Numerical Simulation of Detonation Initiation by Shock-Multiple Discrete Flames Interaction

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1 Introduction

The deflagration-to-detonation transition (DDT) phenomenon is attracting renewed interest in applied research due to its potential applications in hypersonic propulsion systems such as pulse detonation engines (PDE) [1] and in process safety, particularly with the recent interest in the hydrogen economy [2]. Since the direct initiation of detonations requires a significantly large energy deposition relative to deflagrative ignition (several orders of magnitude more), DDT phenomenon is the most probable cause resulting in the formation of detonations in accidental explosions and practically is perhaps the sole initiation scheme feasible in detonation-based engine applications.

For the successful and steady operation of a PDE, repetitive initiation of detonation waves is required. However, experiments showed that in the acceleration of a flame to a detonation, the transition or run-up distance required for deflagration-to-detonation transition is highly irreproducible due to the array of turbulent and instability mechanisms that play a role in promoting transition to detonation (reviewed in Oran & Gamezo [3]). In addition, after a small spark has ignited a deflagration, the transition needs to undergo a complex flow process for the onset of detonation. Much research in pulse detonation engine development is therefore to address the key issue of finding appropriate mechanisms for rapidly generating detonation waves from DDT with a relatively weak ignition source; In other words, to shorten the distance and time required for DDT, and producing reproducible shot-to-shot performance [1, 4].

In DDT, one of the key ingredients for the rapid onset of detonations relies on the proper coupling of energy release and gas dynamic flow field. In the pioneering work by Zel'dovich et al. [5], the coupling

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resulted in the spontaneous onset of detonation is modeled by an initial gradient of auto-ignition delay time through temperature and composition non-uniformities in the pre-conditioned reactive mixture. Similar studies were subsequently carried out numerically and theoretically by a number of researchers, see Bartenev & Gelfand [6] and references therein. The coupling phenomenon was further explored by Lee & Moen [7] leading to the concept of Shock Wave Amplification by Coherent Energy Release (SWACER) which was used to qualitatively explain the photochemical initiation and turbulent jet initiation of gaseous detonations, 'explosion within the explosion' at the onset of detonation [8] and detonation formation from a temperature gradient [9, 10].

In this study, the method of using spatially distributed energy release is investigated numerically as a way to generate the coherent coupling between the gas dynamics and energy release and thus in the goal to achieve very short distances for DDT in smooth tubes. Originally, such ideas of using external sources to facilitate the onset of a detonation was proposed as early as the 1950's by Zel'dovich & Kompaneets [11] theoretically and has been applied experimentally, notably by Frolov et al. [12, 13] using controlled triggering of electric ignition. Hu et al. [14] also simulated the rapid detonation initiation by sparks modelled by a high-energy region with ignition pressure and temperature.

The objective of this work is to study numerically the possibility of deflagration-to-detonation transition resulting from shock-multiple flame interaction by extending the previous works of Khokhlov et al. [15-17]. In this numerical investigation, the phenomenon is described by a relatively weak shock wave travelling along a tube filled with a reactive mixture and an array of laminar flames ignited through different spark sequences as a means of artificially inducing chemical activity to stimulate the strong coupling required for the transition of deflagration-to-detonation.

2 Computational Details

For the present two-dimensional simulations of shock-multiple discrete flame interactions, the governing equations that describe the system are unsteady, compressible, reactive Navier-Stokes equations as detailed in the literature [15-17]. The material and chemistry properties of the reactive mixture model a stoichiometric acetylene-air mixture as a single-gas approximation and are detailed in Table 1. The majority of these values are adapted from [15], only with the transport properties and pre-exponential rate factor updated to match better the laminar flame speed and thickness [18].

