Two-Dimensional Detonations in Ethylene-Air Mixtures with Multi-Step Chemistry

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1 Introduction

Multi-dimensional gas-phase detonations play a central role in a wide variety of practical combustion systems, including novel propulsion designs such as rotating detonation engines (RDEs). In recent years, there has been an increasing interest in using ethylene (C_2H_4) as a fuel in detonation engines, in particular in air-breathing RDEs [1], due to its higher reactivity and better detonability compared to other hydrocarbons. This warrants studies of the dynamics and structure of detonations in ethylene mixtures.

In a pioneering study, Strehlow et.al. [2] carried out experiments in C_2H_4/O_2 and $C_2H_4/O_2/Ar$ mixtures to explore the relation between the detonation cell width, λ, and induction zone length, Δ. Bull et.al. [4] studied detonations in C_2H_4/air and C_2H_4/O_2 mixtures as a function of initial pressure and reported the observed cell sizes. Experiments conducted by Knystautas et.al. [3] and Murray & Lee [7] in hydrocarbon detonations (including ethylene) reported that the empirical correlation between the detonation cell size and the critical tube diameter $d_c = 13\lambda$ holds true even for hydrocarbon mixtures. Bauer et.al. [5] measured cell sizes in ethylene/air mixtures at elevated initial pressures from 1 bar to 10 bar. They further investigated the validity for hydrocarbons of the relation between the cell size and the induction length $\lambda = 29\Delta$ given by Westbrook et.al. [6].

In the context of numerical modeling, majority of prior studies that considered detonations in $C_2H_4/O_2/Ar$ and $C_2H_4/O_2/N_2$ mixtures [8, 9] have been limited to calibrated single-step chemical kinetics. One notable exception is the work by Araki et.al. [10] who performed two-dimensional (2D) simulations of C_2H_4/O_2 detonations using multi-step chemical kinetics at low pressure conditions of 0.1 atm, however, the considered channel size was much smaller than the expected cell width. Therefore, detailed numerical simulations of ethylene/air detonations with realistic chemistry in sufficiently wide channels to produce complex cellular detonation structure remain scarce.

In this study, we present a systematic study of 2D detonations in C_2H_4/air mixtures at atmospheric conditions using complex chemical kinetics. The primary focus is on the near-limit behavior. In particular, we analyze detonation properties as a function of the channel width by considering channels that are both larger and smaller than the expected detonation cell size. We also study the effect of equivalence ratio on the detonation properties by considering $\phi = 1.0$ and 0.7.

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2 Problem Setup

Our numerical simulations solve the unsteady 2D reactive, compressible Navier-Stokes equations. The governing equations are solved on a uniform Eulerian grid using the code `Athena-RFX`, which is a fully compressible reactive flow solver. Over the years, `Athena-RFX` has been extensively used to study a wide variety of reacting flow problems [11–13], including detonation modeling [14, 15]. The solver used in this work employs a directionally unsplit, corner transport upwind, finite-volume scheme with the piecewise linear interpolation for spatial reconstruction [16]. The fluxes at cell interfaces are evaluated using the HLLC-ADC Riemann solver [17]. YASS ODE integrator is used to solve the stiff system of equations for chemical kinetics [8]. The chemical source terms are coupled to the flow equations using operator splitting approach with a global time-step control [18].

Special attention was paid to the choice of a chemical kinetics model. The chemical reaction model is comprised of 30 species and 231 reactions. The model was reduced from the FFCM series of reaction models (see, e.g., FFCM-1 [19, 20]) for high-pressure / high-temperature conditions characteristic of detonations. In particular, the reduction targets 21 combustion responses: i) laminar flame speeds of ethylene-air mixtures at the unburnt gas temperature of 298 K, pressures of $1, 3$, and 50 bar, and three equivalence ratios $\phi = 0.7, 1.05, 1.4$, ii) ignition delays of ethylene-air at 50 bar initial pressure, initial temperatures of $1500, 2000$, and 2500 K and $\phi = 0.5, 1.0$, and 2.0, and iii) ZND induction lengths at an unburnt gas temperature of 470 K, pressure of 3 bar, and $\phi = 0.5, 1.0$ and 2.0. The reduced model was further tested for the ZND structure prediction against the detailed reaction model over a broader range of conditions, with unburnt gas temperatures ranging from 284 to 648 K and pressures from 0.5 to 3.5 bar at the equivalence ratios of $0.7, 1$ and 2. All tests show satisfactory results. The equation of state is that of an ideal gas with the thermodynamic functions computed using NASA seven-coefficient format. The molecular transport coefficients are evaluated using mixture averaging.

