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Modelling of the transition of a turbulent shock-flame complex to detonation using the linear eddy model

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ABSTRACT

In the current study, the influence of turbulent mixing and local reaction rates on the transition to detonation of a turbulent shock-flame complex was investigated using a state-of-the-art large eddy simulation (LES) strategy. Specifically, detonation attenuation by a porous medium, and the subsequent re-initiation for methane–oxygen, a moderately unstable mixture, was considered. The purpose of the investigation was to validate the numerical strategy with previous experimental observations, and to determine what specific roles turbulent mixing and shock compression have on flame acceleration during the final stages of deflagration to detonation transition (DDT). The modelling procedure adopted was a grid-within-a-grid approach: The compressible linear eddy model for large eddy simulation (CLEM-LES). It was found that average turbulent velocity fluctuations greater than the laminar flame speed by an order of magnitude were required in order to maintain wave velocities above the Chapman–Jouguet (CJ)-deflagration velocity threshold, a precursor requirement for detonation re-initiation to occur. It was also found that sufficient turbulent burning on the flame surface was required in order to drive pressure waves to sufficiently strengthen the leading shock wave, locally, in order to trigger auto-ignition hot spots in the wave front. These local explosion events, which were found to burn out through turbulent surface reactions, drive transverse pressure waves outward. Upon subsequent shock reflections or interactions of the transverse waves, new local explosion events occurred, which further strengthened the adjacent leading shock wave above the CJ-detonation speed. Eventually, through this process, the wave sustained the CJ-detonation speed, on average, through the cyclic mechanism of local explosion events followed by turbulent surface reactions. Finally, combustion of the flame acceleration process was found to lie within the thin-reaction zones regime.

1. Introduction

In the current study, the influence of *turbulent mixing* rates and local reaction rates on the transition of a turbulent shock-flame complex to detonation in methane–oxygen was investigated, using a state-of-the-art large eddy simulation (LES) strategy. Particular focus on understanding the physical mechanisms which contribute to the final stages of deflagration to detonation transition (DDT) has been an active area of research in the wake of a number of recent accidents involving compressible gases. One well publicized incident, the Buncefield explosion, highlighted DDT as a major physical fundamental problem, which is not yet clearly understood. In 2005, release of hydrocarbon vapours at the Buncefield oil storage depot, England, triggered an explosion much more powerful than anyone had anticipated. Although it has recently been suggested that possible reasons for the Buncefield accident was due to the episodic combustion concept [1,2], or from a radiation-induced dust explosion [3], the Major Incident Investigation Board (MIIB) determined that detonation occurred as the ensuing flame propagated along a row of trees [4,5]. It was believed that the presence of obstacles allowed for increased turbulence and thus gave rise to enhanced combustion rates. In order to understand how detonations, or powerful explosions occur on the industrial scale, it is necessary to understand the underlying physics of how flames accelerate in compressed fluids and subsequently how transition to detonation occurs, and the mechanisms by which detonations can sustain propagation.

In order to gain insight on the final stages of DDT, a number of past experiments have been conducted using detonation interactions with perforated plates [6], or a series of obstacles, or

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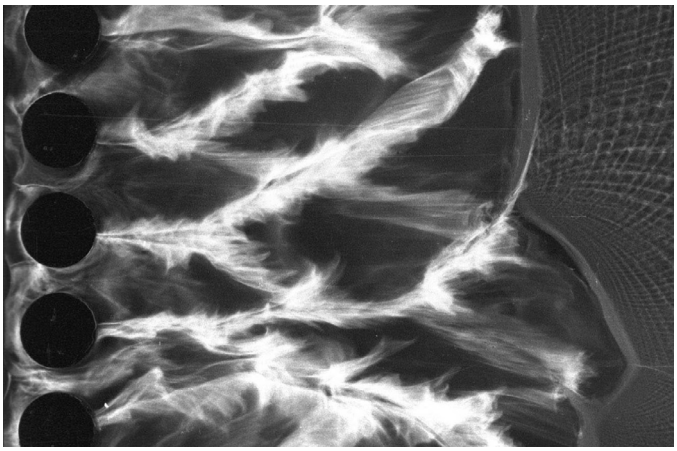

Fig. 1. Open shutter photograph showing DDT of $C_2H_2 + O_2$ at $\hat{p}_o = 5$ kPa, following detonation interaction with a porous medium [9].

blockages [7–9] to create a turbulent shock-flame complex, as shown in Fig. 1. In these experiments, detonation re-initiation was always observed by the subsequent coupling of the turbulent flame dynamics with compressible hydrodynamics, which is not yet fully understood. In general, the re-initiation of the attenuated detonation wave was found to occur through amplification of the incident shock strength resulting from shock reflections or triple point collisions [9,10]. In some cases, several shock reflections were required to accelerate the leading shock wave sufficiently in order to re-initiate the detonation. At each shock reflection, or triple point collision, the incident shock accelerates due to increased reaction rates in the un-burned gases behind the incident shock. In similar experiments, which examined *quasi-detonation* propagation in porous media [11–13], it has been shown that a wave can be sustained below the steady Chapman-Jouguet (CJ) detonation velocity [14]. Due to the velocity deficit, it is believed that *adiabatic compression* alone, from shock interactions, cannot provide the necessary energy to sustain a detonation wave. Thus, it remains unclear whether adiabatic shock compression or turbulent mixing is the dominant mechanism that drives, or re-initiates, the detonation.