The governing flow equations were integrated using the second-order, Godunov-type, Weighted Average Flux (WAF) scheme with an approximate HLLC Riemann Solver [18, 19]. Navier-Stokes fluxes were evaluated using second-order finite differences. The standard Strang's fractional step operator splitting approach is applied to approximate the solutions resulting from different source terms. The numerical solver is implemented in an adaptive mesh refinement (AMR) framework based on a hierarchical system of grids [20] to dynamically increase the resolution of a simulation in regions of interest around shocks, flame fronts and regions of large gradients in density. Five levels of AMR grid refinement are used (2, 2, 2, 2, 2). The

Mixture parameters	Value
Initial pressure P_o	1.33×10^4 Pa
Initial temperature T_o	293 K
Initial density ρ_o	1.58×10^{-1} kg/m^3
Flame temperature T_f	2340 K
Specific heat ratio γ	1.25
Molecular weight M	29
Chemical heat release Q	$35.0\ RT_o/M$
Activation energy E_a	$29.3\ RT_o$
Pre-exponential constant A_k	5×10^8 m^3/kg-s
Kinematic viscosity ν	$2.4 \times 10^{-7}\ T^{0.7}/\rho$
Heat conduction D	$2.4 \times 10^{-7}\ T^{0.7}/\rho$
Diffusion κ	$2.4 \times 10^{-7}\ T^{0.7} c_p$

Table 1. Initial condition and mixture model Parameters (adapted from [15] and [18])

base resolution combined with AMR gives an effective resolution of 7,680 × 320 cells or a Δx in the highest level equal to 47 μm, (equivalent to approximately 5 cells across the initial flame thickness of 2.5×10^{-4} m) for a computational domain 0.36 m × 0.015 m. A schematic of the computational setup for the two-dimensional simulations is shown in Fig. 1 with a computational domain denoted by $L_x \times L_y$, an initial flame radius r, incident shock Mach number M_o, and distance between discrete flames l. The circles shown in Fig. 1 represent initial flame kernels ignited before the shock passage. For simplicity, these are set up as a discontinuity between ambient and adiabatic flame conditions at T_f. The simulation is restricted to half of the domain, with a symmetry plane or reflective boundary condition applied along the lower boundary to minimize the computational expense.