Table 1: Simulation parameters. Here, λ is the corresponding experimental detonation cell size reported in literature [3] and Δx is the computational cell size.

P_f (bar)	T_f (K)	ϕ	D_{CJ} (m/s)	λ (cm)	Δ (cm)	Δ_e (cm)	$\Delta/\Delta x$	$\Delta_e/\Delta x$	L_y (cm)	L_x (cm)
1.0	298	1.0	1832	2.0	6.26×10^{-2}	1.29×10^{-2}	40	8.2	8.0	24.0
1.0	298	1.0	1832	2.0	6.26×10^{-2}	1.29×10^{-2}	40	8.2	1.0	24.0
1.0	298	1.0	1832	2.0	6.26×10^{-2}	1.29×10^{-2}	40	8.2	0.25	24.0
1.0	298	0.7	1704	8.0	1.89×10^{-1}	2.28×10^{-2}	40	5.0	16.0	48.0
1.0	298	0.7	1704	8.0	1.89×10^{-1}	2.28×10^{-2}	40	5.0	8.0	48.0
1.0	298	0.7	1704	8.0	1.89×10^{-1}	2.28×10^{-2}	40	5.0	1.0	48.0

Numerical simulations of ethylene/air mixtures are carried out in a 2D channel of size $L_x \times L_y$. L_x is the streamwise length of the domain (detonation front propagation direction) and L_y is the domain width. The top and bottom boundaries are slip, adiabatic walls. Zero-order extrapolation (outflow) boundary condition is used on the left boundary, while the right boundary is maintained at the CJ state. The details of the simulation parameters for each case are given in Table 1. Here, P_f and T_f are the fuel pressure and temperature respectively, ϕ is the equivalence ratio in the fuel mixture, and D_{CJ} is the Chapman-Jouguet (CJ) detonation velocity. Δ and Δ_e are the induction zone length and exothermic pulse width of a 1D detonation respectively, obtained using the SDToolbox in Cantera [23]. In all cases, the flow field is initialized using the corresponding ZND solution, and the problem is solved in the laboratory frame of reference on a moving grid to limit the streamwise domain length. The ZND solutions at ϕ = 1.0 and 0.7 are shown in Fig. 1. All simulations are well resolved with at least 40 cells per induction length and at least 5 cells per exothermic pulse width.

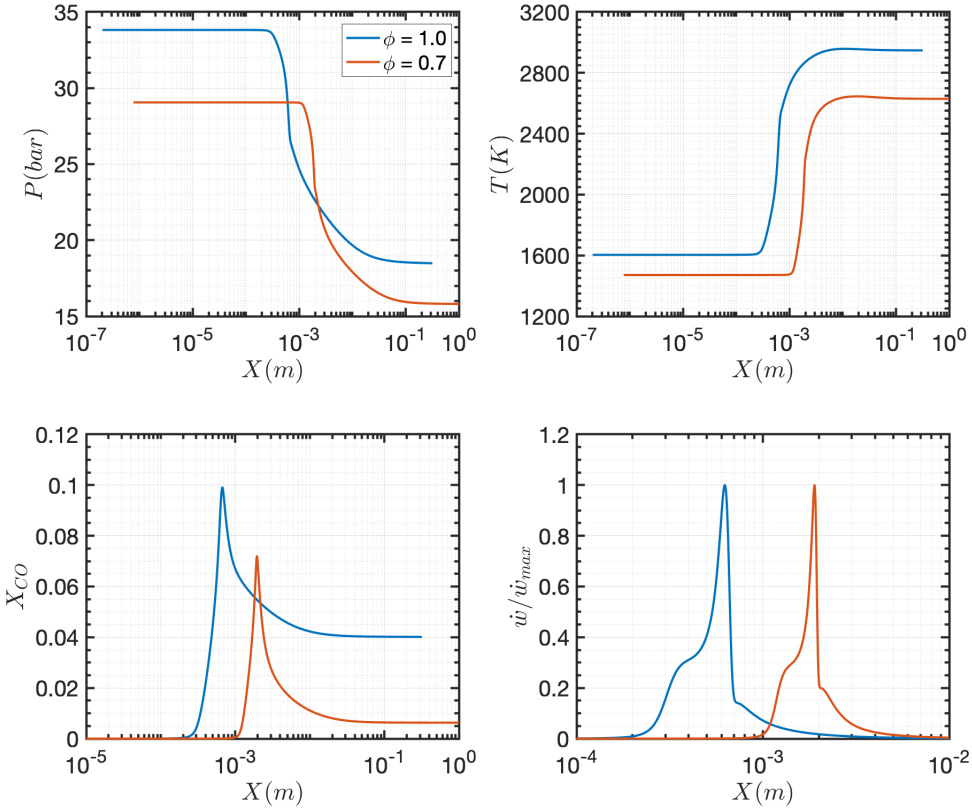

Figure 1: ZND structure of a stoichiometric C_2H_4/air mixture at 1 bar and 298 K at ϕ = 1.0 and 0.7.

