Simplified Numerical Simulation of Gaseous Quasi-Detonation Diffraction

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1 Introduction

Cellular detonation diffraction or the so-called critical tube diameter problem has long been investigated both experimentally and numerically. There is strong evidence that the unstable structure of the Chapman-Jouguet (CJ) detonation emerging from the confined tube plays a prominent role in the failure and detonation re-initiation in the unconfined area [1]. For typical unstable detonation with an irregular cellular pattern, it is believed that at the critical regime sufficient cellular instability must persist for the formation of explosion bubble leading to the detonation re-initiation [2] and the critical tube diameter d_c, above which a planar gaseous detonation propagating in a smooth tube can successfully transform into a spherical detonation, is equal to 13λ [3].

The present study is concerned specifically with the role of the unstable structure of a propagating detonation wave. In our previous studies [2, 4-6], attempts to change the level of instabilities or modify the inherent detonation frontal structure were made by using external means such as a small obstacle to induce flow perturbation or porous media to suppress detonation instabilities, and subsequently observe how the perturbed detonation responds in the critical tube diameter phenomenon. The present study attempts to look at the detonation diffraction of quasi-detonation which has inherently a different reaction structure. Quasi-detonation is referred to detonations being influenced by boundary conditions such as in an obstructed or rough tube, where the detonation velocity becomes less than the Chapman-Jouguet value [7-13]. The structure of quasi-detonations generally consists of an extended turbulent reaction zone with a relatively higher level of instabilities. For quasi-detonation, the competing effects of velocity deficit and increasing instabilities both could affect the outcome of its diffraction and transmission into the open space. It is of interest to see which of these effects play a more dominant role.

In this study, the transmission of a propagating quasi-detonation wave in a rough tube into open space is studied via two-dimensional numerical simulations based on the reactive Euler equations. The roughness required for the formation of a quasi-detonation is simulated numerically by introducing small obstacles at the computational wall boundary, creating velocity deficit and flow instability on the detonation front structure. The resulting transient transmission process and the change in critical diffraction limit for a quasi-detonation are explored. In the two-dimensional scenario, a higher degree

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of instabilities is present within a quasi-detonation structure giving rise to a more irregular cellular pattern and allow the detonation wave to re-initiate in cases where re-initiation is unsuccessful for an inherently CJ detonation initially propagating in a smooth tube without losses.

2 Problem Description

A schematic illustration showing the problem of an incident quasi-detonation wave initially propagating in a rough tube mimicked using small obstacles and subsequently diverging into the open area is given in Fig. 1. The incident quasi-detonation in the small obstacle-filled tube is first simulated separately and allowed to fully develop. The flow fields around the quasi-detonation front are then patched into the detonation diffraction simulation. The computation domain was based on a uniform Cartesian grid. A symmetry boundary condition was applied to the top boundary and hence, $D_{1/2}$ represents only half of the channel width. The bottom, the left and right boundaries of the domain were transmissive. The domain has a mesh size of 1800×600. The length of the rough section L is varied according to each roughness $\delta/D_{1/2}$ considered in this work. Here, in this simulation setup, $D_{1/2} = 250$ which is slightly lower than the critical half tube diameter in the smooth tube case [4]. In other words, at this $D_{1/2}$, the transmission always fails (no-go) in all cases with different cellular front structures emerging from the smooth tube, see Fig. 2.

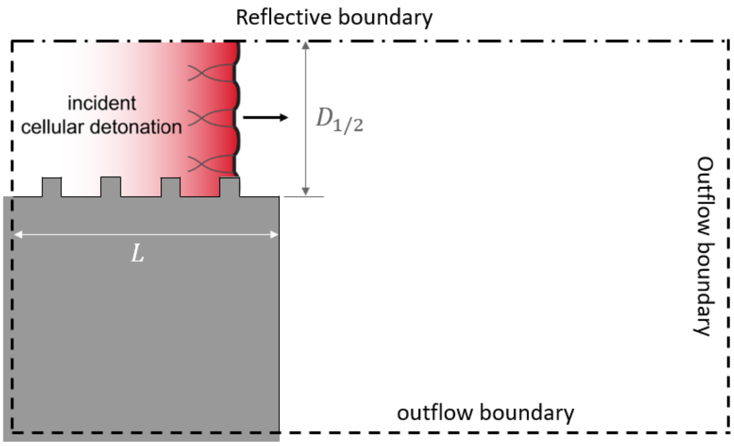

Figure 1 Schematic of the diffraction of detonation from a rough tube to an open area.

