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A numerical study on the influence of increased instability of quasi-detonation on the critical tube diameter phenomenon

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Abstract

At critical conditions, the effect of instability plays a prominent role in the gaseous detonation transmission from a tube into an unconfined space. This study aims to clarify such an effect by investigating the critical tube diameter of quasi-detonations, i.e., detonations under the influence of minor perturbations along the tube walls. The strategy is to conduct two-dimensional numerical simulations using the reactive Euler equations with a two-step induction-reaction kinetic model. The chemical kinetic parameters were adapted to model the detonation wave in the stoichiometric hydrogen-oxygen mixture at 20 kPa and 300 K. The quasi-detonations are obtained in channels with obstacles (attached to the boundaries) of different sizes to mimic wall roughness, σ, which is defined as the ratio between the obstacle size δ and half of the channel width $D_{1/2}$. Below a critical value of σ, the rough wall creates only minor perturbations to the intrinsic cellular detonation. Apart from the velocity deficit, the degree of instability and cellular irregularity increases with roughness, resulting in a broader spectrum in the probability density function of the pressure and induction rate. For $\sigma \gtrsim 0.24$, the intrinsic propagation dynamics are more significantly altered—the cellular structure vanishes locally or small cells re-appear from new re-initiation points. Detonations in these more significantly obstructed channels are not considered quasi-detonations subjected to minor boundary perturbations. The influence of small values of roughness on the critical tube diameter phenomenon is then examined. A shot-to-shot variation in cellular dynamics of quasi-detonations is considered by performing multiple simulations for each value of roughness to assess the probability of successful transmission into an unconfined space. For quasi-detonation diffraction at the sub-critical condition, despite a velocity deficit, increasingly higher instabilities resulting from a rough-walled geometry promote the re-initiation of a detonation in the open

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area. However, if the roughness increases beyond 0.24, both the velocity deficit and different propagation modes in a significantly obstructed channel lead to a lower probability of successful transmission.
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Keywords: Quasi-detonation; Critical tube diameter; Diffraction; Rough-walled tubes; Numerical simulations

1. Introduction

Understanding the effect of boundary conditions on the propagation of detonation waves is of both practical and fundamental interests. When a gaseous detonation wave propagates in an obstructed or rough-walled tube, its velocity could become less than the Chapman-Jouguet (CJ) value due to losses. This propagation regime is usually referred to as $quasi-detonation$ [1–5]. Besides its velocity, the wave structure and even the propagation mechanism could be significantly different from the detonation in smooth tubes. In tubes with a relatively low blockage ratio or roughness, the detonation could retain its cellular characteristics but the reaction structure becomes tortuous and increasingly irregular [6,7]. Previous photographic study [8,9] also indicates a highly turbulent zone behind the leading front of the quasi-detonation. The present study is focused on the transmission of this quasi-detonation wave from a rough-walled tube into an open area and the role of the unstable reaction-wave structure on the so-called critical tube diameter problem.

The critical tube diameter d_c, refers to the minimum tube diameter below which a gaseous detonation propagating in a confined boundary fails to transform into a spherical detonation in an unconfined space [1,10]. Previous studies, either experimentally or numerically, have focused mainly on the critical conditions and diffraction of a CJ detonation emerging from a smooth tube, e.g., [10–23]. For a typical unstable detonation with an irregular cellular pattern, there is strong evidence that the unstable structure of the detonation emerging from the confined tube plays a prominent role in the detonation failure and re-initiation in the unconfined area [22]. In the critical regime, sufficient cellular instability must persist for the formation of an explosion bubble leading to the detonation re-initiation [23]. In our previous studies [24–26], 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-detonations with an inherently different reaction-wave structure. For quasi-detonations, the competing effects of velocity deficit and increasing level of instabilities both could affect the outcome of its diffraction and transmission into an open space. This problem thus sheds light on which of these aforementioned effects play a more dominant role. In our recent experimental study [27], it is shown that the quasi-detonation with a more irregular cellular pattern has essentially the same critical pressure for transmission as for a CJ detonation despite a noticeable velocity deficit. Based on computational analysis, the present work provides an explanatory paradigm to illustrate the details of the diffraction process experimentally examined in [27] and the significance of the unstable reaction-wave structure in the critical phenomena of gaseous detonations.

Although there exist quasi-two-dimensional, inviscid formulations for modeling wall effects into the inviscid core flow, e.g., [28], this study opts for another simplified approach to reduce the computational effort while mimicking the experimental setting [27] and physical characteristics of the critical tube diameters of quasi-detonations. 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 [29]. 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 quasi-detonations are explored. This simplified approach allows us to better isolate gas-dynamic effects and address the role of cellular irregularity on the critical tube diameter phenomenon.

