On cellular multiplicity of detonations in confined channels

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1 Introduction

Behind the apparent detonation cellular structures is the cyclic generation and propagation of local expanding waves: as depicted in Fig. 1, an outwardly propagating wave originates inside a pocket of shock-compressed yet unburnt fuel-oxidizer mixture after the collision of two opposing transverse shock waves. The resulting expanding wave is initially overdriven propagating faster than the detonation CJ speed, and it subsequently decays due to curvature-induced flow divergence. The decaying nature of the wave can be quantitatively described by the separation between the shock front and the heat release region. As shown in the lower part of Fig. 1, the speeds of the pressure front (shock) and the trailing temperature front (location of maximum heat release rate) transition from overdriven to underdriven along a single detonation cell. The increasing separation of the two fronts leads to the formation of the unburnt gas region in between, where a subsequent expanding wave is generated. In a sustained detonation propagation, interactions of neighboring expanding waves carve out the global cellular structures. This conceptual picture of cell formation is consistent with both experimental measurements [1] and numerical simulations [1, 2] for mixtures that produce well-defined cellular structures. It is therefore widely recognized that the detonation cell size and the regularity of its structure are likely governed by these local dynamics, more specifically, the shock-chemistry decoupling characteristics of a given mixture. This geometric description of detonation cell formation forms the foundation of a variety of detonation studies such as cell length scale prediction [3], transverse wave behaviors [4], and physics-based modeling of the cellular structures [5].

The above cell-formation description, however, does not guarantee a unique cellular structure and size for a given mixture. As the detailed dynamics of shock-chemistry decoupling are determined by several parameters such as the initial degree of overdrive of the expanding wave and the size of the unburnt gas pocket, one could imagine that different combinations of physically possible wave parameters may lead to differing detonation cellular structures. While there might be a preferred or stable structure for a particular mixture, this description does not preclude the possibility of multiple solutions.

In this study, we report on detonation cellular multiplicity in hydrogen/oxygen detonations based on simulations in narrow two-dimensional channels. Several cellular structures with the average cell sizes differing by a factor of 3 were observed in simulations of identical mixtures but with different initial conditions. Numerical soot foils and flow fields were analysed to reveal the physical processes that lead to the differing structures. Numerical results were also compared to experimental measurements in an

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attempt to revisit the notion of detonation cell size being a unique and, therefore, fundamental property of a mixture.

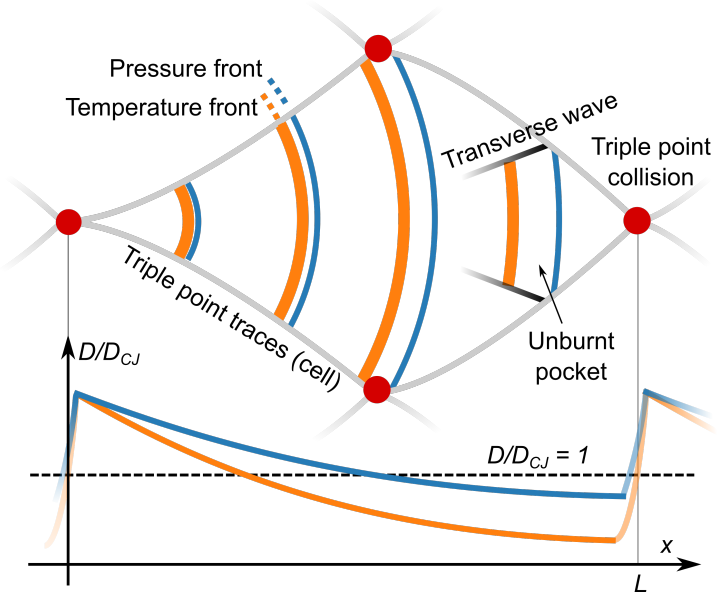

Figure 1: Expanding wave dynamics – pressure and temperature front propagation in a detonation cell.