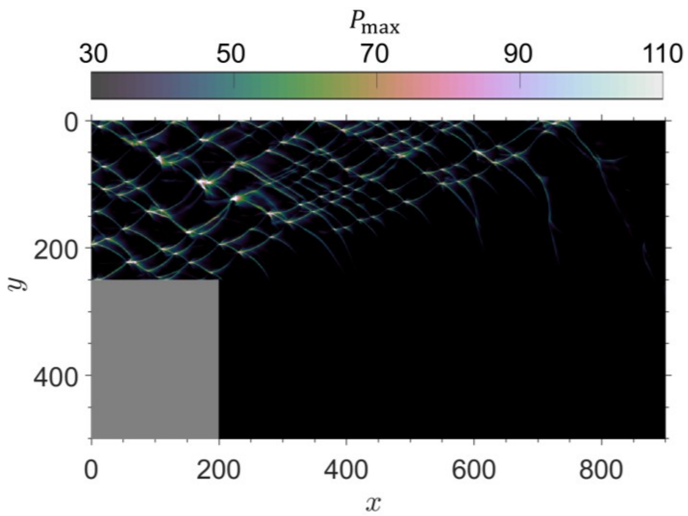

Figure 2 Detonation exiting from a smooth tube under sub-critical condition, $D_{1/2} = 250$.

For simplicity, the strategy adopted in this study is to conduct numerical simulations using an ideal-gas, reactive flow model given by the inviscid Euler equations with a simplified two-step chemical kinetic model [4, 14]. Details of the non-dimensionalized governing equations and different chemical parameters are provided in [4]. The governing equations were solved using the second-order MUSCL-Hancock scheme with a van Leer slope limiter and a Harten-Lax-van Leer-contact (HLLC) approximate Riemann solver [15-17]. A CFL (Courant-Friedrichs-Lewy) number of 0.90 was used and a first-order splitting is used to treat the hydrodynamic and reactive processes separately. Graphic-processing unit-enabled computing was used to accelerate the calculation of the fluxes across the intercell boundaries and reaction rates. This GPU-enabled simulation code has been validated and used in a series of fundamental detonation studies [16-20]. Unless specified, a default resolution of 10 pts per steady ZND induction length is used for the computations.

3 Results and discussion

Figure 3 first shows the numerical soot foil for the quasi-detonation propagating in the tube with small obstacles to mimic wall roughness. In this computational setup, the top boundary is a symmetric boundary so that the length of domain in *y*-direction is half the tube diameter, which is $D_{1/2}$. In this work, the roughness is defined by $\delta/D_{1/2}$ where δ *is* the height of the obstacles. From the numerical soot foil, one can notice the highly irregular cell pattern for quasi-detonation in the rough tube. There exist regions of re-initiation giving birth to new small detonation cells and local quenching leaving behind unburned, shocked reactive pockets (Fig. 4). These instabilities features are thus expected to promote the successful transmission of a quasi-steady detonation into the open area. Figure 5 also shows the local average velocity evolution and the global average velocity. The local average velocity is determined by tracking the mean leading front position in the *x*-direction and the dashed line in Fig. 5 shows the overall average velocity of the quasi-detonation.