This paper is organized as follows. In Section 2, the physical geometry, the ideal detonation model by the two-dimensional reactive Euler equations with a two-step induction-reaction kinetics, and the numerical method for solving the governing equations are described. In Section 3, simulation results are presented, showing that in the two-dimensional scenario, a higher degree of instabilities is present within a quasi-detonation structure propagating in rough-walled channels within a critical roughness degree, giving rise to a more irregular cellular pattern. For increasing roughness, the results become less relevant as the physical scale of the isolated obstacles strongly influences the quasi-detonation dynamics, causing a different propagation mechanism of failure and re-initiation in the obstructed channel. Within the critical roughness, the increased instabilities allow the detonation to re-initiate in cases where re-initiation is unsuccessful for an inherent CJ detonation initially propagating in a smooth tube without losses. The implication of these results on the prominent role of instabilities in detonation diffraction is discussed. The influence of shot-to-shot variation in cellular dynamics is also illustrated from the statistical analysis. Section 4 concludes the paper.

2. Numerical model description

2.1. Governing equations

Following previous studies, e.g., [13,16,19,20,24], this study adopts also the ideal detonation model with governing equations given by the reactive Euler equations:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = \mathbf{S},$$
$$\mathbf{U} = (\rho, \rho u, \rho v, \rho e, \rho \xi, \rho \beta)^{\mathrm{T}},$$
$$\mathbf{F} = (\rho u, \rho u^2 + p, \rho uv, \rho u(e+p), \rho u \xi, \rho u \beta)^{\mathrm{T}},$$
$$\mathbf{G} = (\rho v, \rho uv, \rho v^2 + p, \rho v(e+p), \rho v \xi, \rho v \beta)^{\mathrm{T}},$$
$$\mathbf{S} = (0, 0, 0, 0, \dot{\omega}_{\mathrm{I}}, \dot{\omega}_{\mathrm{R}})^{\mathrm{T}}, \tag{1}$$

with $e = \frac{p}{(\gamma-1)\rho} + \frac{1}{2}(u^2 + v^2 - \beta Q)$ and $p = \rho T$. The variables ρ, u, v, p, T, e, and Q are the density, velocities in x- and y- direction, pressure, energy, and the amount of total chemical heat release, respectively. Although studies have shown that quantitative properties of cellular detonation, such as the cell size and species evolution within the reaction zone, are sensitive to the chemical reaction models used in the numerical simulations, especially those with pressure dependence reactions, e.g., [30,31], this work aims to conduct a comparative study on the overall cellular dynamics of the base case of a weakly unstable detonation in a smooth tube and that of a quasi-detonation in rough wall tubes and their critical transmission into the open area. Therefore, a well-used, simplified two-step induction-reaction Arrhenius kinetic model [16,29,32–34] is considered for the two source terms in Eq. (1):

$$\dot{\omega}_{\mathrm{I}} = \mathrm{H}(1-\xi)\rho k_{\mathrm{I}} \exp\left[E_{\mathrm{I}}\left(\frac{1}{T_{\mathrm{s}}} - \frac{1}{T}\right)\right], \tag{2}$$

$$\dot{\omega}_{\mathrm{R}} = [1 - \mathrm{H}(1-\xi)]\rho(1-\beta)k_{\mathrm{R}} \exp\left[\left(-\frac{E_{\mathrm{R}}}{T}\right)\right], \tag{3}$$

where E_{R} is the activation energy of the exothermic reaction, E_{I} is the activation energy of the thermally neutral induction process, β is the product fraction, T_{s} is the post-shock temperature, and $\dot{\omega}_{\mathrm{I}}$ and $\dot{\omega}_{\mathrm{R}}$ are the induction and reaction rate respectively and the Heaviside step function $\mathrm{H}(1-\xi)$ is given by:

$$\mathrm{H}(1-\xi) = \begin{cases} 1 \text{ if } \xi \le 1, \\ 0 \text{ if } \xi > 1. \end{cases} \tag{4}$$

All the terms, parameters and variables have been non-dimensionalized by reference to the uniform unburned state ahead of the detonation front. The pre-exponential factor k_{I} of the induction step is determined manually to define the reference length scale of the mesh so that the induction length is unit, i.e., $\Delta_{\mathrm{I}} = 1$, or $k_{\mathrm{I}} = -u_{\mathrm{vn}}$. In this study, the same dimensionless thermodynamic parameters of the combustible mixture as in [24] are considered, i.e., $Q = 21.365$, $\gamma = 1.32$, $T_{\mathrm{s}}/T_{\mathrm{o}} = 5.0373$, $E_{\mathrm{I}} = 5.414\ T_{\mathrm{s}}$, $E_{\mathrm{R}} = 1.0\ T_{\mathrm{s}}$, $k_{\mathrm{I}} = 1.0022$, $k_{\mathrm{R}} = 4.0$ and the Chapman Jouguet (CJ) Mach number $M_{\mathrm{CJ}} = 5.0984$ (corresponding to CJ detonation velocity $D_{\mathrm{CJ}} = 5.858$). The procedure to determine these parameters is detailed in [24]. The thermodynamic properties approximately represent the Zel'dovich-von Neumann-During (ZND) detonation structure of the stoichiometric hydrogen-oxygen mixture at 20 kPa and 300 K, determined using the detailed hydrogen combustion kinetic mechanism by Li et al. [35], giving rise to an unstable CJ detonation wave with an irregular cellular pattern. The steady ZND induction length at these conditions is calculated to be 0.253 mm. Using the experimental data from the Caltech detonation database [36], the non-dimensional cell size $\lambda/\Delta_{\mathrm{I}}$ equals 38.9 with a relatively large standard deviation of 14.0 due to the significant variance in the experimental measurement.