2 Numerical setup

Compressible, reacting Naiver-Stokes equations are solved using `Athena-RFX` [6, 7]. Detailed numerical methods include the HLLC-ADC Riemann solver coupled with the 2nd-order corner-transport upwind (CTU) hydrodynamic integrator and piecewise-linear state reconstruction, the 2nd-order finite difference method for transport processes (convection and diffusion), and a semi-implicit ODE integrator YASS [8] for chemistry. Transport and chemistry are coupled through Strang splitting [9]. The simulations were carried out in a 80×20 mm domain, with a stoichiometric hydrogen/oxygen mixture at 298 K and 15 kPa. Detonation is initialized by superimposing spatially perturbed ZND solutions onto the computational domain and propagates along the length direction. The shape of the initial detonation front is specified in the form of sinusoidal waves, similar to several previous studies [7, 10]. Boundary conditions are zero-gradient for the upstream and downstream boundaries, and slip and adiabatic for the top and bottom boundaries. A grid resolution of 20 μm is used, corresponding to about 22 computational cells per induction length of the studied mixture, consistent with the convergence criterion of 25 cells per induction length proposed in [11]. An 8-species hydrogen sub-model of the Foundational Fuel Chemistry Model Version 1.0 (FFCM-1) is used [12] to describe the finite-rate chemistry.

3 Results and discussion

In this study, four simulation cases were carried out. They are identical except for their initial conditions. Specifically, each simulation is initialized with a sinusoidal ZND solution in the spanwise direction, with the period of the sine wave being the only difference among the four simulations. Presented in Fig. 2 are the primary results: the local shock-chemistry dynamics, i.e., averaged velocity profiles of pressure and temperature fronts (as defined in Fig.1) sampled from several detonation cells in each simulation, and the corresponding initial condition schematics along with the numerical soot foils based on the maximum

pressure in each computational cell. Evident from the soot foils are the four different detonation cellular structures, all of which are stable and self-sustaining over the time period simulated, and propagate on average at CJ speed. The top case features one and a half cells across the channel width, and the bottom case has four cells across, differing by a factor of $\sim$3 in cell size. This observation is in direct contrast to the conventional notion of the cell size being unique to a given mixture. Our results are in agreement with one previous study [10], in which detonation simulations with simplified chemistry were performed in much wider channels and a similar cellular multiplicity was observed. Here, the pressure and temperature frontal velocity profiles reveal that the cycle of local expanding waves is able to stabilize with multiple different sets of propagation parameters. In the top case, the expanding wave is initially overdriven at a relatively higher overdriven ratio of 1.51 and has a life time of about 8 μs before the next wave is generated. In contrast, the bottom case shows an initial overdriven factor of 1.29 and a life time of 4 μs. These different local propagation modes result in differing global cellular structures.

