

Detonation Structure at Realistic Pressures: a Differential Diagnosis for the Discrepancy between Numerical Simulations and Experiments

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1 Introduction

Detonation front in any realistic reacting mixture is highly unstable exhibiting complex multi-scale internal structure, which is characterized by the presence of transverse waves, triple-point structures, etc.[1] This structure is essential for the detonation propagation and stability, since it determines such important characteristics of practical systems as the minimum channel size, which can support detonation propagation, or critical tube diameter, from which a detonation can successfully emerge into a larger volume [1]. Therefore, the ability to predict accurately such internal structure, both theoretically and computationally, is essential for the design of detonation-based engines or accident mitigation and prevention.

A convenient visualization technique to represent such complex internal structure of the front is through the soot foils [2]. Soot foils allow one to identify easily the characteristic detonation scales, in particular, spacing between the transverse waves in the front, or equivalently the frequency of their collisions. Any other important dynamical aspects of the front, such as detonation failure/reignition, propagation of transverse detonations, etc., can also be identified in the soot foil traces. Note that other imaging techniques also exist and are often used in the detonation experiments, for instance based on the streak camera imaging [3], which can also reveal the characteristic spatial and temporal scales in the front. At the same time, in numerical simulations of detonations, numerical soot foils have an important benefit associated with their simplicity, as they can be easily created by recording maximum pressure at each spatial location either on the boundary of the channel or anywhere in the interior of the flow.

Prior numerical studies, have suggested that high-fidelity numerical simulations, which utilize modern complex multi-step chemical kinetics, cannot accurately reproduce the cell sizes for hydrogen-air mixtures at atmospheric conditions [4]. In a companion paper submitted in this meeting [5], we present a comprehensive survey of numerical simulations of detonations in a variety of fuel mixtures, from hydrogen to jet fuel, for a wide range of mixture compositions, as well as upstream pressures and temperatures. That analysis shows that indeed simulations, which use state-of-the-art chemical kinetics, cannot capture the internal structure of a freely propagating detonation front, in particular the characteristic cell size, for all hydrocarbons surveyed. For hydrogen mixtures, numerical cell sizes agree with the experimental values only at low upstream pressures. In this study, we analyze systematically various potential sources of such discrepancies, including numerical resolution, thermochemical model, and

Table 1: Summary of mixtures considered and corresponding detonation parameters.

Case	Mixture	ϕ	Pressure (bar)	Temperature (K)	D_{CJ} (Km/s)	ϵ	γ_{vn}
1	H ₂ -O ₂ -3.76N ₂	0.500	1.013	298	1.62	37.71	1.33
2a	2H ₂ -O ₂ -3.76N ₂	1.000	1.000	298	1.98	7.56	1.32
2b	2.965C ₂ H ₂ -2.5O ₂ -7.52N ₂	2.965	1.013	293	2.00	3.88	1.23
3	6.584H ₂ -O ₂ -3.76N ₂	3.292	1.013	300	2.24	18.01	1.33
4a	2H ₂ -O ₂ -3.76N ₂	1.000	1.000	373	1.97	6.56	1.32
4b	2H ₂ -O ₂ -3.76N ₂ -10%H ₂ O	1.000	1.000	373	1.91	12.25	1.30
4c	2H ₂ -O ₂ -3.76N ₂ -20%H ₂ O	1.000	1.000	373	1.85	21.00	1.29
5	2H ₂ -O ₂ -3.76N ₂	1.000	1.000	650	1.93	4.19	1.30

other factors, in order to identify the potential path forward for improving the accuracy and realism of the numerical detonation models.

2 Numerical Setup

The unsteady Navier-Stokes equations are solved numerically using parallel code `Athena-RFX++`, which incorporates dynamic patch-based AMR with Van Leer spatial discretization [6] and the HLLC-ADC Riemann solver with the piecewise linear reconstruction. The stiff chemical kinetics equations are integrated with the semi-implicit YASS method and coupled with the hydrodynamic equations using an operator split approach. Multi-species transport is modeled using mixture-averaging approximation. Reduced multi-step chemical kinetics is based on the FFCM-1 reaction mechanisms [7].

