Numerical Study of Pulse Detonation Engine with One-step Overall Reaction Model

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ABSTRACT

This paper presents an insight for the study of transient, compressible, intermittent pulsed detonation engine with one-step overall reaction model to reduce the computational complexity in detonation simulations. Investigations are done on flow field conditions developing inside the tube with the usage of irreversible one-step chemical reactions for detonations. In the present simulations 1-D and 2-D axisymmetric tubes are considered for the investigation. The flow conditions inside the detonation tube are estimated as a function of time and distance. Studies are also performed with different grid sizes which influence the prediction of Von-Neumann spike, CJ Pressure and detonation velocity. The simulation result from the single-cycle reaction model agrees well with the previous published literature of multi-step reaction models. The present studies shows that one-step overall reaction model is sufficient to predict the flow properties with reasonable accuracy. Finally, the results from the present study were compared and validated using NASA CEA.

Keywords: Pulse detonation engine, numerical simulation, CFD

NOMENCLATURE

PDE	Pulse detonation engine
ER	Equivalence ratio
ρ	Density
u	X-component of velocity
v	Y-component of velocity
P	Pressure
R	Gas constant
γ	Specific heat ratio
q	Released heat
Y	Reactant mass fraction
T_i	Activation temperature
K	Reaction rate multiplier
CFL	Courant number
A_r	Pre-exponential factor
E_r	Activation energy
Δx	Grid size
P_2	Detonation wave pressure
T_2	Detonation wave temperature
P_3	Burned gas pressure
T_3	Burned gas temperature
CJ	Chapman Jouget

1. INTRODUCTION

A detonation is a shockwave sustained by the energy released by combustion. The detonation process is initiated by the shock wave compression and the resulting high temperatures. In recent years there is a vast amount of development in detonation initiation, nozzles and ejectors, and system level performance estimates[1]. The key features of detonation are rapid species and energy conversion. Owing to its advantages of high thermodynamic efficiency, variability of thrust, etc., PDE will be the next generation's engine technology for flight applications. The review by Kailasanath[2] on PDE and its advantages gives a broader insight on the previous attempts made by researchers.

Many attempts are made to understand the unsteady, compressible flow development inside the PDE tube. Some of the early numerical simulation performance estimates are promising for generating performance maps for various thermodynamic properties. Various thermodynamic cycle calculations on the performance of hydrocarbon fuelled PDE developed by Povinelli[3], *et al.* is a major motivation for the present study. They demonstrated the effect of ethylene-air simulation with multi-step kinetics. In the analytical study done by Ma[4,5], *et al.*, it was said that the usage of a single step kinetics yield model errors in performance prediction. Another similar numerical simulation of PDE phenomenon was carried out by Kailasanath[6], *et al.* and He[7], *et al.* with multi-step and single-step kinetics respectively, helped in the investigation of flow conditions developed inside the PDE tube in the present study. A recent study by Watanabe[8], *et al.* also suggest the usage of one-step model for a hydrogen mixture stating the higher complexity in simulations of multistep chemistry. However, the simulations with detailed chemistry model increases the computational cost and time in performance prediction of PDE.

One of the main challenges to make PDEs practical is the requirement for repeated initiation of detonations within the detonation chamber. Pulse detonation engines primarily rely on deflagration-to-detonation transition (DDT) to avoid the high energy required for direct initiation. DDT is the process whereby a deflagration is initiated using a weak energy source (typically tens or hundreds of mille Joules). The subsonic flame is accelerated by creating turbulence with the help of DDT devices like Schelkin spirals, orifice plates etc., via a series of gas dynamic processes, eventually transitioned to a supersonic detonation before exiting the combustion tube. Optimisation of DDT devices is carried out basically depending on the experimental results.

There is a difficulty faced in modelling of detonation flame-front. This is due to the computational load seen in the simulations with the detailed chemical reactions i.e., multi-step reactions. Moreover, simulations with the detailed chemical reactions model take more CPU time and higher computational costs. The requirement to capture the time-accurate motion of detonation waves poses important challenges for any computational approach. So, in the present study a one-step reaction model is used to reduce the computational load.