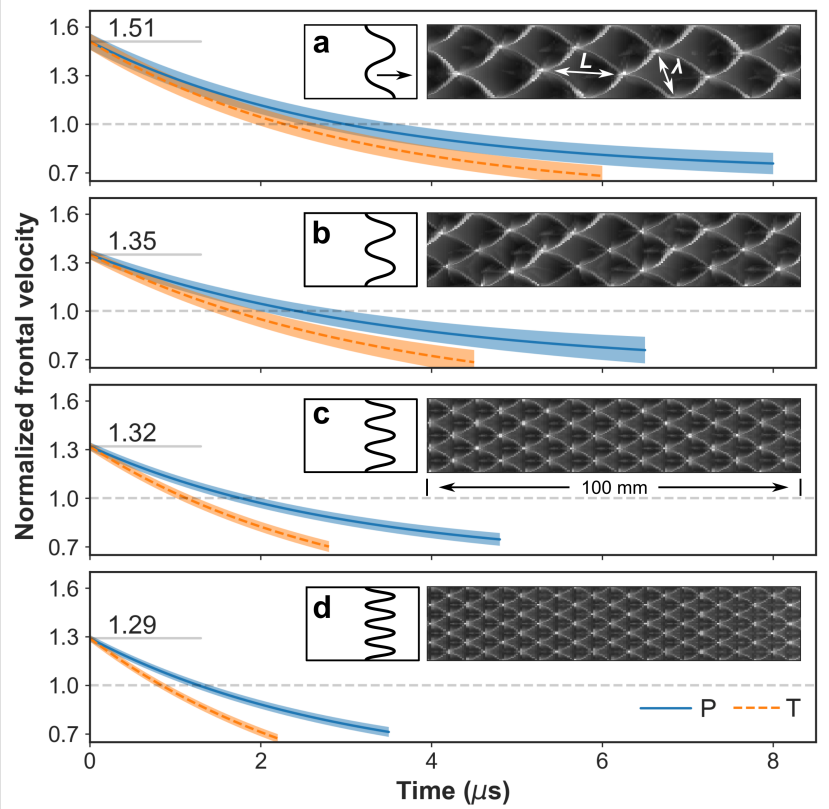

Figure 2: Averaged pressure (solid line and blue band) and temperature (dashed line and orange band) frontal velocity profiles from four detonation simulations of a stoichiometric hydrogen-oxygen mixture at 298 K and 15 kPa with different initial conditions. The velocity profiles are sampled and averaged from several detonation cells in each simulation, and the shaded bands represent one standard deviation. Insets are corresponding initial condition schematics and numerical soot foils. The sinusoidal waves represent the initial shock front based on ZND solution; detonation wave propagates from left to right.

For each of the four simulations, the maximum pressure over the entire computational domain is tracked, along with the corresponding temperature at the same location. The results are shown in Fig. 3. Peaks in the pressure signals correspond to the generations of the local expanding waves, therefore the oscillatory frequencies correlate with the global cellular features: higher frequencies corresponds to smaller cells, and vice versa. The changes in cell size also correspond to a change in thermodynamic states during the local expanding wave generation: the magnitudes of the pressure peaks and the associated temperatures

are around 40 atm and 3,500 K in the top case, and about 20 atm and 3,000 K in the bottom case. These state differences are also consistent with the degree of overdrive observed in the local frontal velocity profiles (Fig. 2). In summary, from the standpoint of detailed physical processes, each of the globally stable cellular structures corresponds to its own local expanding wave dynamics.

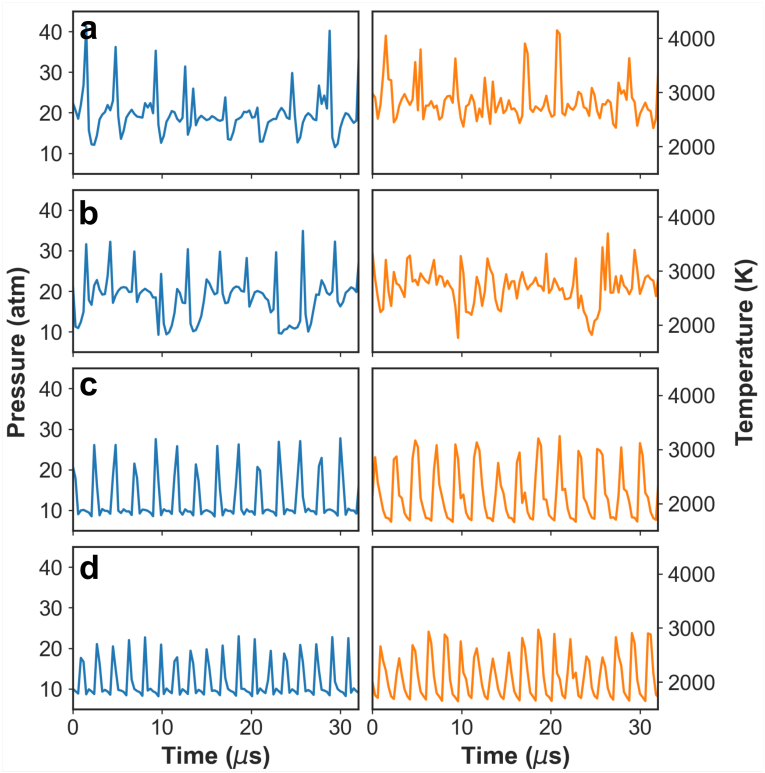

Figure 3: Temporal maximum pressure and corresponding temperature profiles from the four simulations, all of which are done for a stoichiometric hydrogen-oxygen mixture at 298 K and 15 kPa.