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 [37]. 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 (using Nvidia Tesla V100 graphics processing units) was utilized to accelerate the calculation of the fluxes across the intercell boundaries and reaction rates. The GPU-enabled simulation code has been validated and used in a series of fundamental detonation studies, e.g., [38–41]. In this work, the default resolution considered is 10 points per induction zone length Δ_{I}, i.e., $\Delta_{\mathrm{I}}/\Delta_x = 10$. The resolution validation will be given in the next section.

2.2. Simulation setup

Fig. 1(a) shows a schematic of the computational setup with an incident quasi-detonation wave initially propagating in a rough channel mimicked using small obstacles and subsequently diverging into the open area. The computation domain was

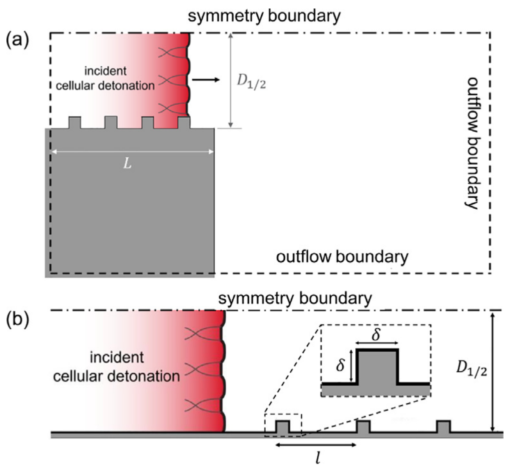

Fig. 1. Schematics of (a) diffraction of detonation from a rough-walled channel to an open area and (b) the incident cellular detonation generated in a rough-walled channel.

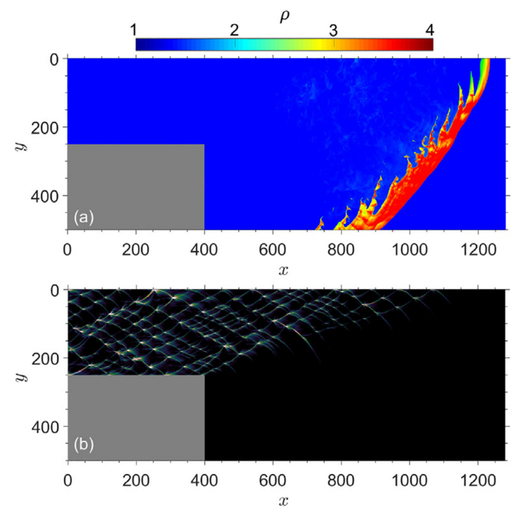

Fig. 2. Detonation exiting from a smooth channel under sub-critical condition, $D_{1/2} = 250$, (a) density flow field, (b) numerical soot foil.

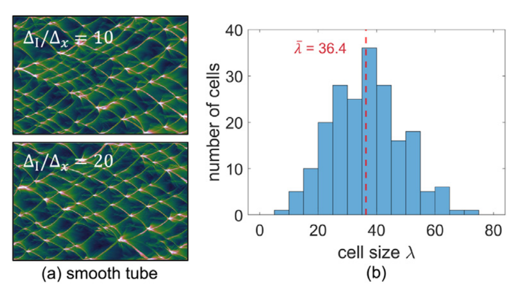

Fig. 3. (a) Numerical soot foils showing the cellular detonation structure in a smooth tube obtained with two resolutions and (b) the numerical cell size distribution counted from 200 cell samples in a long soot foil for cellular detonation propagating in the smooth tube.

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, left and right boundaries of the domain were transmissive. The domain has a mesh size of 1800×600. The incident quasi-detonation in the small obstacle-filled channel is first simulated separately with a very long channel length to allow it to fully develop, see Fig. 1(b). After sufficient propagation, the flow fields around the quasi-detonation front are then patched into the detonation diffraction simulation. The side length of square obstacles is denoted as δ and the distance between two consecutive square obstacles l, is fixed at four times the side length, i.e., $l = 4\delta$. The wall roughness σ is defined by the obstacle side length to the half channel diameter $\sigma = \delta/D_{1/2}$. For the diffraction simulations, the length of the rough-walled section L is varied according to each roughness σ considered in this work. Here, in this simulation setup, $D_{1/2}$= 250 which is slightly lower than the critical half channel diameter in the smooth channel case [24]. In other words, at this $D_{1/2}$, the transmission always fails (no-go) in all cases regardless of the different cellular structures emerging from the smooth channel, see Fig. 2 for the corresponding numerical soot foil and temperature flow field showing the decoupling between the reaction zone and diverging front with cell disappearing.

