Numerical Investigation of the Critical Tube Diameter Problem with Modulated Cellular Detonation Fronts

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1 Introduction

In recent years, the fundamental problem of critical tube diameter has been revisited, contributing new insights into modelling the diffracting detonation front, the introduction of a novel characteristic length scale and notably, the cellular instability effects of detonation on this critical phenomenon, e.g., [1-7]. For the latter, the general observation is 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 [8, 9]. At the critical condition, the detonation re-initiation relies on the persistence of cellular instability to form an explosion bubble and trigger the onset of detonation.

The role of cellular instabilities at the detonation frontal structure on the critical tube diameter problem has been illustrated in recent years by damping the transverse waves of the emerging incident detonation [10], using a small obstacle to perturb the incident or diffracting front and induce instabilities locally [11, 12], and more recently, modifying globally the inherent unstable structure with the use of rough-walled tubes resulting in a quasi-detonation [13, 14]. For the latter, the structure of quasi-detonations generally consists of an extended turbulent reaction zone with a relatively higher level of instabilities [15, 16], providing additional ingredient to promote the successful transmission or re-initiation of the detonation downstream in the open area and overcome the effects of velocity deficit unavoidably accompanied due to the losses from the rough wall.

In a complementary study [17], we have proposed a simple approach to modulate the characteristic of the propagating cellular structure in numerical simulations using a series of micro-plates embedded in the quiescent combustible mixture. Unlike a quasi-detonation [13], while the instabilities and cellular characteristics are being changed, the strength of the detonation remains constant, i.e., no velocity deficit. Using such an approach, this work aims to investigate how the modulated cellular detonation front behaves at the critical phenomenon, and thus further confirm the role of cellular instabilities on the critical tube diameter problem.

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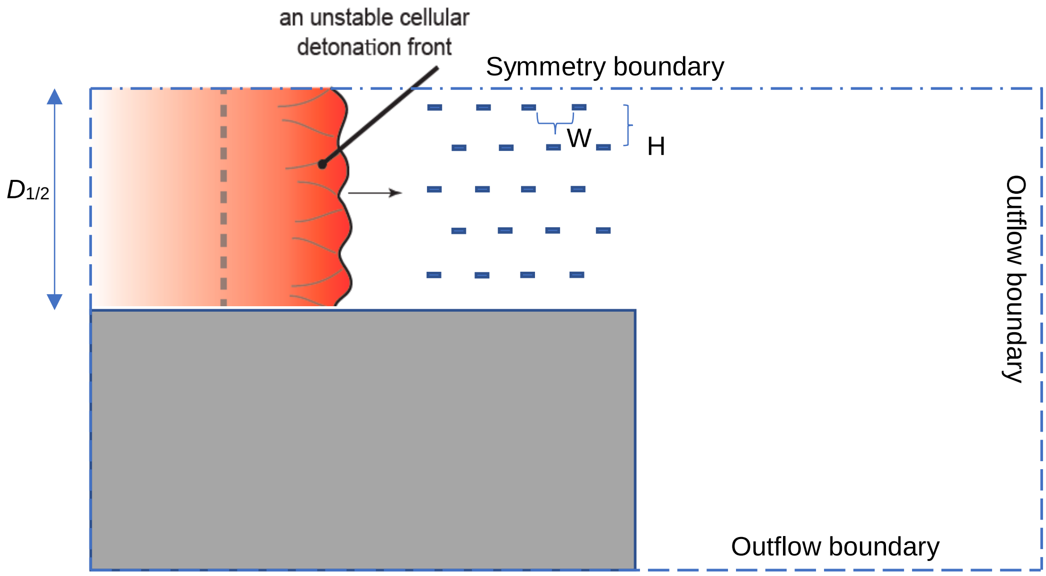


