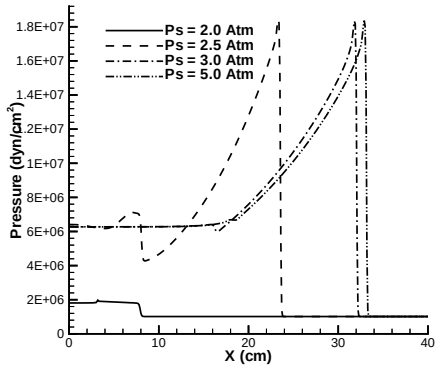


(a)

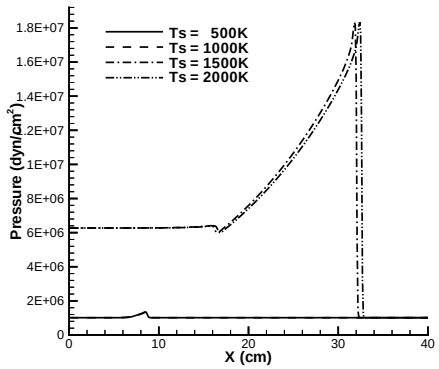
(b)

(c)

Fig. 2: Temporal evolution of the 2D planar pressure field within and external to the PDE over one cycle, with pressure given in units of dyn/cm^2. Data shown are at times corresponding to (a) 0.15 ms, (b) 0.47 ms, and (c) 1.34 ms. A $H_2 - O_2$ reaction was simulated here with full chemical kinetics.



(a)



(b)

Fig. 3: Centerline pressure distribution for the $H_2 - O_2$ reaction with full kinetics, for different computational "spark" conditions: (a) fixed temperature 1500K and variable pressure, and (b) fixed pressure 3 atm and variable temperature, each at time 0.2 msec.