Numerical Simulation of Compression and Detonation Strokes in a Pulse Compression Detonation System

Brian Maxwell[1], Konstyantyn Korytchenko[2], and Olga Shypul[3](✉)

[1] Case Western Reserve University, 10900, Euclid Avenue, Cleveland, OH 44106, USA
[2] National Technical University "Kharkiv Polytechnical Institute", 2, Kyrpychova Street, Kharkiv 61002, Ukraine
[3] National Aerospace University "Kharkiv Aviation Institute", 17, Chkalova Street, Kharkiv 61070, Ukraine
o.shipul@khai.edu

Abstract. At the National Technical University "Kharkiv Polytechnical Institute", an experimental pulse compression detonation (PCD) system was developed to operate on propane-air mixtures while addressing potential issues with regards to efficiency, ignitability of the gas, and the critical tube diameter for detonation. In this PCD system, the reactive gas was pre-compressed within the detonation tube, before ignition. The resulting mixture was found easier to ignite, and the transition to detonation within the tube was much more reliable and consistent. To gain further insight, and to investigate the effect of pressure gradient on the strength/velocity of outflow products and the overall thermodynamic cycle, a two-stage modelling procedure was adopted. First, a 3D inert simulation of the compression process of the PCD system was conducted using ANSYS. The resulting pressure and density profiles within the detonation tube were then prescribed as initial conditions for a 2D detonation stroke and outflow simulation. For this stage, the Compressible Linear Eddy Model for Large Eddy Simulation (CLEM-LES) framework adopted. For the PCD system, it was found that higher peak pressures were obtained at the outflow location of the tube when compared to a detonation tube filled initially at constant pressure equal to the ambient condition. As a result, the higher thermal efficiency of the detonation cycle may be achieved. However, it was found that the outflow products were under expanded, which may adversely affect the generated impulse. Therefore, the use of nozzles should be investigated in future work as part of the PCD system proposed here.

Keywords: Gas compression · Detonation initiation · Pressure and density profiles

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1 Introduction

At the National Technical University "Kharkiv Polytechnical Institute", Ukraine, an experimental pulse compression detonation (PCD) system was developed to operate on propane-air mixtures while addressing potential issues with regards to efficiency, ignitability of the gas, and the critical tube diameter for detonation. In this PCD system, the reactive gas was pre-compressed within the detonation tube, before ignition, using the piston-cylinder arrangement shown in Fig. 1. Similar to the design of the US-Air Force [1], the current design offers an advantage by allowing pre-compression of the gas within the tube while remaining open to the external environment.

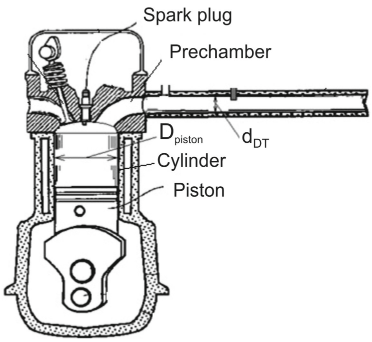


Fig. 1. Diagram of the PCD-system [3].

By pre-compressing the reactive mixture to a state of higher pressure, smaller characteristic cell size may have been achieved [2]. As a result, the mixture was easier to ignite, and the transition to detonation within the tube has been demonstrated to be much more reliable and consistent [3]. Although this experimental system has proved useful to demonstrate these advantages, in concept, the flow diagnostics are limited to pressure sensors mounted at fixed locations and flow visualization was lacking. Therefore, numerical simulations are useful to provide insight into the combustion process within the tube, the external flow field, and also the cycle efficiency.

2 Literature Review

Extensive work has already been performed on modelling detonation tube performance [4–9], such models have been limited to either application of Euler methods or gas-dynamic analysis. Moreover, the effect of viscous friction and heat loss has generally been neglected, except for Radulescu and Hanson [10], who determined that heat loss through tube walls can adversely influence performance. In addition to this past work, Perkins [11] also investigated the influence of the initial concentration gradient in the tube. However, the impact of viscous friction within the tube, and the influence of pressure/density gradients remains to be investigated, both of which are considered in the current study.