Figure 1: Numerical problem setup

2 Problem description and numerical methods

The problem is illustrated in Fig. 1. An incident Chapman-Jouguet (CJ) detonation is initiated in the confined channel and then propagates into the matrix of small, stationary obstacle plates with width ω = 15 and height η = 0.5, separated by W = 20 and H = 10, before it emerges into the open area. The domain is non-dimensionalized with the induction length Δ_I, which for this mixture was found to be Δ_I = 0.21496 mm. 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 present numerical experiment considers again two-dimensional, reactive Euler equations governed by the two-step induction-reaction kinetic model [18]. The MUSCL-Hancock scheme with the van Leer non-smooth slope limiter and a Harten-Lax-van Leer-contact (HLLC) approximate solver for the Riemann problem are used as described by Toro [19]. The state and flow variables are non-dimensionalized with respect to the unburnt state. The non-dimensional parameters are Q = 10.761 and γ = 1.313 and chemical kinetics parameters $\varepsilon_I = 6.2 \cdot T_S$, $\varepsilon_R = 0.7 \cdot T_S$, k_R = 2.371, T_S = 3.074. These parameters correspond to a stoichiometric H_2/Air mixture at p_0 = 1 atm and T_0 = 500 K. The induction pre-exponential constant k_I is scaled such that the induction zone length Δ_I of the corresponding steady ZND solution is unity. For all simulations, a resolution of 10 grid points per ZND induction zone length Δ_I is used. Graphic-processing unit-enabled computing using NVIDIA CUDA programming language (NVIDIA Corp.) was used to accelerate the simulation run-time. This GPU-enabled simulation code has been validated and used in a series of fundamental detonation studies, e.g., [12, 14, 20-23].

3 Results and discussion

The detonation propagation for at tube $D_{1/2}$ = 180 are shown in Figs. 2 to 5. Starting with the intrinsic detonation (Figs. 2 and 3), which exhibits an irregular cellular structure, it can be seen that the large area increase at the corner of the opening causes the detonation to fail locally, with a visible decoupling of the shock and reaction zone. However, the presence of instabilities leads to the formation of local explosion centers, such as the one seen in Fig. 3(d) near the top boundary. This center grows to an overdriven detonation that propagates downwards, along the decoupled front, to reinitiate the detonation and eventually lead to a self-sustained spherical detonation.