In order to investigate the role of shock interactions on detonation re-initiation in unstable mixtures (prone to generate turbulent hydrodynamic structures), following wave interaction with porous media, a numerical strategy based on the Euler formulation was previously adopted [9]. Unfortunately, the numerical strategy, which did not address turbulent mixing, failed to capture exactly the correct number of shock reflections for detonation re-initiation to occur. Furthermore, the transverse detonations observed in the experiments have not been captured numerically. In order to address turbulent mixing in DDT and detonation initiation problems, through inclusion of molecular diffusion effects, some recent investigations have attempted direct numerical simulation (DNS) of the governing Navier–Stokes equations [15–18]. To capture the correct reaction rates and detonation initiation event locations, however, problems are limited to the micro-scale and often include simplified chemistry considerations. This is due to the required expense and resolution to capture mixing on the molecular scale. To address this limitation, LES is currently viewed as a reasonable compromise between accuracy of solution and resolvability of the problem. To date, a LES investigation using a *flamelet* approach [19] has been applied to model the initial states of flame acceleration due to flame interaction with obstacles. Unfortunately, the flamelet approach was not appropriate for capturing the correct reaction rate in the later stages of flame acceleration and DDT, as turbulent fluctuations were expected to increase beyond the flamelet combustion regime. To address this, Gaathaug et al. [20] have applied a hybrid LES strategy to model DDT of hydrogen–air mixtures which treats combustion in both the extreme limits of *flamelet* and perfectly mixed, *well-stirred reactor*, regimes. Unfortunately, detonation initiation events were observed to occur much sooner in the simulations compared to their corresponding experiments. This is likely due to the fact that the hybrid method does not treat combustion rates when turbulent mixing and chemical reaction rates are comparable. Finally, the *flame-thickening* approach has also been attempted with some limited success [21,22]. In this regard, the flame-thickening approach was able to produce grid-independent and converged results for detonation initiation timings and locations resulting from turbulent mixing. This approach, however, has yet to be validated against experiment. Also, the flame-thickening approach relies on the compromise of the sensitivity of the gas to shock-compression, and hence the reaction rate, in order to capture the correct laminar flame speed. This may, therefore, be problematic in predicting accurately the onset of detonation initiation events, quantitatively, for a given fuel mixture. In general, the above proposed LES investigations generally failed to adequately model DDT due to their inability to simultaneously treat autoignition and flame propagation.

To address these modelling limitations, the current study proposes the application of the compressible linear eddy model for LES (CLEM-LES) [23] to address DDT scenarios. This approach is a grid-within-a-grid approach, based on the linear eddy model for large eddy simulation (LEM-LES) [24]. The CLEM-LES was recently validated to experiments and applied to investigate the role of *turbulent mixing*, due to turbulent velocity fluctuations, on unobstructed and unstable detonation propagation in a narrow channel filled with premixed methane–oxygen at low pressures [23,25]. In this recent investigation, it was found that altering the turbulent mixing rates had a significant impact on the detonation hydrodynamic structure, cell size, and formation of un-burned pockets in the wake. It was therefore concluded that turbulent mixing, and turbulent surface reactions, are a dominant mechanism which contribute to detonation propagation.

In the current work, detonation attenuation by a porous medium, as depicted in Fig. 1, and the subsequent detonation re-initiation was modelled, numerically, using the compressible LEM-LES (CLEM-LES) approach. Accordingly, the solutions obtained were compared to recent experiments [26–28], where turbulent shock-flame complexes were generated by the passing of detonation waves through a perforated plate. Owing to the principal advantage of the CLEM-LES strategy to ensure adequate coupling of the turbulent flame dynamics with compressible hydrodynamics, and simultaneous treatment of autoignition and flame propagation, we thus address the influence of turbulent mixing on the subsequent detonation re-initiation process. As such, the application of CLEM-LES on the transition to detonation of a turbulent shock-flame complex, with strong compressible effects, has been investigated.

2. A Review of the validating experiments

2.1. Methodology

For the experiments conducted in references [26–28], whose data serves to validate the numerical investigation conducted here, a shock tube technique was used, as illustrated in Fig. 2. The shock tube was 3.4 m in total length and had a rectangular cross section whose height was 203 mm by 19 mm wide. The narrowness of its cross section in one direction permitted the establishment of flow fields with high aspect ratios whose flow structure was essentially two-dimensional. A large-scale Edgerton shadowgraph technique [29] was implemented using a 2 m by 2 m retro-reflective screen, a hig-speed Phantom v1210 camera, and a Xenon arc continuous light source [30]. Images were obtained from experiments