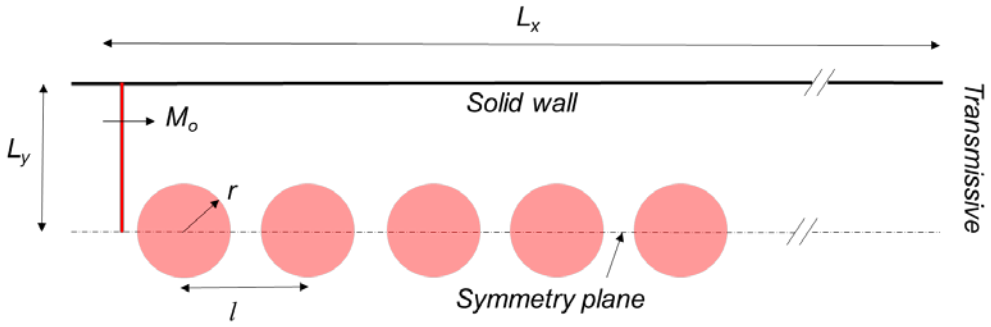


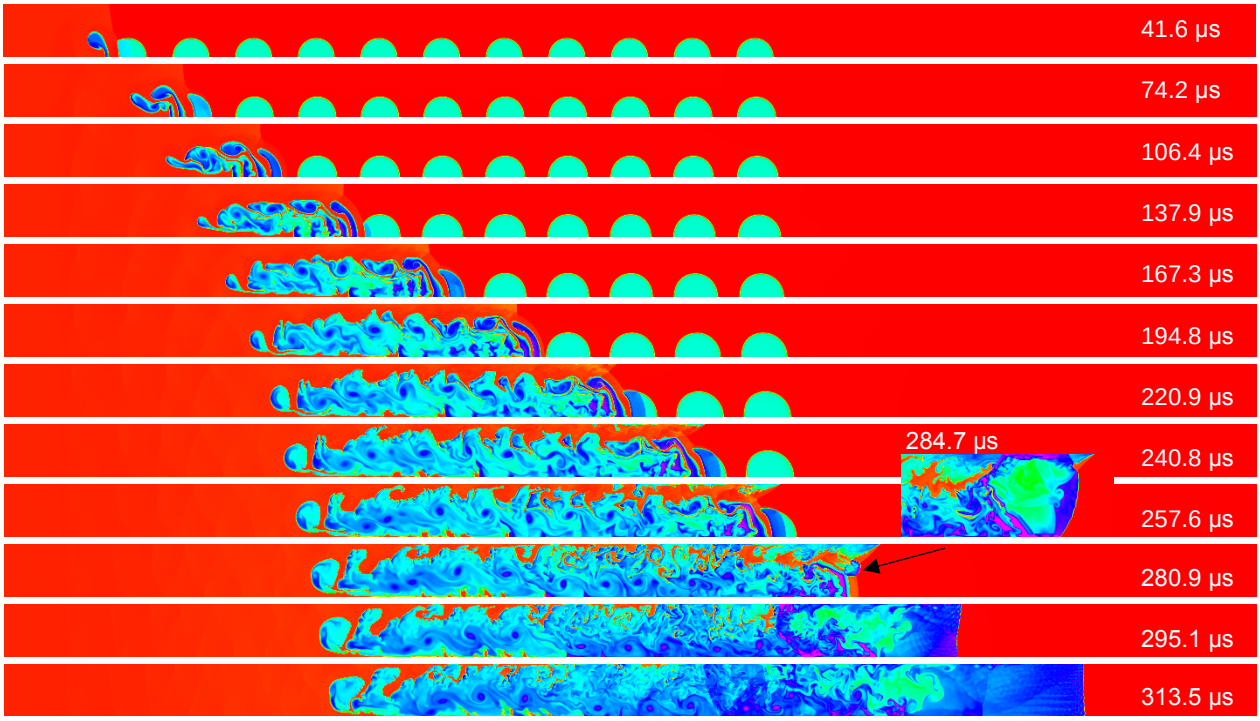
Figure 1. Schematic of the computational setup for the two-dimensional simulation. M_o, r, l and $L_{x,y}$ denote the incident shock Mach number, flame radius and distance between discrete flames, and the domain size, respectively

3 Results

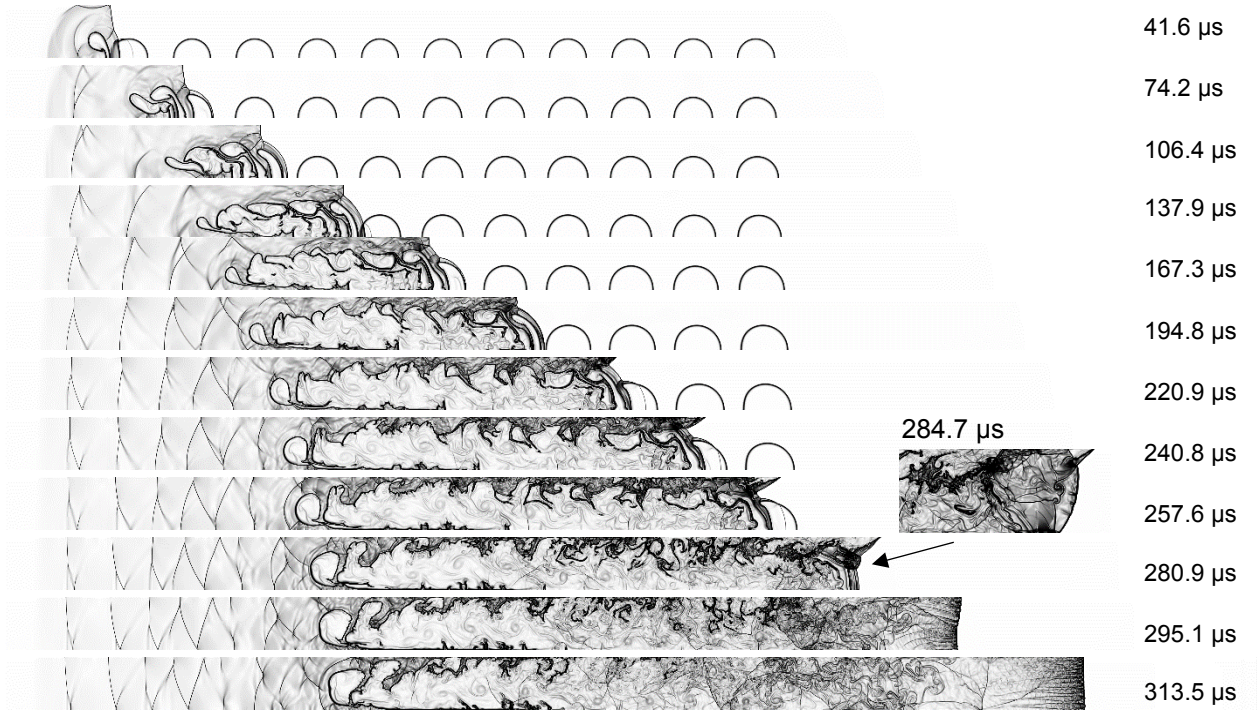
Temperature fields and Schlieren plots at different time steps with an incident shock Mach number M_o = 1.80 and twelve cylindrical flames of radius r = 5 mm equally separated by l = 18 mm are given in Fig. 2 showing the evolution of the simulation. The twelve discrete laminar flames embedded in the computational domain approximate a sequence of low energy ignitions.