To investigate the effect of pressure gradient on the strength/velocity of outflow products and the overall thermodynamic cycle while considering tube friction, on the detonation outflow process and cycle efficiency, a two-stage modelling procedure was adopted. First, a 3D inert simulation of the compression process of the experimental PCD system [3] was modelled using a commercial CFD software (ANSYS). The resulting pressure and density profiles within the detonation tube were then prescribed as initial conditions for a 2D detonation stroke and outflow simulation. For this stage, a grid-within-a-grid approach was adopted using the Compressible Linear Eddy Model for Large Eddy Simulation (CLEM-LES) framework [12].

3 Research Methodology

Two-Stage Numerical Approach was applied as a research methodology. The compression stroke was modelled first, using ANSYS, to determine the initial pressure and density distribution within the tube before detonation initiation. The detonation and outflow process was then modelled separately using the CLEM-LES strategy, a relatively new approach to modelling highly compressible and reactive flows [12]. Justification for this approach was based on the principal assumption that time scales associated with the detonation process ($\sim 5.6 \times 10^{-4}$ s) were much shorter compared to the compression process ($\sim 1 \times 10^{-2}$ s) by at least an order of magnitude.

The compression stroke simulation was a three-dimension solution of the Navier-Stokes equations, supplemented by the SST turbulence model, using a resolution of 15 μm. The numerical domain was constructed to scale with the experimental setup and is sketched in Fig. 2a.

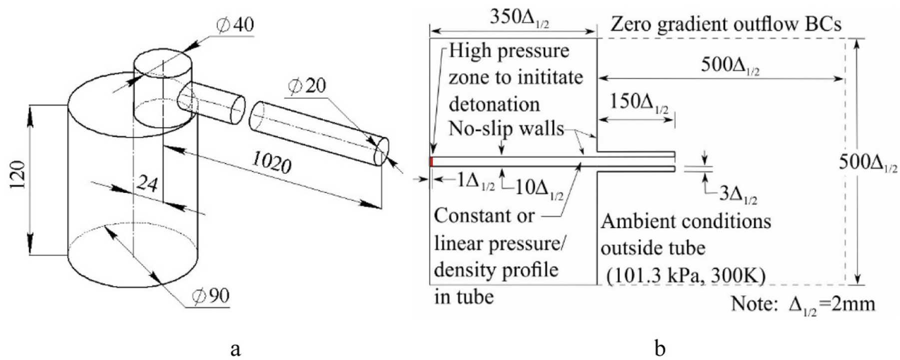


Fig. 2. Numerical domains for a) the compression stroke (in mm) and b) the detonation and outflow process.

The working fluid considered was stoichiometric propane-air, and the piston was treated as a moving wall boundary with a prescribed sinusoidal motion,

$$\upsilon_p = 18.85 \sin(\pi t/0.01), [\mathrm{m/s}] \tag{1}$$

The sinusoidal dependence approximately corresponds to a transformation of a rotate motion of the crank-shaft into the linear motion of the piston. A rotation frequency of the crank-shaft and a maximum of the piston velocity were chosen in such a manner that there is a gas compression into the detonation tube. The action of the piston, once the tube was filled with the propane-air mixture, was found to generate a linear pressure distribution within the tube, with a maximum pressure of approximately ~4 atm at the closed end.