Both one and two-dimensional numerical simulations were performed in this study. The present study mainly focuses on the performance characteristics of a PDE with a one-step overall reaction model. Comparison is done with the flow conditions obtained in the simulations done by previous published literature to validate the present study. A separate study is also done on the effect of grid resolution using flow-adaptive grids. Simplified reaction kinetics is used so that a straightforward estimate of engine parameters may be made.

2. COMPUTATIONAL DOMAIN AND TEST DESCRIPTION

In the present numerical simulation the geometry of the detonation tube selected for the analysis is similar to those of Povinelli[3], *et al.* The tube has a length of 1000 mm and a diameter of 66 mm. This tube is entirely filled with ethylene and air having an ER of 1.0. The geometries used for present analysis are 2-D axisymmetric. This is done since He[7], *et al.* in their paper said that the pressure evolution at the head thrust wall and within the tube is not very different between the planar and axisymmetric configurations. Simulations were run to see the effect of one-step reaction model. Further CFD simulations are done to study the exhaust dynamics of ethylene-air mixtures in a PDE tube.

Computations are done by completely filling the tube with the test gases. The direct initiation is done near to the closed end of the tube. So, to initiate the combustion a small region of high pressure and high temperature is used. The pressure is 4.5 MPa and temperature is 3000 K. These values are similar to those used by Povinelli[3], *et al.* for the ethylene and air simulation. After the direct ignition, the shockwave generated is transitioned into a detonation wave.

2.1 1-D Case

Flow-adaptive grids are used to resolve regions of high gradient by increasing the numerical resolution in that region.

Since, detonation is approximated as a one-dimensional problem; resolution in x-direction is done in the present study. Mesh with different grid size is used for the present study to better predict the flow properties such as detonation velocity, *CJ* Pressure, Von-Neumann spike developing inside the PDE tube. Firstly, the grid points are started with no-refinement, corresponding to the grid point size of $\Delta x = 0.20$ mm as shown in Fig. 1. Secondly, the grid points are increased to a level as refinement -1 corresponding to the grid point size of $\Delta x = 0.066$ mm in the reaction zone. Thirdly, a final refinement is done as refinement -2 corresponding to the grid point size of $\Delta x = 0.031$ mm. Mesh refinement is done in x-direction in the whole tube; no particular refinement zone is selected for refinement. Figure 1 (a) and (b) are used only for representation purposes. A brief overview of the 1-D mesh is shown in Fig. 2.
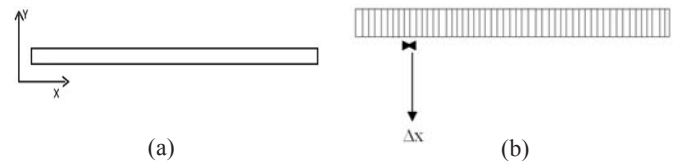

(a)   (b)

Figure 1. **(a) Dimensional Representation of the PDE tube, and (b) Grid resolution in X-direction of the PDE tube.**
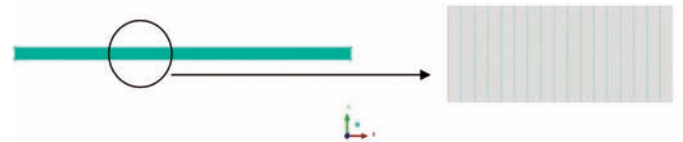

Figure 2. **Overview of mesh generated for 1-D case and a zoomed view of the mesh generated.**

2.2 2-D Axisymmetric case

In the 2-D axisymmetric simulations the computational domain consists of mainly 2-D grids. To study the exhaust dynamics of PDE tube, the computational domain is extended well downstream of the tube. This computational domain is helpful in capturing the flow characteristics external to the PDE tube. The grid generated for the 2-D axisymmetric case is shown in Fig. 3.
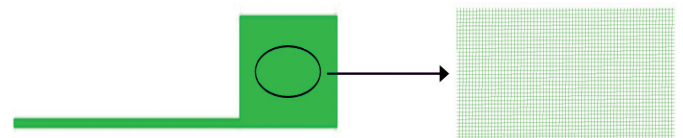

Figure 3. **Mesh generated for 2-D Axisymmetric case with zoomed view of the mesh.**

3. NUMERICAL MODELLING AND SETUP

The governing equations employed for the flow characteristics are the 2-D Euler equations. The following sets of equations are used in the simulation of PDE tube[7].