3 Results and Discussion

We first consider ethylene/air detonation at ϕ = 1.0 in an 8 cm wide channel. At this equivalence ratio, the expected cell size is 1.95 cm [3], which is smaller than the channel width. The corresponding numerical soot foil is shown in Fig. 2a. The soot foil is constructed by recording the history of maximum pressure in each computation cell. It can be seen that detonation cells are highly irregular with a hierarchy of cell sizes, which is characteristic of unstable detonation mixtures. Second, when the detonation is about to fail (shown by marker A), a strong transverse detonation is formed and it propagates across the channel width (shown by marker B) re-igniting the mixture and producing a series of extremely small cells (shown by marker C). More specifically, when the detonation is about to undergo failure, the incident shock becomes weaker. This reduces the post-shock temperature, which creates a large induction zone behind the incident shock. At this point, a transverse detonation is initiated and it starts to consume the hot dense post-shock fuel mixture formed in the large induction zone created by the incident shock. This results in very high pressures and shorter induction length in the post-shock state of the transverse detonation and ultimately leads to the formation of very small cellular structures in the soot foil. Previously, Gamezo et.al. [21] observed similar detonation dynamics in mixtures with high effective activation energy modelled using single-step chemical kinetics at near-limit conditions. We also note that the simulation produced a wide range of cells sizes that are all substantially smaller than those observed in experiments.

Figure 2b shows the numerical soot foil in a 1 cm wide channel. In this case, the channel width is smaller than the expected cell size. However, even in such a narrow channel, the detonation produced a range of detonation cell sizes. The dynamics is similar to the 8 cm channel case with frequent failure/re-ignition events dominating the propagation. Markers A, B and C in Fig. 2b also show respectively the

global detonation failure, the subsequent formation of a transverse detonation wave, and the creation of extremely small cellular structures. Further decrease of the channel width to 0.25 cm causes the detonation to fail even in a lossless adiabatic channel (soot foil not shown here). Therefore, for ϕ = 1.0 case, the minimum channel width required for detonation propagation is $\approx 0.5 - 1$ cm. The detailed mechanism of detonation failure in a narrow lossless channel will be discussed in a separate study.

Figure 3 shows the numerical soot foils for ϕ = 0.7. For this equivalence ratio, the expected cell size from experiments is around 8.0 cm [3]. We find that as the mixture gets leaner, a much wider channel is required in order to propagate a detonation. In case of ϕ = 0.7 (see Fig. 3), the detonation propagates in a 16 cm wide channel with irregular cellular structure and with cells again smaller than the expected cell size of 8 cm. In the lean case, the detonation propagation is also dominated by the failure-reignition events similar to the ones observed in the stoichiometric case. However, once we reduce the channel width from 16 cm, we observe that the detonation fails promptly in both the 8 and 1 cm channels. Therefore, for $\phi = 0.7$, the minimum channel width required is in the range 8.0-16.0 cm. Overall, it can be concluded that in cases where robust detonation propagation is observed, the formation of transverse detonations is inevitable and in fact it is crucial to sustain healthy propagation.

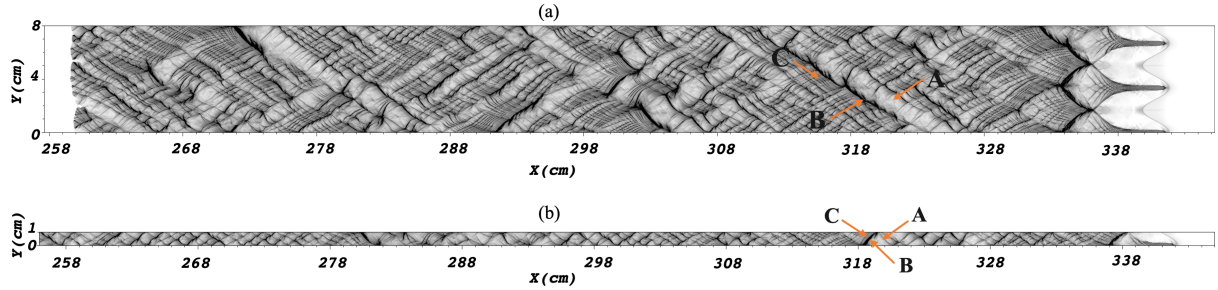

Figure 2: Numerical soot foils for C_2H_4/air detonations at P = 1.0 bar, T = 298 K, ϕ = 1.0 in a channel of size a) 8 cm; b) 1 cm.