The linear pressure distribution obtained from the compression simulation was the initial condition for the detonation stroke and outflow process simulation. A two-dimensional simulation using the CLEM-LES approach was adopted, using physical scales comparable to the compression simulation and experiment. The corresponding numerical domain is sketched in Fig. 2b, which contains no-slip boundary conditions within the tube. The pressure and density distributions in the tube:

$$p(x) = 4p_0 - 3p_0(x/L) \text{ and } \rho(x) = (p(x)/p_0)^{\frac{1}{\gamma}} \tag{2}$$

where isentropic compression was assumed. Here, $p_0 = 1$ atm and L/x represented the normalized length along the tube from the closed end, where $l = 1$ m. We note, however, that experimental evidence suggests the tube is never able to fill, resulting in concentration gradients near the open end of the tube [13]. This is currently not addressed. To initiate the detonation, sufficient energy in the form of pressure, $p = 400p_0$, was deposited within the first half-reaction length ($\Delta_{1/2}$) from the closed end of the tube. We note, however, that the actual initial flame acceleration and transition to detonation process, not modelled here, is a much more complex phenomenon originating from within the cylinder, and would likely have some impact on the cycle and performance.

Although specific details of the CLEM-LES procedure are published elsewhere [12], the chemical parameters in this study (Q = 15, E_a = 60, A = 33.000, and γ = 1.37) were calibrated to reproduce the correct detonation velocity of M_{CJ} = 5.3

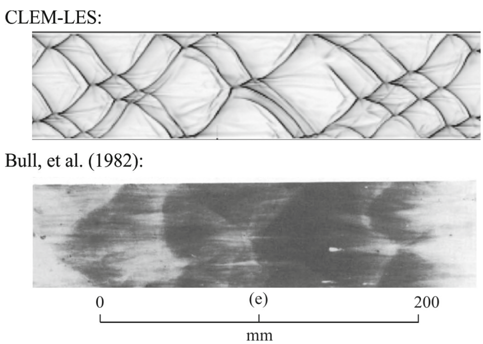


Fig. 3. To scale comparisons of sootfoils obtained using the CLEM-LES and from experiments of Bull et al. [14], for detonation propagation in stoichiometric propane-air at 1 atm.

(1807.1 m/s), half-reaction length ($\Delta_{1/2} = 2.1$ mm), post-shock laminar flame speed (S_L = 6.64 m/s at $M_D = 0.7M_{CJ}$), and cell size ($\lambda \approx 50$ mm) for stoichiometric propane-air at atmospheric conditions. A resolution of $\Delta' = \Delta_{1/2}/8$ with 64 subgrid elements within each LES cell, providing an effective resolution of $\Delta'_{eff} = \Delta_{1/2}/512$, was found sufficient to resolve both the post-shock laminar flame speed and experimentally observed cellular patterns [14] (see Fig. 3).

4 Results

A typical flow field for the outflow process of the PCD system, with initially linear pressure distribution profile, is shown in Fig. 4. Here, the outflowing hot product gases have been found to expand rapidly while driving a strong incident shockwave. Within the expanding jet, internal shock structures followed by rapid expansions were found to form, with a diamond-like pattern. This is a characteristic of typical underexpanded jet bevaviour when there exists a high pressure at the jet exit, followed by the same diamond pattern of rapid expansions and shocks [15] as the outflowing gas attempts to equilibrate with the surroundings.