We performed eight calculations to explore various potential sources of the discrepancy in the detonation cell sizes. All calculations are initialized with a perturbed ZND profile in a rectangular channel with width $4\lambda_{exp} \times 40\lambda_{exp}$ with slip adiabatic walls (unless specified otherwise), where λ_{exp} is the experimentally measured detonation cell size. Grid cell size ensures that the corresponding ZND induction length, Δ_i , is resolved with ≥ 40 grid cells and the ZND thermal width, Δ_r , with ≥ 5 numerical cells. The domain length, grid resolution, or the boundary conditions are varied in tests below to analyze their impact on the numerical detonation cell size. Details of the mixtures used in the calculations, along with the upstream pressure and temperature, as well as other related detonation parameters, are listed in Table 1. Here, ϕ is the equivalence ratio, D_{CJ} is the Chapman-Jouguet speed of the detonation front, and

$$\epsilon = \frac{E_a}{RT_{VN}} = \frac{1}{T_{VN}} \frac{\partial \ln \tau}{\partial (1/T)} \quad (1)$$

is the normalized effective activation energy based on the logarithmic temperature sensitivity of the ignition delay time, τ , and T_{VN} is the temperature at the von Neumann state.

3 Results

We analyzed the potential impact of the following two large groups of factors on the resulting detonation cell size: (i) numerical method and simulation setup, and (ii) physico-chemical model.

3.1 Numerical model

Domain length. Prior studies [8] have suggested that the internal structure of a detonation front can relax to a freely propagating CJ state much more slowly than the overall detonation speed. To investigate this effect, in Case 1 (lean, atmospheric H₂-air), detonation was allowed to propagate the distance $40\lambda_{exp}$ (1.6 m) and $160\lambda_{exp}$ (16 m). In both cases (see Fig. 1), cellular structure is virtually unchanged with

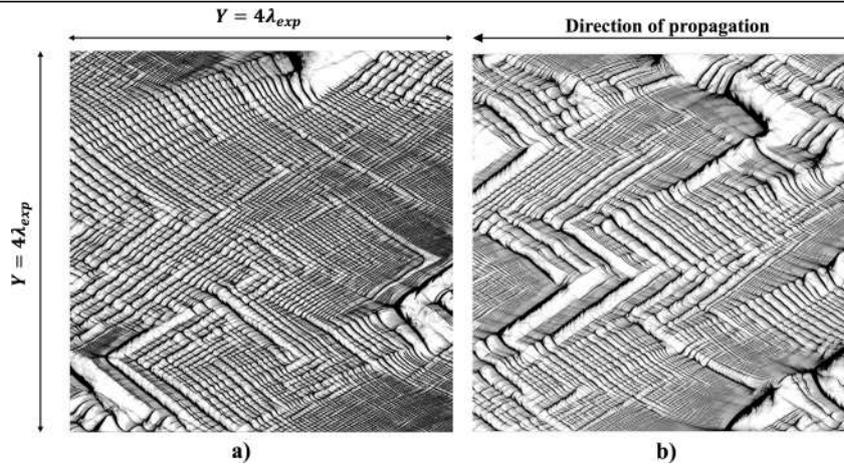


Figure 1: Numerical soot foils for the lean H₂-air mixture at atmospheric conditions (Case 1) after detonation propagation over the distance a) $40\lambda_{exp}$ and b) $160\lambda_{exp}$.

cell sizes much smaller than the experimental value [9] (channel width is $4\lambda_{exp}$). This suggests that the discrepancy in the cell size cannot be due to the insufficient distance of detonation propagation.

Grid resolution. Detonation front is comprised of structures spanning a wide range of scales, from hydrodynamic scales, associated with the shock thickness, to the characteristic combustion scales, associated with the local ignition and reaction lengths. Resulting detonation structure obtained in a simulation depends on how well such scales are resolved. Traditionally, simulations primarily aim to resolve the combustion scales, in particular the induction, Δ_i , and reaction, Δ_r , zones in a ZND solution of a CJ detonation. We performed simulations (Cases 2a and 2b) with varying resolution to assess the potential effect of under-resolving both the hydrodynamic and chemical scales. In Case 2a (stoichiometric H₂-air), Δ_i resolution varied from 2.5 cells to 160 cells (cell size $1\mu\text{m}$). In agreement with prior observations of [10], cell size showed little variation past $40\Delta x$, remaining $\approx 1/3 - 1/4\lambda_{exp}$, though cells became progressively more irregular with increasing resolution. Similar observations were made in Case 2b (rich C₂H₂-air at atmospheric conditions), in which resolution of Δ_i was varied from 70 cells to 274 (cell size 700 nm). In this case, cells were $\approx 5 - 10$ times smaller than λ_{exp} . In both cases, numerical resolution approached ≈ 10 times the mean free path, below which the continuum assumption in the Navier-Stokes equations would be violated. Despite this, grid-independent detonation cell size was obtained, which was $\sim 3 - 10$ times smaller than the experimental cell size [11].