$$\vec{U}t + \vec{F}(\vec{U})x + \vec{G}(\vec{U})y = \vec{S}(\vec{U}) \qquad (1)$$

where $\vec{U}$ is a conserved variable with flux vectors $\vec{F}$ and $\vec{G}$. Furthermore,

$$\vec{U} = \begin{Bmatrix} \rho \\ \rho u \\ \rho v \\ E \\ \rho Y \end{Bmatrix} \vec{F}(\vec{U}) = \begin{Bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (E+p)u \\ \rho uY \end{Bmatrix} \vec{G}(\vec{U}) = \begin{Bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (E+p)v \\ \rho vY \end{Bmatrix} \vec{S}(\vec{U}) = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ -K\rho Y e^{-\left(\frac{T_i}{T}\right)} \end{Bmatrix}$$

(2)

and where E can be written as

$$E = \frac{p}{\gamma-1} + \frac{\rho(u^2 + v^2)}{2} + \rho qY$$

(3)

Here, ρ represents density, p represents static pressure, u and v are the x- and y- components of the velocity vector.

One-step chemical irreversible reactions are employed in the detonation calculations. The test gas mixtures are completely pre-mixed and are also considered that the burned gas is isentropically expanded. The Arrhenius rate equation used and the rate constants agree with the following reaction.

$$K_{f,r} = A_r T_r^\beta e^{[-Er/RT]}$$

(4)

To justify the selection of flow solver, the goals of the present study must be considered. The major goal of the present study is to evaluate performance characteristic of the internal flow of a PDE. Other major requirements for a solver are – it should able to simulate compressible flows and model detailed chemical reactions. The commercial code FLUENT, an Ansys[9] product is used for the present study. Stoddard[10,11], *et al.* also performed their detonation simulation using FLUENT which gave an insight for our present study. This code allows easy inclusion of complex chemical mechanisms.

This code employs Roe's 2nd order upwind scheme for discretization and Runge-Kutta method for time integration[12]. The standard limiter is the default limiter function in ANSYS FLUENT and is derived from the work of Barth and Jespersen[13]. This limiter is of a non-differentiable type and uses the Minmod function (Minimum Modulus) to limit and clip the reconstructed solution overshoots and undershoots on the cell faces. This limiter is employed in the current study. Since, the reaction time is very small, of the order of 1×10^{-8} s, time-steps of these order are employed.

Approximation of the chemical source term can trigger pre-detonation, producing unphysical detonation wave speeds. Although the particular details are different, all customary methods for finite difference, finite rate combustion computations suffer from this difficulty[14]. A fairly low CFL number (0.1 to 1) is applied based on the grid size of the model. This is done to maintain the time accuracy, since the reaction time is very small.

Initial conditions for mass fraction of reactant species, velocity, pressure and temperature are provided in the simulation. Since, the mixture used is stoichiometric ethylene-air mixture, the mass fraction of ethylene is 0.06375, oxygen is 0.21815 and rest is nitrogen. In experimental studies, self-sustained detonation is achieved using traditional deflagration to detonation transition (DDT) devices that accelerate the transition of a deflagration wave to a detonation wave. In simulations, self sustained detonation can be easily attained using high pressure and temperature as ignition conditions. This technique is known as direct initiation[15].

The detonation wave moves from the closed end to the open-end at supersonic speeds. So, to simulate this phenomenon, appropriate boundary conditions are applied in the simulation problem. The closed end of the PDE tube is considered with 'rigid wall' boundary condition and the open end is considered with 'pressure-outlet' boundary condition. The upper side of the tube is considered as 'wall' and the lower side as 'axis'. An in-viscid model is selected for the simulation.

