Preliminary Investigation into the Influence of Transverse Waves in PDE Simulations

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1 Introduction

Pulse detonation engines (PDEs) are inherently difficult to model due to the large disparity in length scales presented in the problem. Calculations using the Zeldovich-von Neumann-Doring (ZND) detonation model show that reaction zone thicknesses for stoichiometric fuel-oxygen mixtures at standard temperature and pressure are typically on the order of 1e-5 m [1]. In actuality, this length scale is only a first approximation to the smallest inviscid scale as the unsteady, multidimensional structure of realistic detonations leads to shock strengths that can be significantly larger than the Chapman-Jouguet (CJ) estimates used in ZND calculations. Several previous studies have shown that sufficient resolution can be achieved in numerical simulations when between 10 and 50 grid points are placed in the reaction zone [2-5]. The largest length scale in a practical PDE configuration can be expected to be on the order of 1 m. Consequently, even a one-dimensional simulation of a practical device using uniform, non-adaptive, grid spacing would require over one-million grid points in order to fully resolve the smallest length-scale.

Due to the aforementioned difficulties, PDE simulations presented in the literature are typically done at resolutions which are orders of magnitude larger than the smallest physical length scale [6]. Despite being under-resolved, these simulations are typically capable of predicting detonation velocities and post-reaction-zone flowfield quantities that are consistent with equilibrium CJ theory [7]. Ideally, these under-resolved simulations represent a spatial and temporal average of the underlying physics; however, a systematic study has not been presented to assess the validity of this approach for PDE performance predictions. In this work we will focus on whether the typically unresolved transverse wave structure in multidimensional cellular detonations has an impact on performance.

2 Numerical Model

The model equations in this study are the two-dimensional, reacting Euler equations in curvilinear coordinates written in conservative form. Curvilinear coordinates are used so that non-uniform grids can be implemented with points concentrated in the reaction zone. A continuity equation is written for each of the chemical species present in the system and Strang-splitting [8] is used to incorporate the chemical source term. The convective fluxes are evaluated by applying the nominally 5^{th}-order-accurate Weighted-Essentially-Non-Oscillatory (WENO) method in individual characteristic fields, and with the use of the Local-Lax-Friedrich's (LLF) Riemann solver [9-11]. After all spatial derivatives have been approximated; the resulting semi-discrete equation is advanced in time using an explicit, total-variation-diminishing, 3^{rd}-order, Runge-Kutta algorithm [12]. The code is parallelized using the Message-Passing-Interface (MPI) standard and a one-dimensional domain decomposition in the transverse direction is used to divide the problem amongst available computer resources.

3 Results & Discussion

Of primary concern in PDE performance evaluations is the stagnation pressure produced at the closed wall behind the propagating detonation. This stagnation pressure, which will be referred to as the plateau pressure, is responsible for the vast majority of the impulse generated by a PDE. In the case of straight-tube, nozzle-less

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PDEs it is the only contribution to the generated impulse. The objective of the present work is to investigate whether transverse waves generated in the reaction zone lead to losses that lower this plateau pressure.

The primary motivation for investigating the influence of the transverse waves is the ongoing discrepancy between the plateau pressure predicted by current PDE models and that measured in experiments. This discrepancy is illustrated in Figure 1 where the plateau pressure is plotted for a stoichiometric mixture of C_2H_4/O_2 at initial temperature and pressure of 300 K and 1 atm, respectively. The simulated result is based on a 1-D form of the model described previously. The chemical mechanism used is a slightly modified version of the 21-species, 33-reaction mechanism developed by Varatharajan [13]. A grid refinement study was performed ensuring that the plateau pressure was independent of the grid resolution. Interestingly, measurements performed by Cooper and reported in Reference 14 indicate an average plateau pressure of approximately 10.8 atm for the same mixture at 300 K and 1 bar. Their measurements were made in a tube which is twice the diameter of that used for the experiment in Figure 1. The discrepancy between Cooper's measurement and that reported here suggests the possibility of some dependency on the transverse dimension.