Boundary conditions and problem dimensionality. Heat and viscous losses on channel walls can affect the detonation cell size [12]. Such losses are always present in experiments, and thus a question arises whether the observed discrepancy can arise when numerical simulations fail to properly account for such losses. To investigate this, for Cases 3 (rich H₂-air at atmospheric conditions) and 5 (stoichiometric H₂-air at 650 K upstream temperature), simulations were performed in a two-dimensional (2D) channel with adiabatic, slip walls and a three-dimensional (3D) channel with isothermal, no-slip walls. In both cases, the channel height was $4\lambda_{exp}$, while in the 3D case, the channel width was much smaller equal to Δ_i in Case 3 and $4\Delta_i$ in Case 5. Such narrow channels resulted in a significant velocity deficit relative to D_{CJ} , namely 14% in Case 3 and 11% in Case 5. At higher velocity deficits, detonation failure would occur. Figure 2 shows the numerical soot foils for Case 3 in a 2D (panel a) and 3D channels (panel b). Wall loss effects indeed increase the cell size, however, detonation propagation becomes much more unstable with quasi-failures (extended light regions in the soot foil) and re-ignitions (dark bands), resulting in a wide range of cells, which are all nevertheless significantly smaller than the experimentally reported values. In contrast, in case 5 with preheat, cell size was in close agreement with experiments

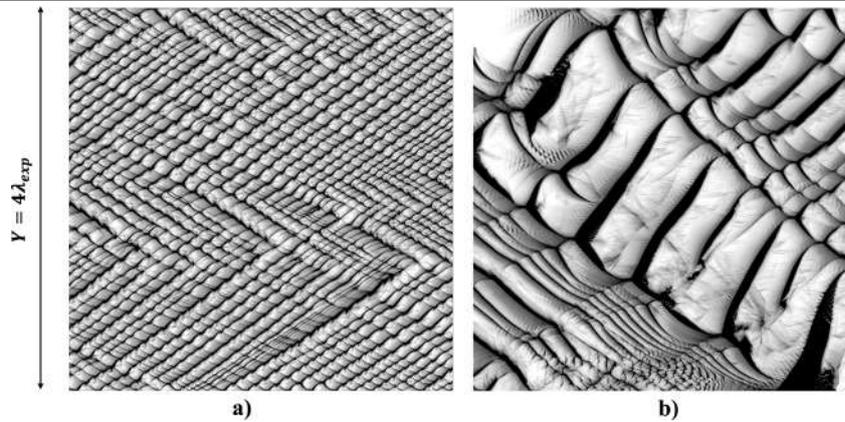


Figure 2: Numerical soot foils for the rich H_2 -air mixture at atmospheric conditions (Case 3) in a) a 2D domain with adiabatic slip walls and b) a 3D channel with isothermal no-slip walls.

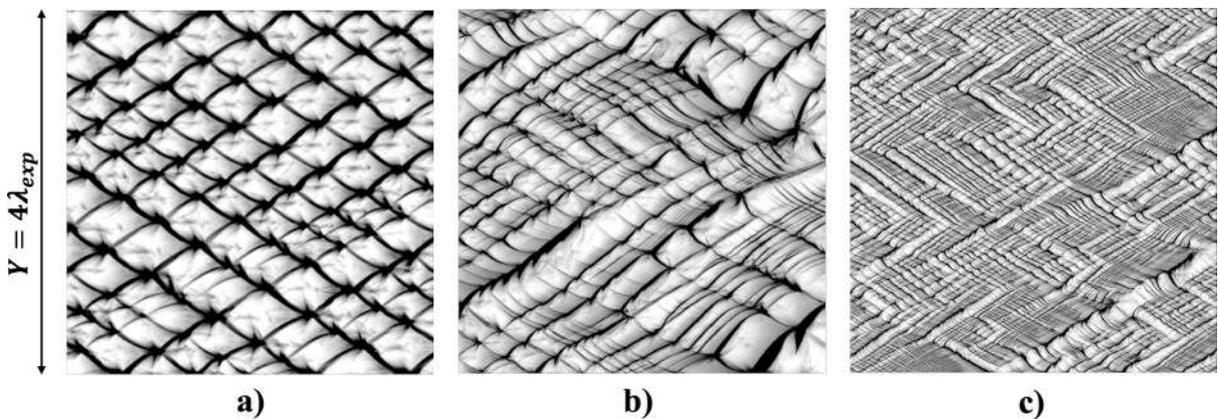


Figure 3: Numerical soot foils for stoichiometric H_2 -air mixture at 1 bar and 373 K with a) 0%, b) 10%, and c) 20% steam dilution.

in 2D, and in 3D with wall losses, cell size was ≈ 2 times larger. This shows that modern multi-step kinetics can give good agreement in experimental cell size at atmospheric conditions with significant preheat of the upstream mixture. On the other hand, in mixtures with significant disagreement with experiments, large wall losses cannot account for such discrepancy.