As explained earlier the simulation of the reaction model is compared with the Povinelli[3], *et al.* simulation with ethylene-air as detonable mixture. They have used a short multi-step mechanism of Li[16], *et al.* and consists of 36 reactions among 20 species with nitrogen being treated as an inert i.e.; non reacting species. The computational target of our study is a two-dimensional axisymmetric single tube PDE. For the one-step model the parameters are chosen to be pre-exponential factor $A_r = 1.125 \times 10^{10}$, activation energy $E_r = 1.256 \times 10^8$ J/Kgmol.
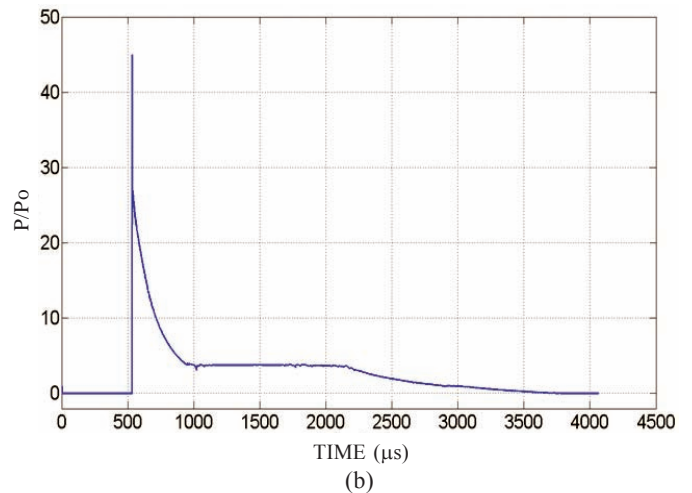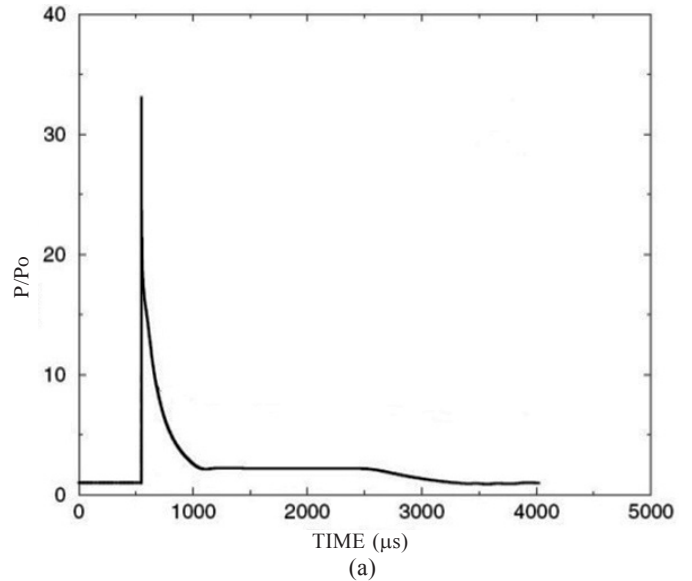

(a)

(b)

Figure 4.   Numerical comparison of pressure profile at the exit of the tube: (a) Pressure profile from Povinelli[3]. *et al.*, and (b) Pressure profile obtained from present one-step simulation.

4. VALIDATION

Figure 4 shows the pressure evolution at the exit of the detonation tube for the ethylene-air mixture for ER of 1.0. The passage of the initial detonation pressure spike rise occurred at 0.5 milliseconds which is same as the time obtained in Povinelli[3], *et al.* tests. The Von-Neumann spike observed in the present study is 4MPa which is higher than the Povinelli[3], *et al.* model. The plateau region where the pressure remains at a level value of 0.37 MPa is seen to persist up to about 2.3 milliseconds in the present study which is higher by 0.14 MPa. A brief comparison of the pressure plots from the simulation and the published literature are shown below.

The Chapman Jouguet detonation parameters were calculated using NASA CEA code[17]. The detonation speed is 1848.5 m/s in the simulations. The CEA code predicted Chapman Jouguet detonation wave speed as 1823.7 m/s.

Default value of Arrheneius rate constants were chosen for the present study which are available in FLUENT database. Stoddard[11,12], *et al.* also performed their simulations in FLUENT comprising of a single step kinetic model. It is observed and validated that the similar set of simulations were performed by Stoddard[11,12], *et al.* with the available Arrhenius rate constants. And it is also observed that the results obtained in the present study are well within the limit.

A brief qualitative comparison of the experimental shadowgraph data from University of Cincinnati[18] and the present numerical simulation of 2-D axisymmetric is shown in Fig. 5. The results of the simulations show the same characteristics as experiments with PDE. The pressure contour and shadowgraph image correspond well over time. The simulation is for ER 1.0 ethylene-air mixture and the shadowgraph is of a stoichiometric ethylene-air mixture. The times are shown below each frame, and correspond to the same time step between each frame this is basically because of variation in tube lengths.