As part of a resolution study, Fig. 3(a) shows a direct comparison of the cellular detonation structures in a smooth tube obtained with $\Delta_I/\Delta_x = 10$ and 20. The cell irregularity shown in the soot foils is qualitatively similar and the cell size λ agree approximately with each other. Fig. 3(b) also shows the numerical cell size distribution counted from 200 cell samples in a long numerical smoked foil for cellular detonation propagating in the smooth tube. The non-dimensional cell size λ/Δ_I is found to be 36.4 and the standard deviation is 12.3, which agrees well with the experimental data considering the irregularity of the cell patterns. Fig. 4(a) also shows a comparison of the cellular detonation structures in a rough-walled tube obtained with two resolutions. The average detonation velocities with different roughness values converged with both grid resolutions, see Fig. 4(b). Another equivalent resolution study is also reported in [24]. Shi et al. [19] using a one-step Arrhenius kinetics also demonstrates a similar resolution range, i.e., a 16 pts per half-reaction zone length $l_{1/2}$, is sufficient to determine the critical condition for the detonation diffraction. To this end, considering also the goal of this comparative study, the mixture condition and roughness level, a grid resolution of $\Delta_I/\Delta_x = 10$ is deemed sufficient and used for all simulations.

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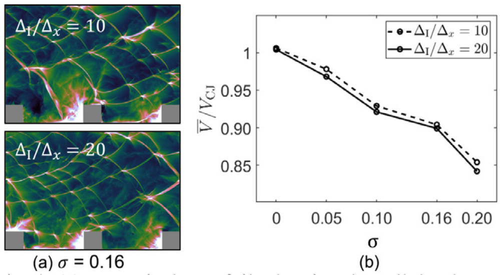

Fig. 4. (a) Numerical soot foils showing the cellular detonation structure in a rough-walled tube $\sigma = 0.16$ and (b) the average detonation velocity with different roughnesses obtained with a resolution of $\Delta_I/\Delta_x = 10$ (dashed line) and 20 (solid line).

3. Results and discussion

3.1. *Quasi-detonations in rough-walled channels*

Figs. 5 and 6 show the numerical soot foils and frontal velocity evolution for the quasi-detonation propagating in rough-walled channels with different sizes of small obstacles to mimic various degrees of wall roughness: $\sigma = 0$ (smooth channel) to $\sigma = 0.28$. Recalled that the numerical soot foils record the maximum pressure in place to present the trajectory of the triple points in detonation front and the local average velocity is determined by tracking the mean leading front position in the x-direction. To record the oscillation features of the detonation velocity, the velocity data is collected over 1200 transient snapshots.

From the numerical soot foils, one can notice the increase of roughness in the wall channel resulted in highly irregular cell patterns for quasi-detonations. Fig. 5(a) first gives a cellular structure of the CJ detonation propagating in a smooth channel as a reference. As shown in Fig. 5(b) and (c), i.e., the rough-walled cases with $\sigma = 0.1$ and 0.16, the cellular patterns are strongly disturbed and cells are enlarged in some regions while relatively unperturbed cells remain in the most part of the channel. The cell sizes of quasi-detonations in rough-walled channels are also greater than those resulting from a smooth channel. Overall, for relatively low σ (up to 0.2), the cellular frontal structure of the quasi-detonation is retained. In other words, the presence of the wall roughness only generates perturbation and induces irregularity to the cellular quasi-detonation front.

For $\sigma = 0.2$, the cellular quasi-detonation pattern is highly irregular. At some propagation instances, the wall roughness causes cell enlargement and partial decoupling of the leading front from the reaction zone, leaving behind unburned, shocked reactive pockets as shown in Fig. 7. Subsequently, there exist regions of re-initiation giving birth to new small detonation cells. These instability features, as in a highly unstable detonation wave, are ingredients to promote the successful transmission of a quasi-steady detonation into the open area.

By increasing further σ, the strong perturbation from the large physical scale of the obstacles at the wall becomes significant on the quasi-detonation propagation dynamics. For $\sigma > 0.24$ (Fig. 5(e) and (f)), triple point tracks (and hence cells) in some prolonged regions of the numerical soot foils (highlighted by a red box) vanish. Subsequently, behind the highlighted regions, there exit strong local explosion and abrupt re-initiation giving birth to small detonation cells. Unlike the cases with low σ, the larger scale of the obstacles for $\sigma = 0.24$ and 0.28 can no longer be treated as rough-walled boundary conditions. The detonation structure and its dynamics are also different and dominated by the presence of each discrete obstacle. The wall roughness no longer creates only small perturbations on the cellular detonation and the flow field associated with the detonation front. Instead, the obstacles change the overall propagation mechanism where the diffraction of the detonation and reflections from the obstruction and the tube wall of the diffracted front causes the failure and then ignition as the detonation propagates past the obstacles [3–5]. The scenario with high σ is less relevant to answering the question of the effect of instability on the critical tube diameter phenomenon as it introduces a different propagation mechanism and destroys the inherent cellular frontal structure of the quasi-detonations.