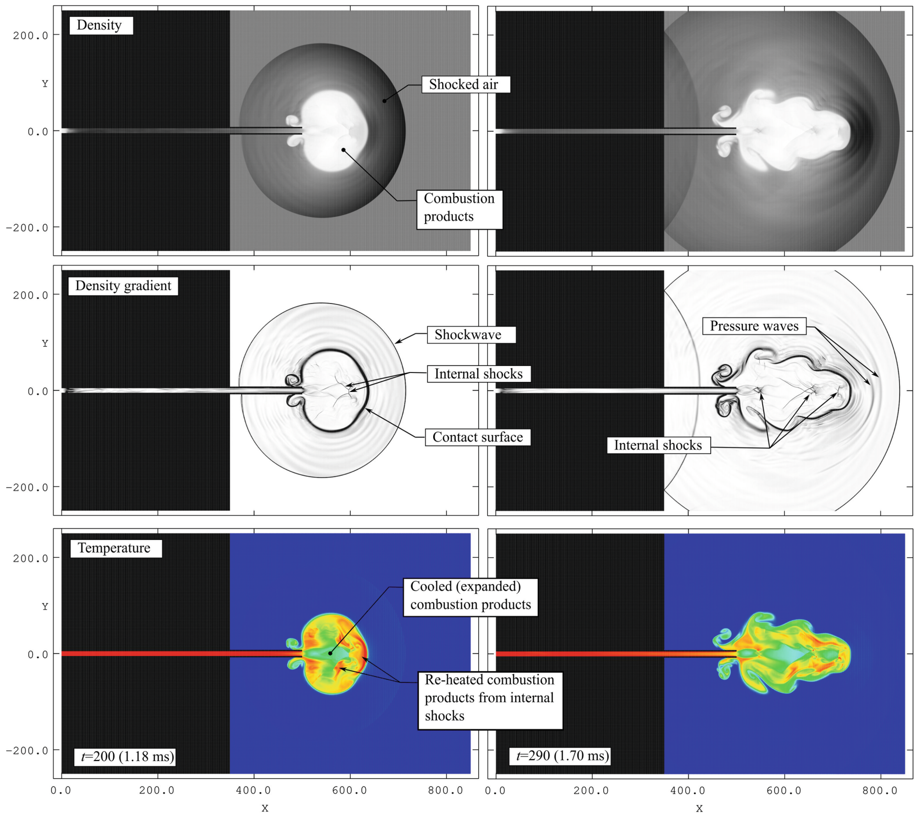


Fig. 4. Flow fields of density, density gradient, and temperature for two instances in time.

This outflow behaviour was also observed in previous investigations of pulse detonation tubes [5, 7], and is generally undesirable and leads to loss of performance. This cyclic expansion (cooling) of product gases, followed by shock-induced re-heating of the jet gas resulted in zones of varying temperature gas within the jet, with hotter regions near the jet head and outer edges of the jet outside the core regions. This behaviour is further analyzed by examining pressure and density evolutions along the centreline, y = 0, at several instances in time, as shown in Fig. 5. Here we first note the continual decay of the incident shockwave as the flow jets out of the tube. We expect the rapid expansion of the wave since there is no confinement outside the tube. We also note the development of inward-facing shocks, as labelled in the figure, which acts to continually shock the outflowing gas.

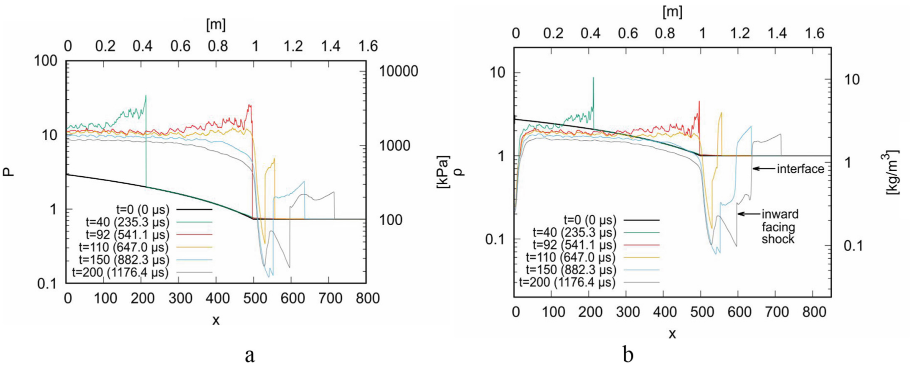
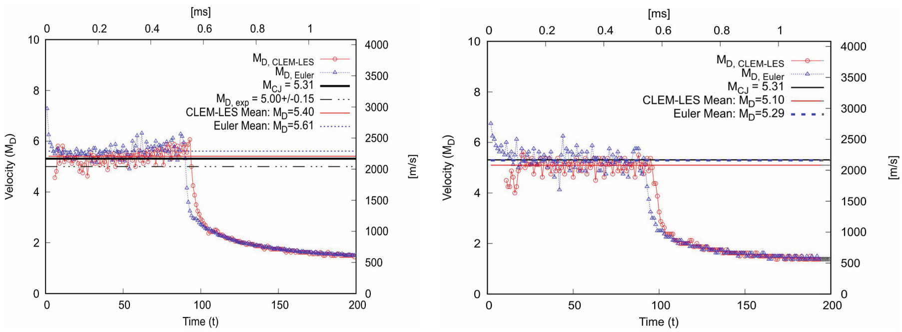