The numerical results are also compared to existing experimental data. Figure 4 compares the global cellular features from the present simulations with the experiments reported in [13], which were performed in the same mixture and at the same conditions. The experimental cells were recorded and measured using the soot foil technique. In Fig. 4, the x axis is the normalized detonation cell size, i.e., the ratio of cell width (λ) to the ZND induction length, while the y axis is the cell aspect ratio, or the ratio of the cell length (L) to cell width. The definitions of L and λ are denoted on the numerical soot foil shown in Fig. 1a. For the simulation results, each symbol with its respective error bar represents the statistics of numerical detonation cells from each simulation. Experimental results are presented as individual points, each of which represents a single detonation cell measured from experimental soot foils. Overall, the range of the numerical cell sizes overlap with the spread of the experimental cell sizes (often referred to as cell regularity). A discrepancy in terms of the cell aspect ratios is observed, with the simulations producing somewhat more "stretched" cells with larger aspect ratios as compared to experiments. This discrepancy is likely to result from a three-dimensional effect present in the experiments and a potential impact of curvature as the experimental cells are measured from the inner wall of a round tube. Note that despite the apparent similarity between two-dimensional numerical cellular structures and experimental measurements which are a result of three-dimensional dynamics, it remains to be further studied whether the two-dimensional dynamics is representative of the three-dimensional phenomenon.

The above comparison implies that varying detonation cell sizes in a single experiment could be considered as a statistical superposition of multiple solutions in the context of cellular multiplicity. This

offers an alternate understanding as compared to the traditional notion of flow responses to local disturbances [14]. When examining detonation cells across multiple experiments, it remains unclear whether a dominant size of detonation cells exists as an intrinsic property of a given mixture and condition, or detonation cellular structures are a mere consequence of the interaction between a mixture and its surrounding environment, and therefore such structures always remain subject to the specific confining geometries and boundaries. In fact, there has not been any systematic, unambiguous experimental and computational evidence supporting the notion of a unique detonation cell size. Computational detonation cell sizes vary widely because of different numerical methods and models, and most calculations do not explore exhaustively different initial and boundary conditions and their impact on the cellular structure. Meanwhile, cross comparisons among experimental measurements are also difficult as wide discrepancies and experimental uncertainties exist among different facilities. The relationship between cell multiplicity and cell regularity, and the corresponding underlying physics remains to be studied.

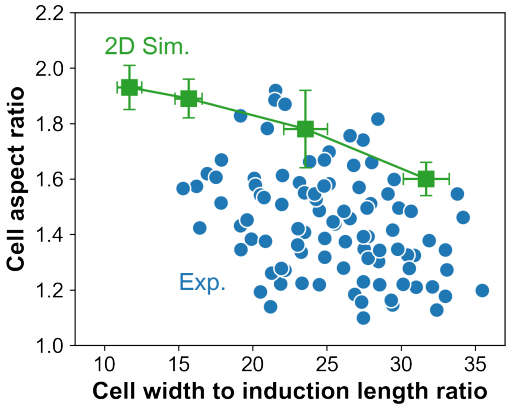

Figure 4: Detonation cell statistics between the present numerical simulations and experimental measurements.

4 Conclusions

We have shown evidence of detonation cellular multiplicity in two-dimensional hydrogen/oxygen numerical detonations in narrow channels. Different initial conditions can lead to different stable cellular structures. These differing structures are physically possible through variations of the local expanding wave dynamics, with larger detonation cells resulting from stronger and longer-lived local expanding waves. This observation challenges the traditional notion of a unique detonation cell size for a particular mixture, and indicates the possibility that detonation cellular structures are a result of both the mixture properties and the properties of its confining geometry, boundary conditions, and propagation histories. Moreover, cellular multiplicity provides an alternative explanation of the cellular regularity: different mixtures may have varying solution surface structures, comprising a range of possible cellular structures. A series of future studies are planned on several topics including the existence of cellular multiplicity in other mixtures, its sensitivity to numerical resolution and boundary conditions, and whether in three-dimensional detonations the multiplicity is suppressed.

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