The very early results showing the interaction of the weak shock with the first cylindrical flame demonstrate very good agreement with the results obtained by Khokhlov et al. [15]. The incident shock impacts the flame, causing a distortion of the flame front due to Richtmeyer-Meshkov instability. The interaction leads to the formation of a funnel of unburned reactants intruding into the burned region. The energy release continues to accelerate after the interaction due to the increase in flame surface area and higher, shock-induced, temperature of the surrounding reactants. The other laminar, cylindrical flames in front of the shock are seen to have maintained their circular shape as they continue to burn outward. It is clear that a single weak shock–flame interaction was not enough to cause prompt DDT as concluded in [15].

In the second collision, the funnel penetrates into the second flame and pushes the interface ahead. These effects repeat, resulting in intense mixing, coalescence of flame areas and compression waves generation. Through the interaction with subsequent discrete flames, the leading shock strength continues to amplify and a wrinkled flame brush is formed from the merging of the multiple flame surfaces. A series of compression waves is emitted from the shock-flame interactions and reflected from the upper solid wall. These effects create small variations in the temperature ahead of the flame brush and act to increase the overall rate of energy release in the system. At t ~ 257 μs, local ignition of unreacted materials starts to appear near the top wall. The shock interactions with multiple flames eventually trigger a transition to detonation. The transition is observed to originate from a localized explosion occurring near the domain centerline at t ~ 280 μs, as indicated by an arrow and shown in an inset. The last frame in Fig. 2 shows the onset of the detonation with the appearance of cellular structure at the wave frontal surface.



(a)



(b)

Figure 2. Two-dimensional evolution of shock-multiple discrete flames interaction and the onset of detonation starting with a weak shock M_o = 1.80. a) Temperature flow fields; and b) density Schlieren plots