5. RESULTS AND DISCUSSIONS

The study initially investigated the basic aspects of detonation in a tube using previous study of fuels and oxidizers. One-step chemistry is employed in the present study since these were sufficient to enable reasonable estimates for performance parameters to be derived from the computations. The study then progressed from these to compare with published literature. Investigation is done to find the effects of different grid-sizes and effect of one-step chemistry in detonation computation. This provides a simple and fast method to estimate engine parameters.

5.1 Effect of Numerical Resolution in Detonation Simulation

Since, the size of the shock front is in the order of microns, there is a need to study the mesh size effect on the fundamental detonation structure and related parameters. In the present study the two dimensional detonation computations is repeated using three different mesh sizes as mentioned previously. All the computations employ the same initial boundary conditions.
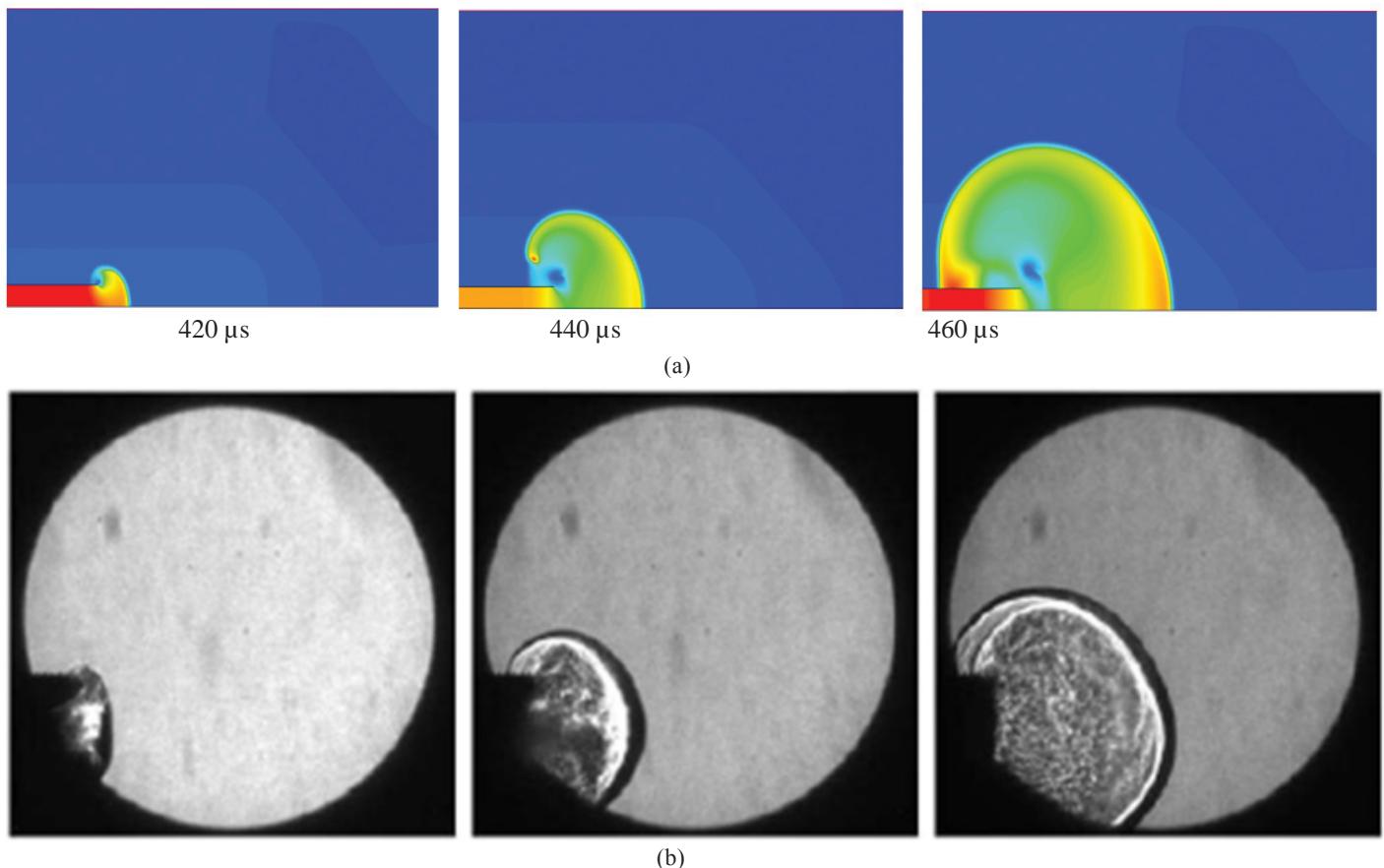

| 420 μs | 440 μs | 460 μs |
| (a) |

(b)