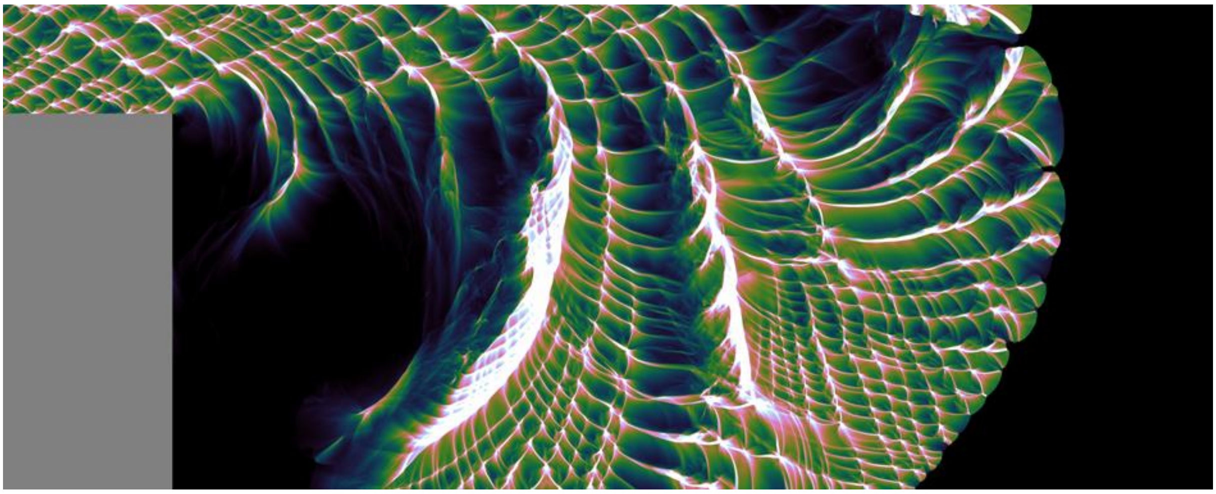
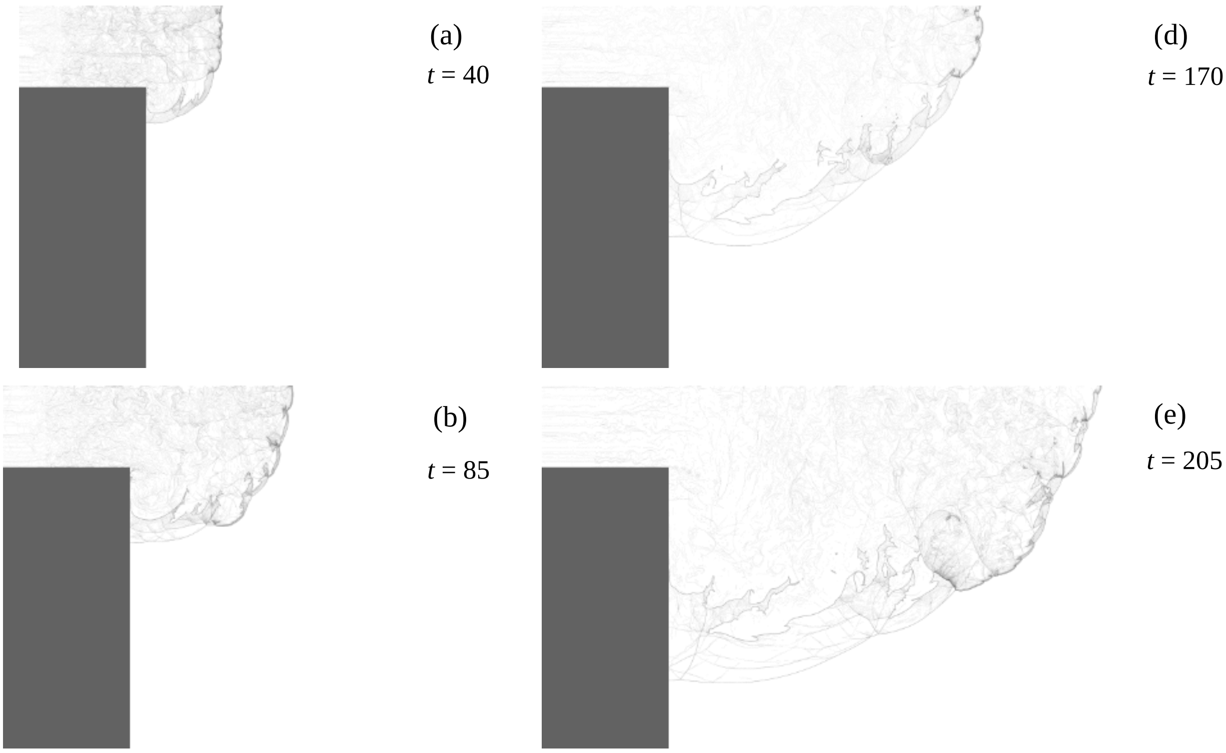


Figure 2: Soot foil of intrinsic detonation propagating to the unconfined space



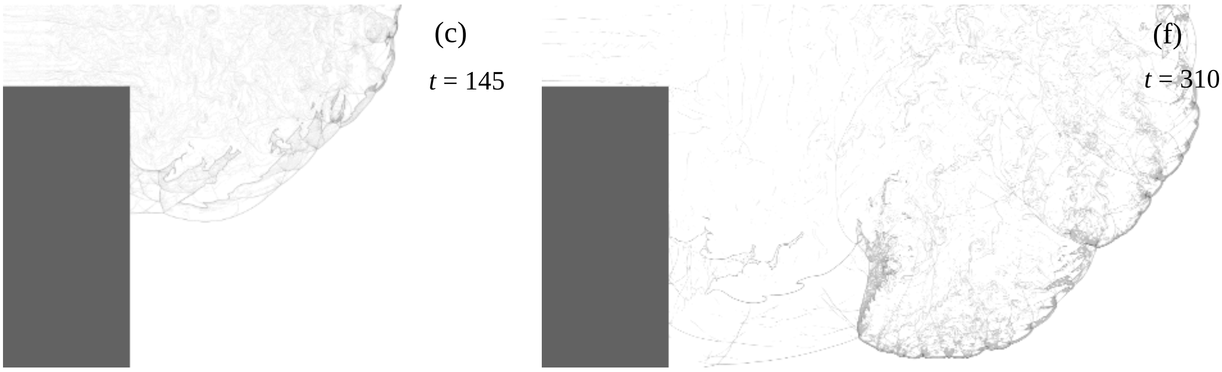


Figure 3: Schlieren plots of intrinsic detonation propagating to the unconfined space at different timings