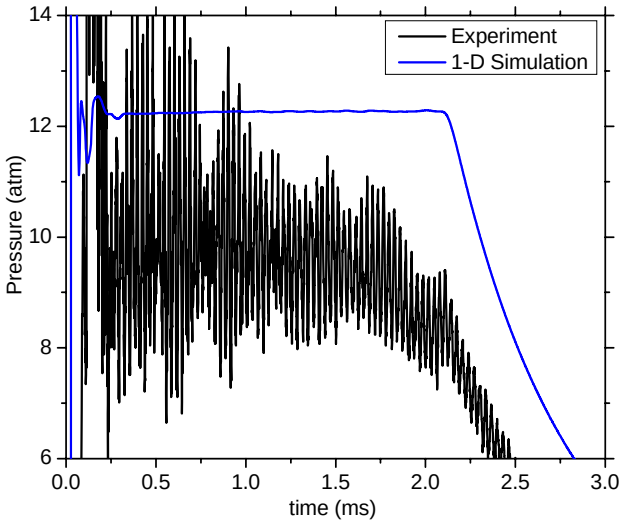

Figure 1. Plateau pressure for stoichiometric C_2H_4/O_2 at T=300 K and P=1 atm.

In order to investigate whether the transverse wave structure in a cellular detonation has an effect on the plateau pressure, simulations are initially performed in a shock-fixed frame until the transverse structure has evolved for a sufficiently long time such that the solution is independent of the initial condition. The resulting solution is then shifted to the laboratory frame and a closed wall condition is applied at the upstream boundary. The solution is then advanced in time and the pressure at the wall is recorded.

In this preliminary work we first consider a room temperature (298 K), low pressure (6.67 kPa), stoichiometric H_2/O_2 detonation diluted with 70% Ar. While this low reduced activation energy mixture is not representative of what will be used in a practical PDE, it has been studied extensively in the literature [2-3] and serves as a starting point for the investigation. This case is also particularly amenable to simulation because the ZND reaction zone length is relatively large (1.8 mm) and previous experiments have demonstrated the cellular structure to be very regular [2-3]. Simulations of mixtures with less regular structure, which are of more practical importance for PDEs, are currently being investigated and will be included in future results.

The shock-fixed-frame simulation is initialized by placing the 1-D ZND solution onto the 2-D grid and assuming unburned reactants enter the inflow boundary traveling at the CJ wave speed (1626.9 m/s). The ZND initial condition is constructed using the tools described in Reference 15. A perturbation in temperature and pressure is applied in a small region behind the front as described by Oran [2] in order to accelerate the development of the transverse instability. The top and bottom walls are specified to be symmetry lines, while the outflow boundary is specified using a zero-gradient condition. The rectangular domain size is set to be 10 cm in the longitudinal direction by 3 cm in the transverse direction and a 1000 x 200 uniformly spaced grid is utilized. The transverse domain width was chosen to be the height of one detonation cell and the longitudinal grid spacing places 18 grid points in the ZND reaction zone. The hydrogen/oxygen mechanism used in the simulations was extracted from the hydrocarbon mechanism developed by Westbrook [16].

After the detonation has developed a periodic cellular structure in the shock-fixed frame, the simulation is halted and then shifted into the laboratory frame with a closed wall boundary condition applied 43 mm behind the shock front. The described initial condition is shown in Figure 2a. The plotted quantity depicted in Figure 2 is a scaled magnitude of the density gradient which gives a schlieren-like shading pattern. Several snapshots of the cellular detonation are shown in Figure 2 as it propagates down the 30 cm length of the test section. This test section length was chosen based on 1-D simulation results which revealed 30 cm to be the minimum distance for the expansion wave generated at the closed wall to merge smoothly with detonation front. One-dimensional simulations are also used in order to represent the pressure field that is predicted when the transverse wave

structure goes unresolved. The 1-D simulations are initialized by placing the shock front of the ZND solution 43 mm from the closed wall boundary as shown in Figure 3b.