Figure 5. Bow shock comparison: (a) Comparison of numerical simulation to (b) Shadow graph data from University of Cincinnati[19].

The numerical computation shows that the mesh size has negligible influence on some detonation parameters. Table 1 lists the related detonation parameters for various mesh sizes. It is found that the integrated variables like detonation velocity, *CJ* pressure and wall pressure are fairly insensitive to mesh size, this was put forward by Qung[19] in his thesis. And we observe the same in the present study.

Table 1. Detonation parameters vs Mesh size

Mesh Size (Δx) (mm)	Detonation velocity (m/s)	Head wall pressure (MPa)	Von-neumann pressure (MPa) (In tube)
0.20 (No- refinement)	1848.5	1.48	7
0.066 (Refinement-1)	1848.5	1.48	6.4
0.031 (Refinement-2)	1848.5	1.48	6.2

5.2 Detonation Velocity

The detonation velocity is reproduced on all grid resolutions. The mean detonation velocity obtained from the profile of the detonation wave is about 1848.5 m/s, which is close to the theoretical *CJ* value of 1823.7 m/s calculated using chemical equilibrium code NASA CEA. The detonation velocity obtained by povinelli[3], *et al.* is same as in the present study.

The downstream mach number after the flame front is shown in Fig. 6, at time 2.24×10^{-4} s and at a distance of 0.42 m from the head end. It is evident that the mach number after the flame front is near to unity.

5.3 Pressure Evolution

Figures 7, 8, and 9, respectively show the evolution of the pressure at the exit of the detonation tube for different mesh refinements. Pressure trace at the head wall of the tube is shown in Fig. 10. The combined traces of pressure for all five positions are shown in Fig. 12.

5.3.1 Chapman-Jouget Pressure

Theoretical values of detonation parameters are predicted using NASA CEA. Ethylene-air mixture is used with
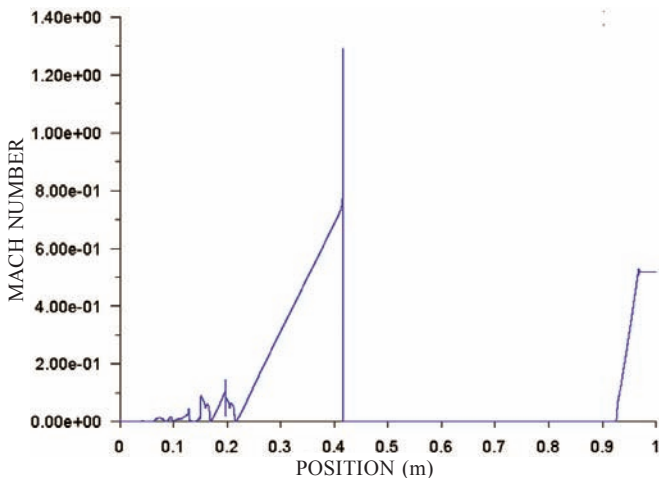
equivalence ratio 1. Standard initial pressure of 0.1 MPa and temperature 298 K is used to calculate the *CJ* parameters. Mach number obtained in the detonation problem is used further as an initial parameter for Von-Neumann pressure prediction in NASA CEA. It is observed that the *CJ* pressure obtained using NASA CEA is comparable with the present study.
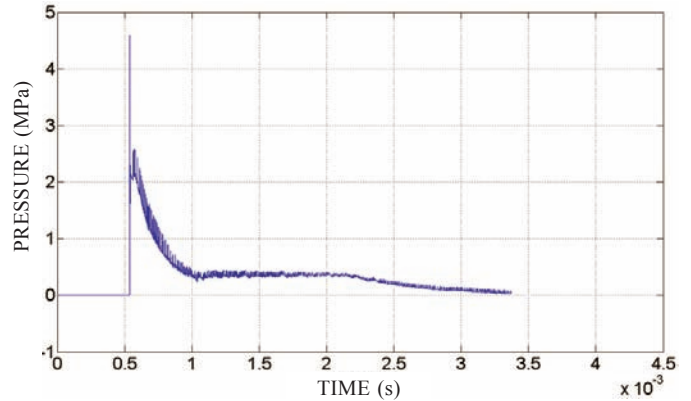