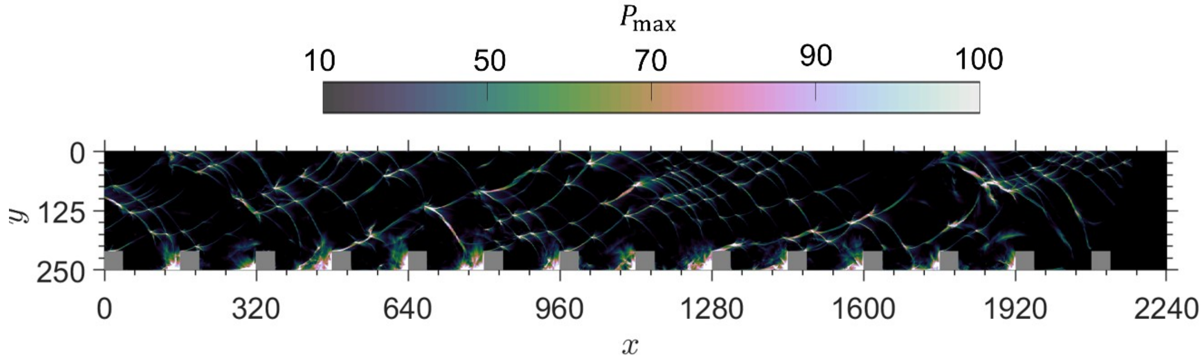

Figure 3 Cellular pattern of a quasi-detonation propagation in a rough tube with $\delta/D_{1/2} = 0.16$.

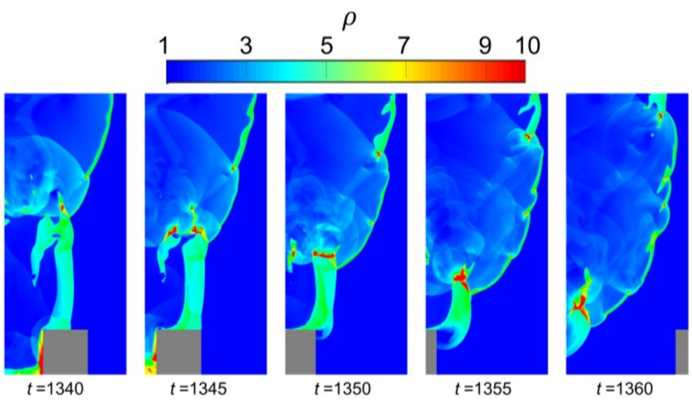

Figure 4 The unstable features at the quasi-detonation front ($\delta/D_{1/2} = 0.16$).

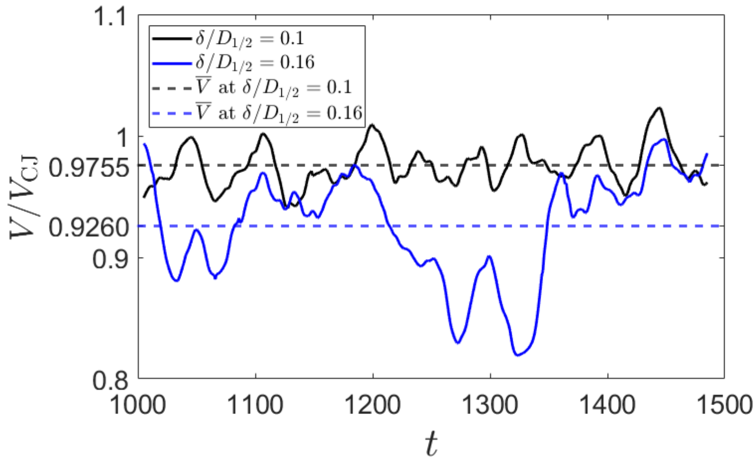

Figure 5 Local and global average velocity of the quasi-detonation propagating in tube with different degree of roughness.