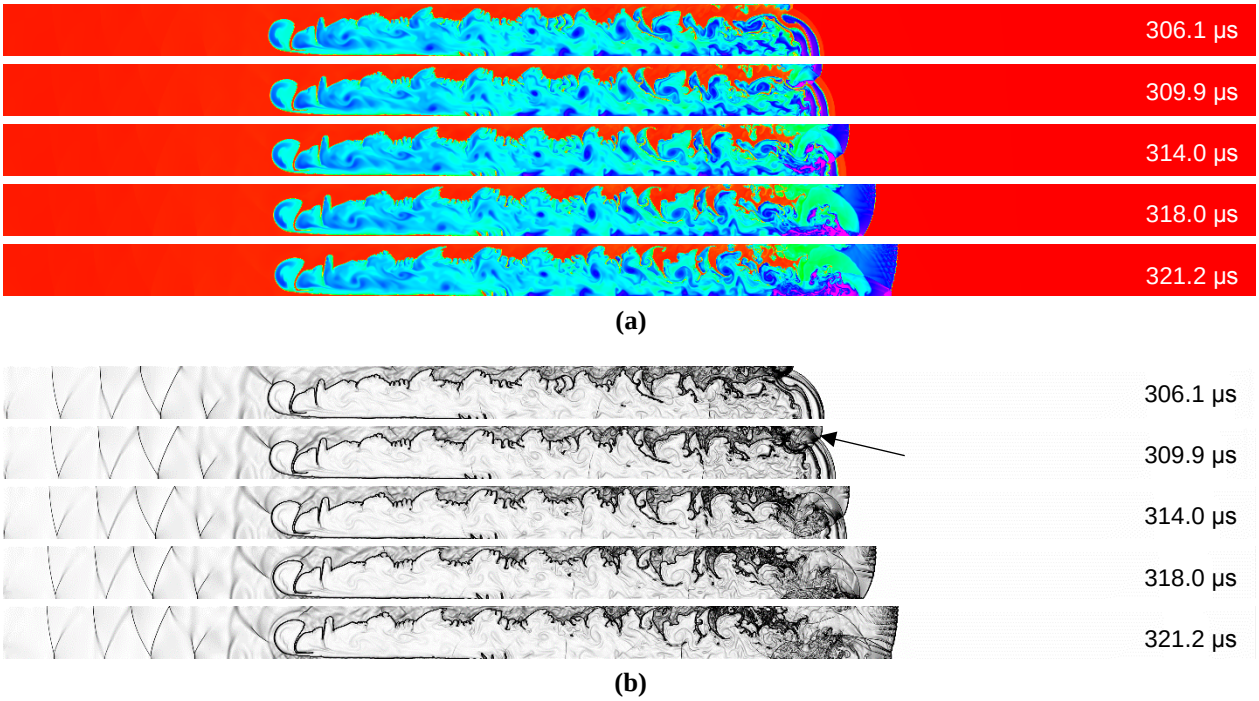


Figure 3. a) Temperature contours and b) Schlieren plots at later stage of the evolution for M_o = 1.60 showing the detonation initiation from a localized explosion near the top solid wall

Figure 3 shows the results obtained for a lower incident Mach number of M_o = 1.60. The flow field inside the flame brush formed from the shock interaction and coalescence of individual flames is relatively less turbulent. The onset of detonation is again seen from a localized explosion created in the flow by various wave interactions ahead of the flame. However, in this case, the hot spot is produced near the top solid wall. With a weaker incident shock, the onset of detonation occurs at a much later time t ~ 306 µs. However, the run-up distance for the detonation onset is close to the previous condition with M_o = 1.80. From the present results, it is found that the DDT occurs at random locations, where an appropriate condition is produced through a series of shock-flame interactions for the coupling between the heat release and gas dynamics.

4 Concluding Remarks

In this study, two-dimensional numerical simulations have been performed to observe the propagation of a weak incident shock wave into multiple cylindrical flames and its subsequent amplification via various wave interactions and reflections. Through these effects and flow disturbances, the present simulation results demonstrate that the transition to detonation is possible. The series of shock-flame interactions eventually produces a hot spot ahead of the flame brush through an increase in the energy release caused by the increase of flame surface area and the higher shock temperatures. This hot spot leads to the onset of a detonation wave. In order to assess the influence of various components of the model on the transition event and to explore any scaling relationship among different physical parameters, a parametric study is on-going with a range of simulations considering varying computational resolution and domain size, ignited flame arrangements, mixture and initial conditions, boundary conditions, and model equations (Euler or Navier-Stokes).

Acknowledgment

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