Figure 7. Profile of pressure at the exit of detonation tube (1.0 meter) as a function of time, ER 1.0 for No-Refinement mesh model.
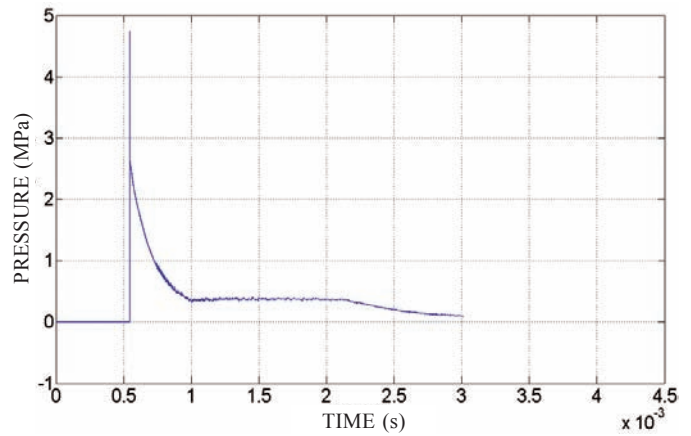

Figure 8. Profile of pressure at the exit of detonation tube (1.0 meter) as a function of time, ER 1.0 for Refinement - 1 mesh model.
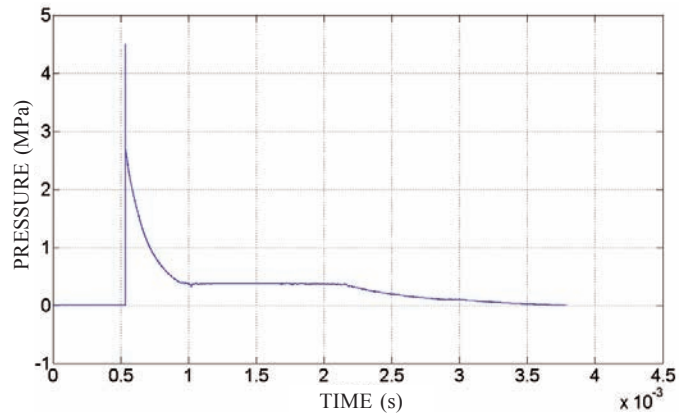

Figure 6. Plot for the downstream mach no. after the flame front in time 2.24×10^{-4} s and at a distance of 0.42 m from the head end.

Figure 9. Profile of pressure at the exit of detonation tube (1.0 meter) as a function of time, ER 1.0 for Refinement-2 mesh model.

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5.3.2 Von-Neumann Pressure

In the present study a one-step chemistry is considered, the Von-Neumann pressure spike value obtained is comparable to the value obtained by the one-step chemistry in NASA CEA. These comparisons are shown in the Table 2. Considering the present study, in NASA CEA the Ethylene-air mixture is used

Table 2. Von-Neumann pressure spikes comparison with NASA CEA and CFD

	CFD	NASA CEA
Present study (one-step global reaction)	6.8 MPa	6.7 MPa
Povinelli *et. al.* study (Multistep reaction)	3.4 MPa	3.2 MPa

with equivalence ratio 1 to validate the one-step chemistry. Here, the products are limited only to CO_2, H_2O, and N_2 such that NASA CEA solves for an incident shock condition of purely one-step chemical reaction.