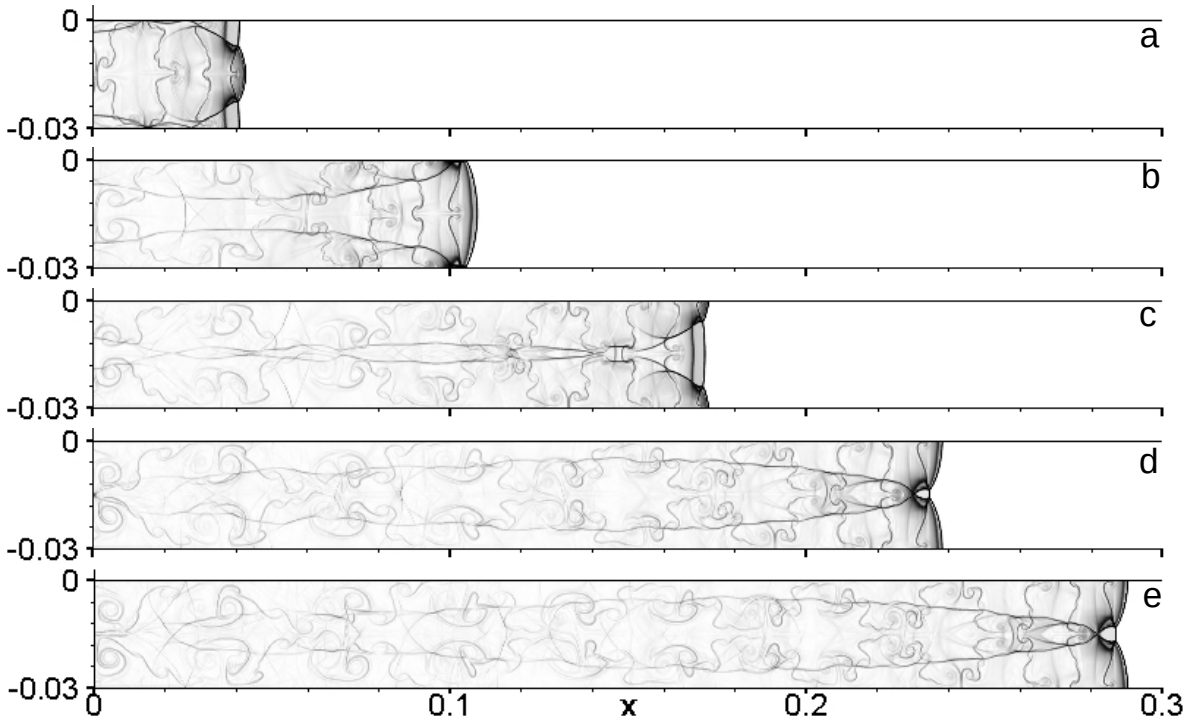

Figure 2. Schlieren-like plots of detonation propagation in laboratory coordinate system. Frame a) 0 µs, b) 40 µs, c) 80 µs, d) 120 µs, e) 152 µs.

As evident in Figure 3 the pressure field behind the 2-D, multi-headed detonation is quite different from the smooth profiles predicted using the 1-D model. The pressure oscillations produced in the 2-D model occur due to transverse wave interactions as well as the varying strength of the shock front as it evolves through its periodic cell cycle. In particular, large pressure spikes are evident a short distance behind the front in the 120 µs and the 152 µs profiles which are the result of triple-point collisions shown in Figure 2. Despite the substantially different pressure profiles, both models reveal the average speed of the front to be consistent with CJ theory.