Fig. 6 shows the time-dependent detonation velocity evolution and the global average velocity normalized by CJ speed V_{CJ}. Increasing σ causes a more significant overall average velocity deficit, as well as local velocity fluctuation. In the absence of viscous dissipations, the velocity deficit is caused by the energy scattering, in all possible components, by the rough wall, diminishing the strength of the detonation front itself. Apart from the momentum loss in the wave propagating direction, the velocity deficit comes from the modified front structure, enhanced by the global wrinkled curved front, as a result of the interactions with the rough wall. Despite the fact that only chemical-gasdynamic effects and a two-dimensional configuration are considered, the velocity deficits for increasing wall roughness degrees are nonetheless in agreement with the experimental study using helical wire spirals to mimic wall roughness in a circular tube with $D_{1/2} = 19.05$ mm [7]. For a roughness $\sigma = \delta/D_{1/2}$ from 0.08 to 0.26 where δ is the wire diameter, the V/V_{CJ} value at 20 kPa for $2H_2 + O_2$ ranges approximately from about 0.85 to 0.75, respectively. With a relatively small tube diameter used in the experiment [7], a velocity deficit of about 5% is already present in the smooth tube. The two-dimensional geometry used in the simulation where the possible curvature in one other direction is neglected.

When the roughness approaches a critical value, i.e., $\sigma = 0.24$, the detonation velocity evolution

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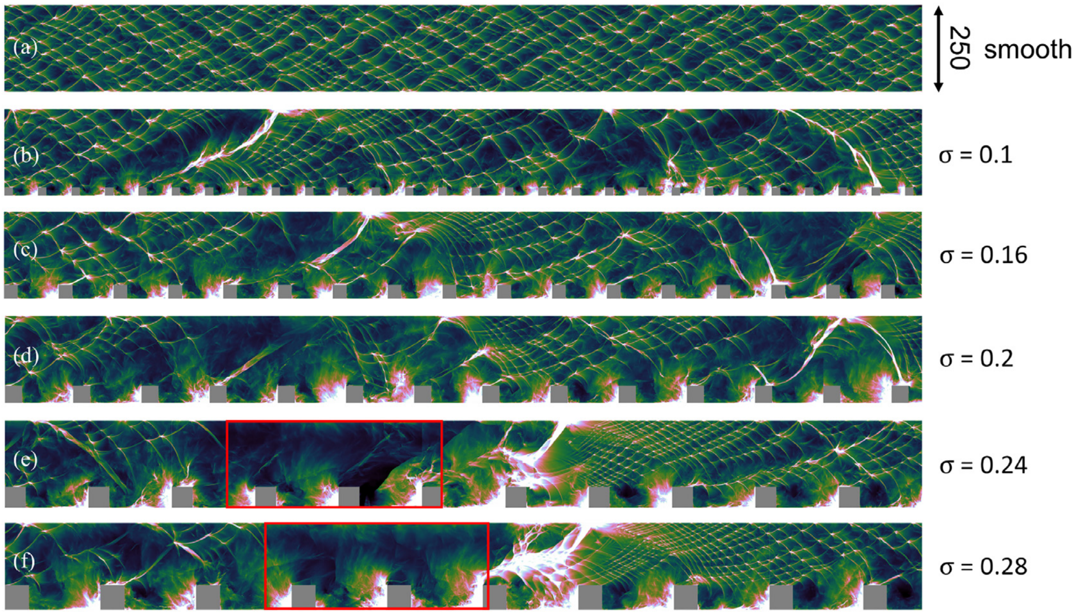

Fig. 5. Soot foils showing cellular patterns of quasi-detonations in (a) a smooth channel and rough-walled channels with (b) $\sigma = 0.1$, (c) $\sigma = 0.16$, (d) $\sigma = 0.2$, (e) $\sigma = 0.24$ and (f) $\sigma = 0.28$. The red boxes in (e) and (f) highlight the regions where the cellular structure vanishes. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

reproduces the wave behavior as observed from the cellular pattern, i.e., a low-velocity period indicating a failure or decoupling of the leading front and reaction zone, followed by an abrupt increase to as high as $1.2V_{\mathrm{CJ}}$ due to a strong local explosion. Due to a different propagation mechanism and quasi-detonation frontal structure, the focus should be limited to the case with relatively low σ where only perturbations are introduced, inducing additional instabilities without significantly modifying the overall dynamics features.

The induction-reaction-zone dynamics of an intrinsic cellular detonation resulting from a smooth channel and quasi-detonations in rough-walled channels with $\sigma < 0.24$ are further scrutinized via statistical analysis. The simulation data of the pressure field p and induction rate $\dot{\omega}_{\mathrm{I}}$ is collected in a window following the non-planar pattern of the detonation front as shown in Fig. 8. This data-collection window has two wings of 20 and 60 times Δ_{I} ahead and behind the shock front, respectively. The top and bottom boundaries of the data window are aligned with the inner surface formed by the top of obstacles to reduce the disturbance from the reflection between the wall and obstacles. In order to minimize the noise introduced by the transient fluctuations of an unstable detonation, data were collected throughout 1200 transient flow-field snapshots, including propagation over many obstacles and cycles of cellular patterns.