Fig. 5. Evolution of a) pressure and b) density, along the tube centreline (y = 0).

Behind each inward-facing shock, the gas always expands to lower than ambient pressures and therefore requires the formation of further shocking downstream as the jet further develops. It has previously been shown that such behaviour can adversely affect the specific impulse and thrust of the pulse detonation tube, owing to outflow pressures below ambient and entropy generation through the shocking process. As such, the use of nozzles has been suggested for promoting the expansion of the gases sufficiently before outflow into ambient to further boost efficiency [5, 7, 16, 17]. We obtained the velocity history of the wave front measured along the centreline (y = 0) to assess the performance of the PCD system. It is shown in Fig. 6.

For comparison, the PCD wave velocity was compared against a case where the tube pressure was not pre-compressed, also using the CLEM-LES. In this comparative case, the tube pressure was initialized with $p(x) = p_0$. Also, for both cases (linear and constant p), results are compared against Euler simulations. Here, wave velocities obtained for the initially linear pressure distribution profile were always found to accelerate toward the tube end, at velocities above the CJ-speed. This observation was found, in part, to be influenced by the forward motion of the unreacted gas resulting from the pressure gradient, ahead of the wave, as the pressure attempts to equilibrate with its surroundings. The detonation wave was therefore advected forward, to some



a b

Fig. 6. Wave velocity histories for the cases: a) linear pressure distribution, b) constant pressure.

extent inside the tube, leading to faster-observed wave propagation. However, the flow velocity ahead of the wave was found to be on the order of $u \sim 0.3$, at most, inside the tube. Therefore, we attribute the overdriven wave velocity to the increased pressure behind the wave as the detonation evolved in the tube.

Next, the average wave velocities obtained from the CLEM-LES, inside the tube, were found to be lower than their counterpart Euler simulations by roughly 5%. We attribute this discrepancy to boundary layer development at the tube walls. Flow divergence due to boundary layer formation behind detonations has previously been shown to produce significant velocity deficits for flows within comparatively thin channels and tubes [18–22]. We acknowledge, however, that the recorded experimental velocity was 10% lower compared to the Euler simulation, which does not account for such losses. We also note that while a 5% deficit was observed in the CLEM-LES compared to the Euler case, there are several factors not accounted for. First, the simulations were two-dimensional and did not capture the actual boundary layer development of a three-dimensional pipe. Moreover, heat loss through the pipe walls, which has not been accounted for here, may also contribute to a slower wave, and consequently a loss of specific impulse [10]. Finally, we note difficulties in ensuring perfectly stoichiometric mixtures in the experimental PCD system, which also contribute to velocity deficits.

To further investigate the performance of the PCD system, $p\text{-}v$ diagrams were constructed in Fig. 7 for the detonation cycles of both the initially linear and constant pressure distributions, using the CLEM-LES. To construct the $p\text{-}v$ diagrams, the pressure and specific volumes were obtained at $(x, y) = (500.0)$ for several time steps over the outflow process, which corresponds to the centre of the open end of the pipe. Also shown in the figure is the theoretical detonation-cycle for a wave corresponding to the perfect gas ZND-structure associated with the CJ-detonation for the parameters for Q and γ used in the numerical model. We first note that the peak pressure is never attained in the simulations. Since the cellular structure is larger than the tube, peak pressures always occur at the tube walls and not along the centre. As a result, the peak pressure along the tube centreline is always lower than the von-Neumann pressure associated with the detonation. Despite this, we note that the simulation starting with the linear pressure distribution can achieve a higher peak pressure compared to the case where the tube is initially at ambient pressure by roughly $\sim 10\%$.