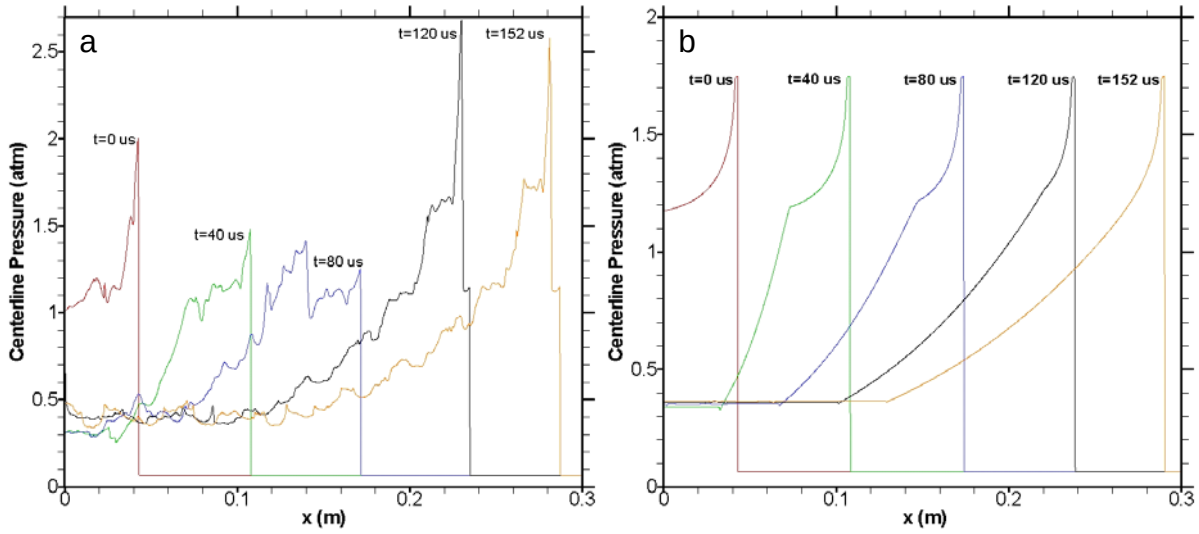

Figure 3. Centerline pressure from a) 2-D simulation versus b) 1-D simulation.

In Figure 4 the plateau pressure is plotted for both the 1-D and 2-D simulations as a function of time. The 2-D result is constructed by taking the spatially-averaged pressure over the entire wall. The small perturbation in the 1-D profile at 80 μs originally arises just behind the detonation front at the beginning of the simulation and then travels back towards the head wall. It is believed to be a startup transient caused by the use of a steady ZND initial condition.

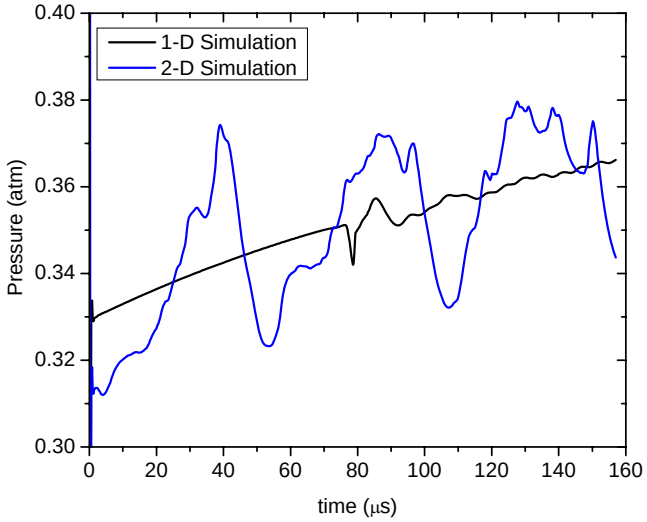

Figure 4. Comparison of 1-D versus 2-D (spatially-averaged) head wall pressure.

The small positive slope evident in both simulated results in Figure 4 is believed to be a chemical kinetic effect. Fluid particles closest to the end wall undergo the most rapid expansion as evident from the large slope of the Taylor wave visible in Figure 3 at early times. The expansion here is so rapid that the chemistry is effectively frozen throughout the Taylor wave. As the detonation moves further from the closed wall the expansion widens sufficiently such that the process is less rapid and chemical reactions now occur throughout the Taylor wave. As demonstrated by Witenberger [14] the plateau pressure is higher when a fluid particle travels through the Taylor wave along an equilibrium isentrope than when it travels along a frozen isentrope. This is due to the heat released from recombination reactions taking place during the expansion process. The magnitude of this effect is highest for fuel-oxygen mixtures with low levels of dilution [14], and in this case accounts for a small gradual pressure rise at the head wall.

The important conclusion to draw from Figure 4 is that the 1-D result effectively represents an average of the 2-D result. This indicates that transverse wave effects in this particular mixture have a negligible impact on impulse. The time-averaged, head-wall pressures predicted in both simulations are within 0.06% of one another. In future work the objective is to verify whether the role of transverse waves continues to be negligible in mixtures more commonly used in PDEs. These more practical mixtures are characterized by highly irregular cellular structure, unlike the mixture considered in this preliminary work.

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