Fig. 9 presents the probability density function (p.d.f.) distribution of the pressure p and induction rate $\dot{\omega}_{\mathrm{I}}$ in the data window. Although the p.d.f. distribution of different cases, both for smooth and rough-walled channels, peaks at different values, the spread of the distribution indirectly gives us some description about the degree of instability or fluctuation level within the detonation flow field. As seen in Fig. 9(a) and (b), although the overall distribution of pressure p and induction rate $\dot{\omega}_{\mathrm{I}}$ and their peak values shift leftwards for quasi-detonations with increasing σ, this also results in a wider spread of the p.d.f. spectrum. These results suggest that, although the bulk reaction rates and transverse pressure wave strength of a quasi-detonation is reduced by the obstacles, primarily due to the decrease in average detonation velocity in an increasingly rougher channel, the instabilities induced by the wall roughness broadens the probability distribution of the reaction rates and pressure fluctuation range of the quasi-detonation.

3.2. *Detonation diffraction from rough-walled channels*

The previous section shows conclusively that for quasi-detonation propagating in rough-walled channels (with $\sigma < 0.24$), an increase in instability can be manifested within the cellular detonation structure and it is this effect of increased instability we would like to explore on the critical tube diameter problem. Since the cellular pattern of quasi-detonation is irregular, a shot-to-shot variation in cellular dynamics of the emerging quasi-detonation

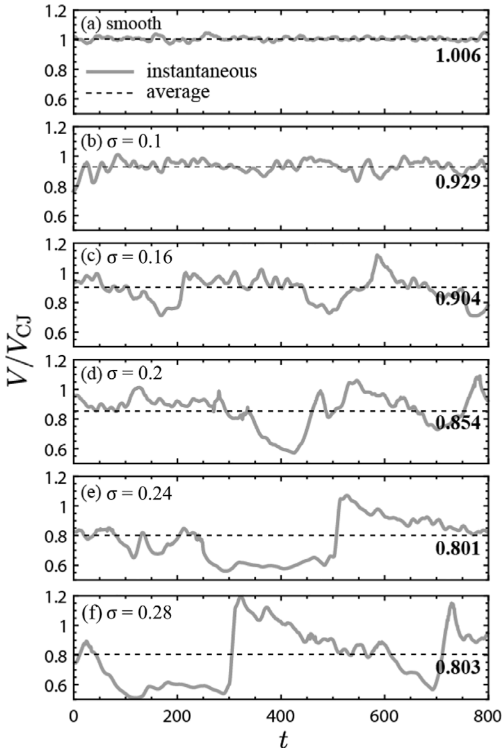

Fig. 6. Time-dependent transient velocity evolution (gray line) and global average velocity (black dashed line) of the quasi-detonation propagating in rough-walled channels with different degree of roughness σ.

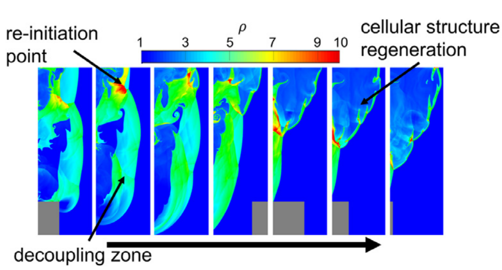

Fig. 7. A sequence of density contours showing the unstable features of the quasi-detonation propagation with $\sigma = 0.2$.

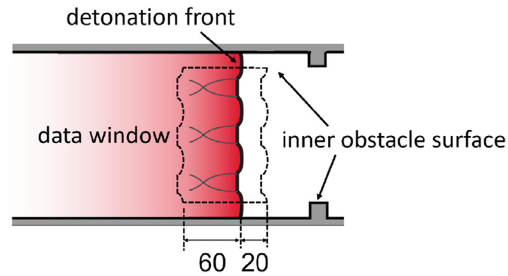

Fig. 8. The schematic for the data window near the detonation wave shock front, collecting the data required in the probability density function distribution.

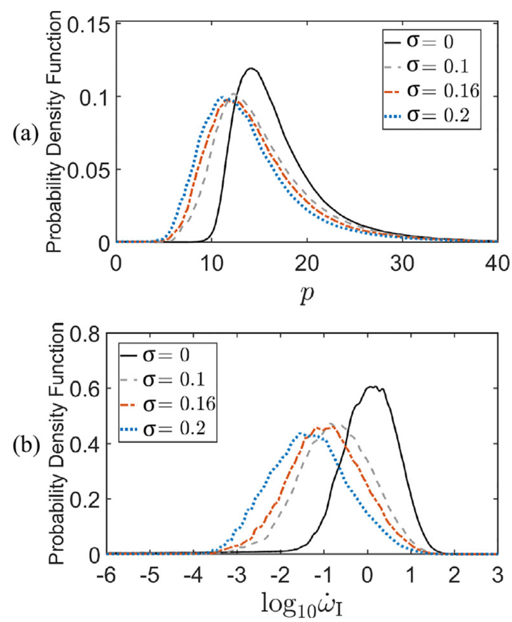

Fig. 9. The probability density function of (a) pressure p and (b) induction rate $\dot{\omega}_{\mathrm{I}}$ with roughness $\sigma = 0$, 0.1, 0.16 and 0.2.

from the rough-walled tube should be considered. A large number of simulations are thus 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 channel.