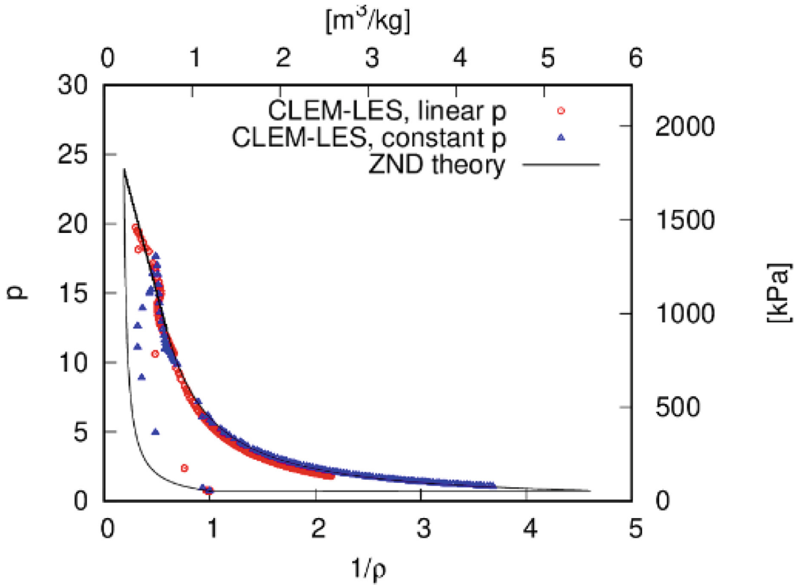


Fig. 7. *p-v* diagram for the detonation cycle.

As a result, the higher thermal efficiency of the cycle is realized by pre-compressing the gas in the tube using the PCD system. This is consistent with theoretical predictions of Wintenberger et al. [8], who found that the impulse per unit volume of the tube was directly proportional to the initial pressure, or mass of reactant in the detonation tube, i.e. $I \propto m$. In this case, the linear distribution of pressure in the tube resulted from an increase of reactant mass in the tube by a factor of 1.93 from the case where the pressure in the tube was kept constant at atmospheric conditions. In theory, the PCD system under investigation should result in nearly twice as much impulse as the constant pressure case. However, regarding thermal efficiency, a full analysis of the PCD system power input and output would be required to determine the actual useful efficiency gain of the system for practical applications.

5 Conclusion

In this work, a two-stage digital strategy was applied to model a pulsed compression detonation system. In general, the compression-detonation device allowed to permit better control the distribution of pressure, temperature and concentration of reactive gas before detonation initiation. The linear pressure profile case had M_D = 5.5 (1875 m/s), the constant pressure case had M_D = 5.1 (1739 m/s), lower than CJ (M_CJ = 5.3, 1807 m/s) due to no-slip condition in the tube walls. From this, we can conclude that the pressure gradient results in an 8% increase in wave velocity over the constant pressure case. As a result, controlled gradients of pressure in the detonation tube were realized. This was found to give rise to higher peak pressures, obtained at the outflow location of the tube when compared to a detonation tube filled initially at constant pressure equal to the ambient condition. As a result, we may conclude that a higher thermal efficiency of the detonation cycle may be achieved. However, further detailed analysis is required. Finally, it was found that the outflow products were under expanded, which contained complex gas dynamic features such as repeating inward-facing shocks and rapid expansions of the outflowing gas. It is believed that such features may adversely affect the generated impulse owing to the presence of below ambient pressures and entropy generation in the jet gas. To remedy this issue, the use of nozzles have proved useful [5, 7, 17, 23] and should be investigated in future work as part of the PCD system proposed here.

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