5.4 Temperature Evolution

Figure 11 shows the temperature evolution at the exit of the detonation tube for ethylene-air mixture. It is seen that similar to pressure spike the temperature spike occurred at 0.5 milliseconds followed by a rapid decay within 1 millisecond.
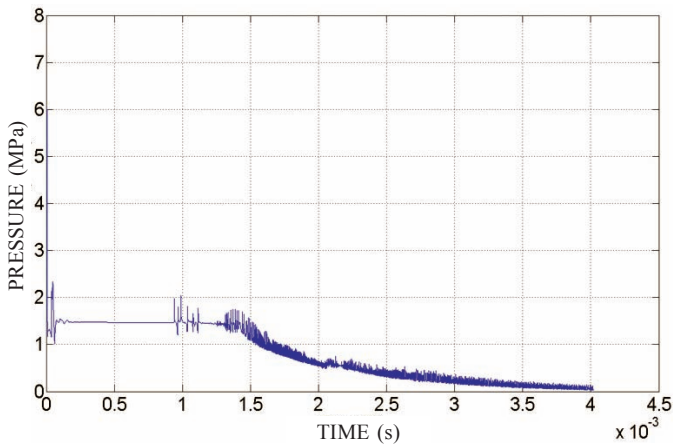

Figure 10. Profile of pressure at the head-end of detonation tube (1.0 meter) as a function of time, Equivalence ratio 1.0 for Refinement-2 mesh model.
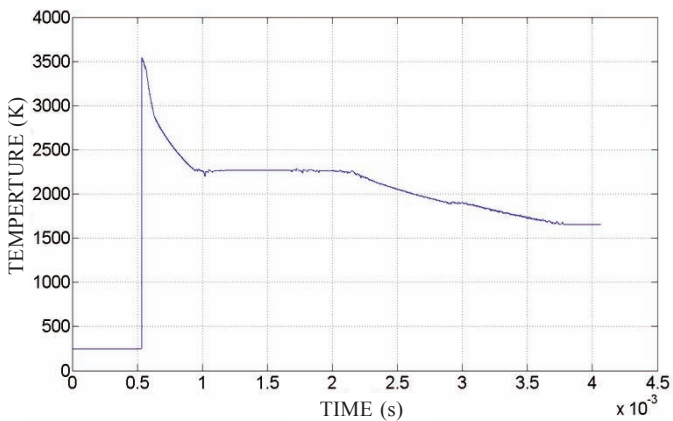

Figure 11. Profile of Temperature at the exit of detonation tube (1.0 meter) as a function of time, ER 1.0 for Refinement-2 mesh model.

6. CONCLUSION

An elementary chemical reaction model with one-step chemistry is developed for a stochiometric ethylene-air mixture. Grid dependence study is also made to understand the influence of grid sizes to the integrated variables like detonation velocity, *CJ* pressure, and head wall pressure. The thermodynamic properties and mass fractions were calculated theoretically, obtained by the chemical equilibrium code NASA CEA. Necessary comparisons made with the model are shown here. The present study gives an insight in estimating the flow conditions developed in the PDE tube by using a one-step overall reaction model. And it is observed that one-step overall reaction model is sufficient to predict the detonation velocity and detonation wave profile with reasonable accuracy.

Validation of the present numerical study is done with previously published literature. Investigation is done on the prediction of Von-Neumann pressure and is compared with NASA CEA. It is shown that the integrated variables like detonation velocity and wall pressure are fairly insensitive to mesh size. Various physical features for the detonation propagation in the detonation tube are observed in this study. This preliminary approach appears as a feasible method in predicting the parameters in a detonation tube.
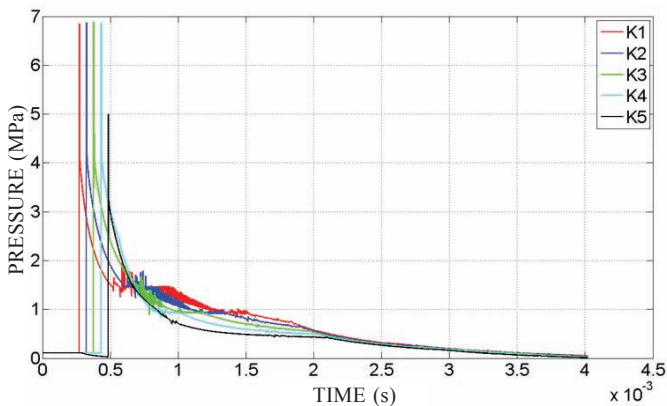

Figure 12. Profile of pressure at different locations in the tube as a function of time. *K1* is located at a distance of 500 mm from the head end and the location of *K2, K3, K4, K5* at intervals of 100 mm each.

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