Fig. 10 shows some typical results obtained from these simulations for four levels of roughness (up to the critical level of $\sigma = 0.24$). Depending on the instantaneous unstable quasi-detonation structure emerging from the rough-walled channel, some instabilities can indeed lead to the re-initiation and successfully transmit a detonation into the open area. On one hand, from the left column of Fig. 10, the diffraction will highly possibly result in a *no − go* case if the incident detonation is maintaining a well-formed regular cellular structure or partially failing at the exit. On the other hand, the right column shows that if a re-ignition point from the unstable quasi-detonation structure is close to the exit of the channel, the detonation will re-initiate and result in *go* case. This demonstrates how the irregularity of the detonation structure could facilitate transmission and give rise to the possibility of a *go* mode in a sub-critical condition of the CJ detonation case in a smooth channel.

The number of successful and unsuccessful re-initiation of the diverging detonation wave with

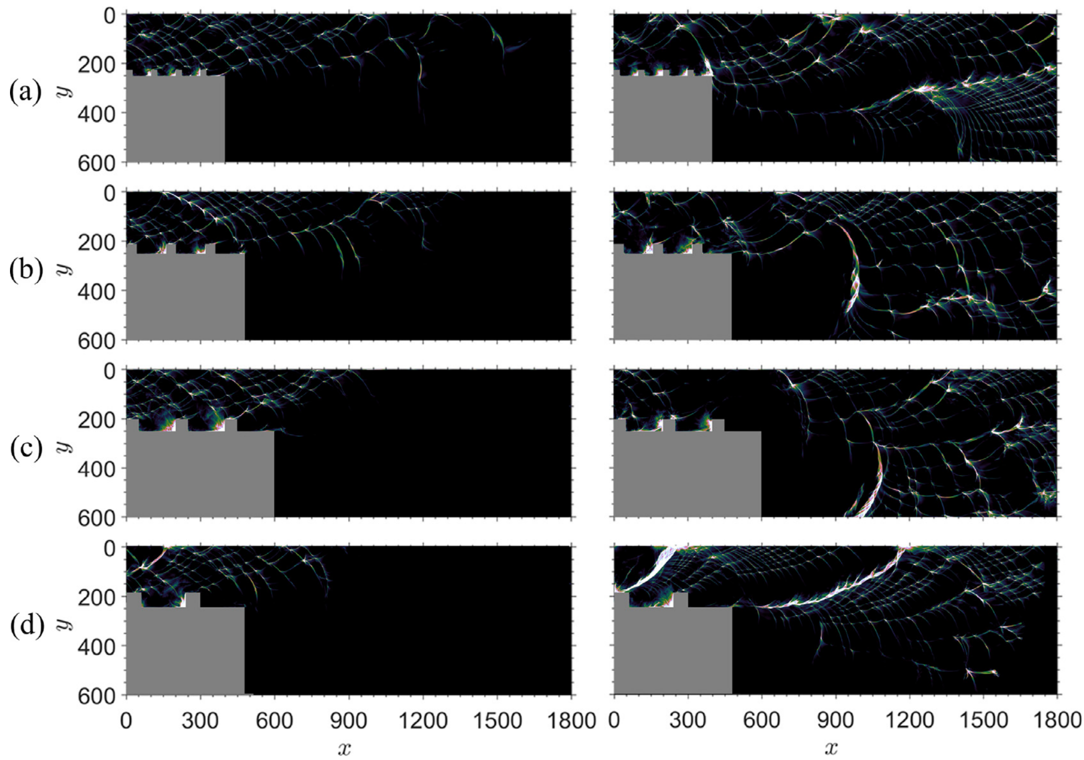

Fig. 10. Numerical soot foils showing a example case of the no-go mode diffraction (left) and go mode diffraction (right) with roughness (a) $\sigma = 0.1$; (b) 0.16; (c) 0.2 and (d) 0.24.

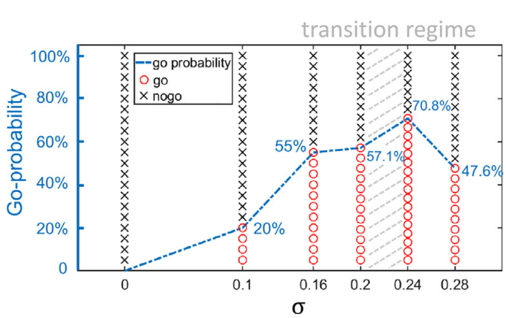

Fig. 11. Successful (go-mode) and failure (no-go mode) detonation transmission cases and the probability curve (blue dashed line) for successful detonation transmission (go-mode) at $D_{1/2} = 250$ with different roughnesses σ values. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