3.2 Physico-chemical model

Induction length (or time) behind a shock is often identified as the most important parameter in a detonation, as it controls the timescale of heat addition to the gas, which in turn controls the subsequent flow evolution that manifests as a cellular structure. Previous studies [13, 14] have suggested various correlations between the induction length and the resulting cell size. At the same time, Cases 1 and 2 (lean and stoichiometric H_2 -air) have similar values of Δ_i , namely ≈ 200 and $300 \mu\text{m}$, respectively. Yet, while in Case 2, numerical cells are $\sim 3 - 4$ times smaller than λ_{exp} , in lean H_2 , this disagreement is more than an order of magnitude (Fig. 1a). This suggests that the induction length in a ZND structure can serve as a rather poor predictor of the detonation cell size.

Vibrational non-equilibrium. Previous studies [4] have suggested that vibrational non-equilibrium (VNE) formed behind strong shocks, such as those present in a detonation front, can be important as the VNE relaxation timescale can be comparable to the chemical ignition timescale [4]. As a result,

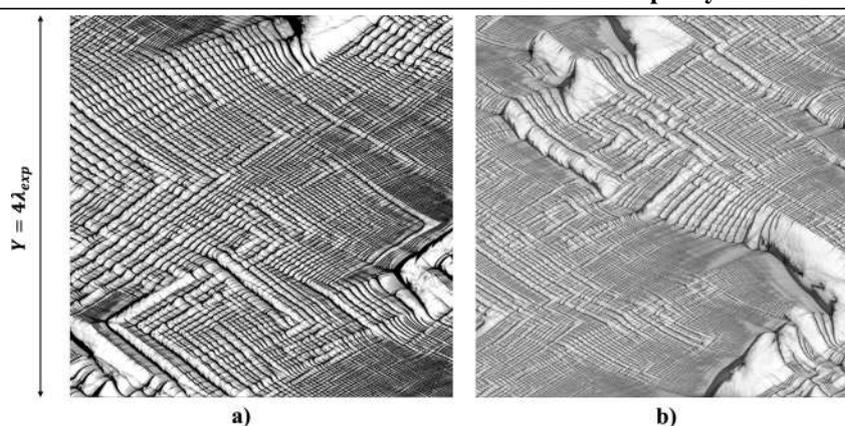


Figure 4: Numerical soot foils for the lean H_2 -air mixture at atmospheric conditions (Case 1) for two different chemical mechanisms: a) FFCM1, and b) UCSD.

it was previously suggested that accounting for the VNE could also act to increase the cell size [15]. In order to investigate the potential importance of the VNE, we considered several mixtures with steam addition (Cases 4a - 4c, from no steam to 20% steam). Due to its large collision cross section, presence of H_2O can efficiently equilibrate the VNE. Therefore, increasing amounts of steam in the mixture would be expected to suppress the VNE considerably and thus improve the agreement in the cell size with observations. Figure 3 shows the numerical soot foils for Cases 4a - 4c. Note, in all three cases, channel width is equal to $4\lambda_{exp}$ [16]. Contrary to the expectation, addition of steam drastically worsens the agreement with the experiments. This thus suggests that while proper treatment of the VNE in the physical model of a detonation is important, it may not serve as the main explanation of the observed discrepancy in the cell size.

Chemical mechanisms. The sensitivity of the detonation cell sizes to the chemical mechanism was investigated by comparing the FFCM1 and UCSD chemical mechanisms [7, 17] for Case 1 (Fig. 4). Both mechanisms result in a very similar cellular structure, with extremely small cells and highly unstable detonation dynamics. Furthermore, virtually all other published hydrogen mechanisms also show very similar ZND solution structure. This suggests that the observed results are representative of all existing hydrogen reaction kinetics models.

4 Conclusions

We performed a series of numerical simulations of the freely propagating detonations using multi-step chemical mechanisms to investigate potential causes of the observed discrepancy between the numerical and experimental detonation cell sizes in hydrogen-air and hydrocarbon mixtures at realistic pressures. In particular, we investigated various aspects of the numerical simulations, including domain length, grid resolution, problem dimensionality, and boundary conditions, and of the physico-chemical model, including thermochemical conditions, vibrational non-equilibrium, or the details of the thermochemical model. We found that while these effect can affect the resulting cell size, none of them can fully account for the observed disagreement by bringing the numerical cells within a factor of 2 or less of the experimental values. Thermal and viscous wall losses can increase the cell size by a factor of ~ 2 , which is not sufficient to explain the observed disagreement, which, for many mixtures exceeds an order of magnitude. We also found that steam addition, which would be expected to quench vibrational non-equilibrium, increases the discrepancy in cell size considerably. Finally, variations in the existing chemical kinetics models were found to have only minimal effect on the large difference between the numerical and experimental cell sizes.

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