The modulated detonation (Fig. 4) exhibits a very regular cellular structure before reaching the open area. Again the detonation starts failing near the corner of the opening, with a visible decoupling of the shock and reaction zone. However, unlike before there is no re-initiation, with the whole front fully decoupling and the detonation failing completely. The suppression of instabilities caused by the presence of the obstacles prevents the formation of any local explosions centers that could cause re-initiation and potentially survival of the detonation in the open space.

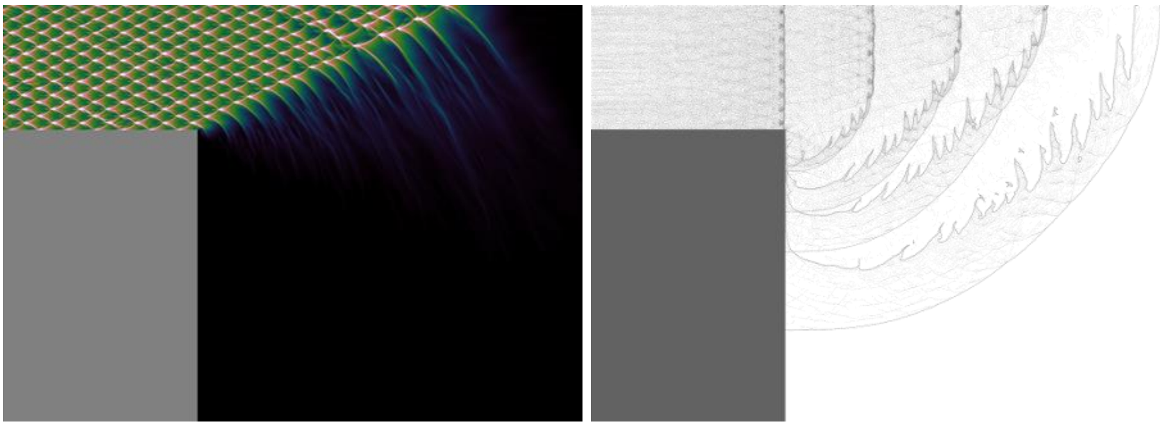


Figure 4: (Left) Soot foil of modulated detonation in the open space **(Right)** Overlay of Schlieren plots at different times for the perturbed detonation propagating to the open space at t = 0, 30, 60, 90 and 150

The outcome of the detonation transmission for different channel widths is also studied, and can be seen in Table 1. The intrinsic detonation is able to successfully transmit for much lower tube diameters compared to the modulated. The minimum diameter for the intrinsic is close to the predicted value from the closed form model [7], which estimates that for this mixture, this chemical kinetics model and parameters, the critical value is $W_*/2 = W_{*1/2} = 133\cdot\Delta_I$. For the modulated detonation, the critical diameter value is about 24 times the modulated cell size ($\lambda_m = 20$), which agrees with the 20 - $30\cdot\lambda$ criterion for detonations with regular cellular structure.

$D_{1/2}$	100	120	140	160	180	200	220	240
Intrinsic	no go	no go	go	mixed	go	go	no go	go
Modulated	no go	no go	no go	no go	no go	no go	no go	go

Table 1: Outcome of successful (go mode) or failed (no-go mode) for detonation transmission at different half- tube diameters $D_{1/2}$.

5 Concluding remarks

In this study the critical tube phenomenon was explored for an unstable detonation whose cellular structure was modulated with the placement of a series of staggered obstacles. The results showed that the modulated detonation, unlike the intrinsic, was unable to survive in the open channel due to the suppression of instabilities by the obstacles. The results also showed a much lower critical tube diameter for the intrinsic detonation compared to the modulated.

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