different degrees of roughness is presented in Fig. 11. For each roughness degree, the numerical experiments were carried out using the fixed-initial-condition incident quasi-detonation waves obtained at different transient frames. Each of the roughness degrees was repeated over 20 times. In essence, the plot shows the probability of getting detonation re-initiation for successful transmission from the total number of runs performed for each roughness. The results for roughness σ between 0.2 and 0.24 are considered to be in a transition regime where, as indicated in the previous section, the propagation mechanism differs with stronger effects of each isolated obstacle. These large obstacles can no longer be considered wall roughness introducing only mild disturbances to the intrinsic cellular structure. Here, the results show that within the critical roughness value, 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. For reference, when the wall roughness is further increased over a critical degree, i.e., $\sigma > 0.28$, the resulting velocity deficit, together with a different propagation mechanism relying on failure and re-initiation, as well as the presence of a prolonged decoupling between the shock and reaction zone or local failure indicated by the disappearance of cellular structure will, in turn, reduce again the possibility of re-initiation. A similar trend for slightly narrower tube diameters where $D_{1/2} = 230$ and 240 was also found by repeating the whole numerical experiment

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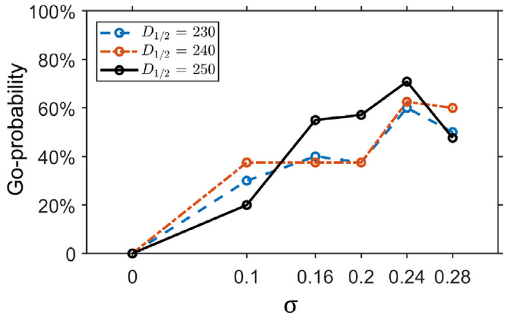

Fig. 12. The probability curve for successful detonation transmission (go-mode) with different degrees of roughness, at $D_{1/2} = 230$, 240 and 250.

with altered initial conditions as shown in Fig. 12. Notably, the successful transmission probabilities for $D_{1/2} = 230$ and 240 were obtained by repeating the numerical experiments 12 times only at each roughness degree. It could be less convincible, but enough to illustrate that when the half tube diameter is slightly lower $D_{1/2}$ than the critical value, which equals 250 according to this initial condition setup, the competing mechanism between velocity deficit and cellular instability overtakes each other, dominating the quasi-detonation diffraction process based on the degree of roughness.

4. Concluding remarks

The present study clarified the role of instability and unstable structure in the critical tube diameter phenomenon. This is addressed numerically by considering the dynamics of quasi-detonations. The results show that the quasi-detonation in rough-walled channels has a higher degree of instabilities (or a higher level of cell irregularity). It is important to emphasize the focus is on the effect of roughness which aims to generate only perturbation and additional instabilities to the cellular quasi-detonation. The present results demonstrate that, above approximately $\sigma = 0.24$, the detonation propagation dynamics changes to a different mode where the larger roughness (or more appropriately blockage ratio) no longer generates only minor perturbations, but causes failure and re-initiation due to the wave diffraction and reflection as the detonation past the obstacles.

To answer the fundamental question being posed in this work, an important finding is that, below a critical value of wall roughness, despite the velocity deficit of the leading detonation front, the additional inherent instabilities of the quasi-detonation are shown conclusively to provide additional ingredients to promote the successful transmission or re-initiation of the detonation downstream in the open area. This finding is consistent with the previous experimental results indicating that the increase of quasi-detonation cellular irregularity compensates for losses from the rough wall facilitating the successful detonation transmission into the open area. Above the critical value, both the decrease in the wave front strength and a switch to a different propagation mechanism described by a continuous diffraction, flow jetting, failure and re-initiation of the quasi-detonation via diffracted shock reflection reduces again the probability of successful detonation transmission.

Altogether with [22–27], the present numerical results further support that the failure and re-initiation mechanisms of the diffracting detonation wave are related to the degree of cellular instabilities of the unstable detonation front structure emerging from the confined tube.

At last, this study aims to provide a qualitative analysis of the role of instability on the critical tube diameter by considering the increased cellular irregularity of quasi-detonation induced by various rough walls as compared to the propagating CJ detonation in a smooth tube. The inviscid model is appropriate while the propagating quasi-detonation cellular structure retains and only the effect of perturbations caused by the rough wall on its irregularity is considered and hence, its consequence on the transmission and re-initiation in the open area. Nonetheless, in order to establish a more quantitative dependency between the roughness and the critical condition for transmission, as well as to predict accurately the viscous losses, the reactive Navier-Stokes equations and a more detailed rough-walled boundary model will need to be considered in future work. For very large roughness or blockage beyond the limit interested in this work, with additional propagation mechanisms being introduced, the wave propagation could resemble a deflagration-to-detonation transition (DDT) process wherein a decoupled front and large unburned pockets in an extended reaction zone are formed. Diffusive and turbulent transport in turn becomes significant for flame acceleration and burning of those relatively large gas pockets which thus relies on the need of the Navier-Stokes simulations.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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