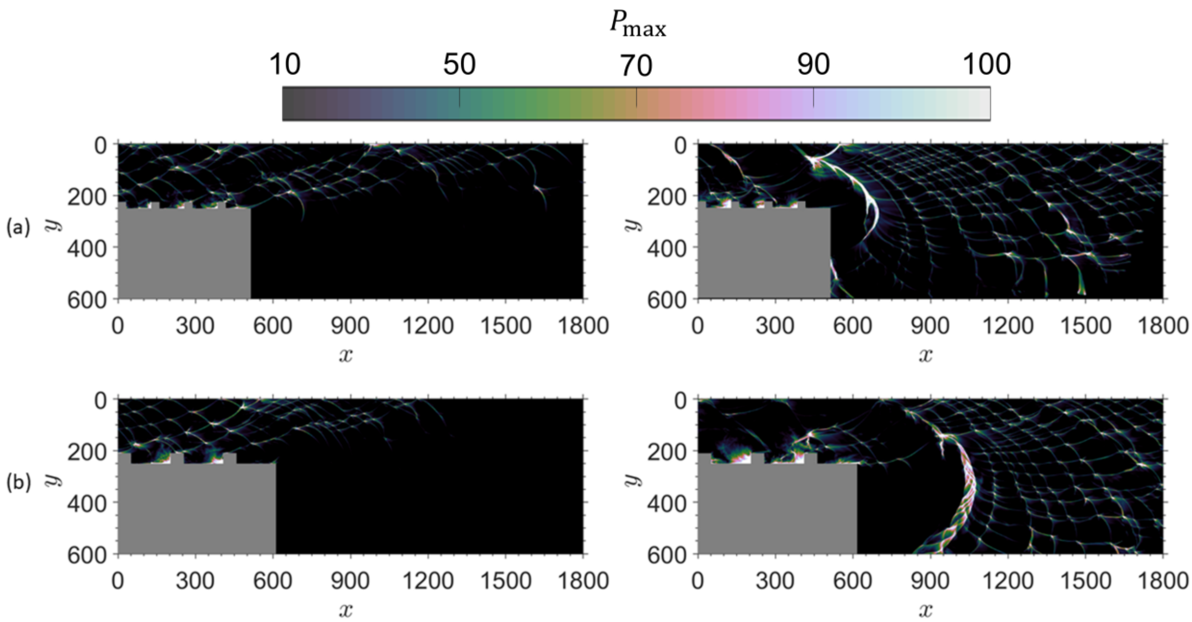

Figure 6 Numerical soot foils showing the No-go mode (left) and Go mode (right) with (a) roughness $\delta/D_{1/2} = 0.1$ and $L = 400$; (b) $\delta/D_{1/2} = 0.16$ and $L = 480$.

Since the cellular pattern of quasi-detonation is highly irregular, a significant number of simulations are repeated for each roughness by initializing the incident quasi-detonation at different locations. This resulted in different unstable quasi-detonation frontal structures exiting the rough tube. Figure 6 shows some typical results obtained from all these simulations for the two levels of roughness considered in this work. Depending on the instantaneous unstable structure of the quasi-detonation emerging from the tube, some instabilities can indeed lead to the re-initiation and successfully transmit a detonation into the open area.

Roughness $\delta/D_{1/2}$	Total number of simulation	Number of successful transmission (Go mode)	Go mode probability
0	8	0	0
0.10	20	4	20%
0.16	20	11	55%

Table 1 The probability for successful detonation transmission for different tube roughnesses

In summary, Table 1 illustrates the probability of getting detonation re-initiation for successful transmission from the total number of runs performed for each roughness. The results show that the larger the roughness, the higher probability of re-initiation. Hence, the higher instabilities at the detonation front caused by the rough wall appear to provide an additional mechanism to facilitate the transition, creating an explosion bubble and subsequently the detonation re-initiation in the open area.

4 Concluding remarks

Simplified two-dimensional numerical simulations of quasi-detonation diffraction process based on the reactive Euler equations with two-step induction-reaction chemical kinetics are performed. The results show that the quasi-detonation in rough tubes has a higher degree of instabilities (or a higher level of cell irregularity). Despite the velocity deficit of the leading detonation front, the additional inherent instabilities of the quasi-detonation appear to provide additional ingredients to promote the successful transmission or re-initiation of the detonation downstream in the open area. The present numerical results thus further support the conclusion that the failure and re-initiation mechanisms of the diffraction detonation wave are related to the degree of cellular instabilities of the detonation front emerging from the confined tube. The role of unstable features in quasi-detonation particularly their effects on the critical tube diameter phenomenon will be further explored in future work.

Acknowledgement

This work is supported by the Natural Sciences and Engineering Research Council of Canada (NSERC).

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