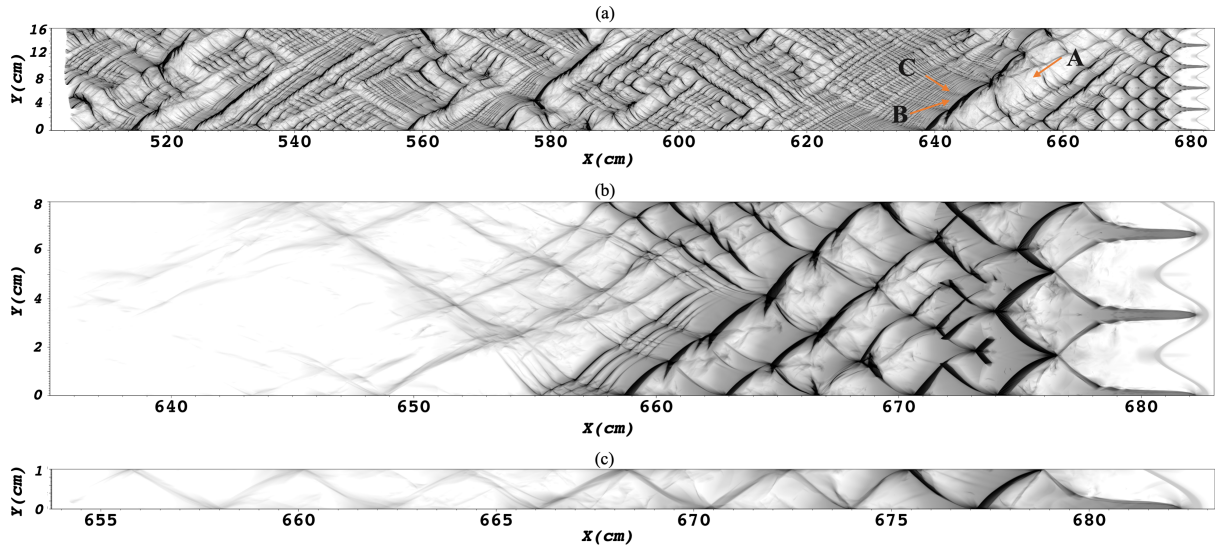

Figure 3: Numerical soot foils for C_2H_4/air detonations at P = 1.0 bar, T = 298 K, ϕ = 0.7 in a channel of size a) 16 cm b) 8 cm c) 1 cm.

4 Conclusion

We performed a series of numerical simulations to study the near-limit dynamics of detonations in ethylene/air mixtures at atmospheric conditions in a lossless channel. The cellular structure is highly irregular with a wide range of cell sizes characteristic of an unstable mixture. Detonation propagation is also studied as a function of channel size. In all cases, failure/re-ignition events involving the formation of a transverse detonation are observed, which are central for the detonation propagation. A minimum channel width required for detonation propagation is found to exist even in lossless channels. For $\phi = 1.0$ this width is $\approx 0.5 - 1.0$ cm and for $\phi = 0.7$, it is $\approx 8.0 - 16.0$ cm. Finally, in all cases that propagated, detonation cells were found to be significantly smaller than the expected experimental values. Similar observation was previously made for hydrogen mixtures [22]. It is not clear at present what causes this discrepancy, e.g., inaccuracies in the chemical kinetics model, thermal non-equilibrium effects, or other effects not accounted for in the calculations. This important question requires further investigation. Future analysis of the detonation dynamics in ethylene-air mixtures at near-limit conditions will include consideration of much leaner mixtures, as well as the effects of wall losses (isothermal, no-slip walls) on the minimum channel width. That analysis will be presented in a separate study.

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References

[1] Sato T, Voelkel S, Raman V. Analysis of detonation structures with hydrocarbon fuels for application towards rotating detonation engines. In2018 Joint Propulsion Conference 2018 (p. 4965).

[2] Strehlow RA. Transverse Waves in Detonations: II. Structure and Spacing in H_2-O_2, C_2H_2-O_2, C_2H_4-O_2, and CH_4-O_2 Systems. AIAA J. 1969;7:492-6.

[3] Knystautas R, Lee JH, Guirao CM. The critical tube diameter for detonation failure in hydrocarbon-air mixtures. Combustion and Flame. 1982 Jan 1;48:63-83.

[4] Bull DC, Elsworth JE, Shuff PJ, Metcalfe E. Detonation cell structures in fuel/air mixtures. Combustion and Flame. 1982 Jan 1;45:7-22.

[5] Bauer PA, Presles HN, Heuze O, Brochet C. Measurement of cell lengths in the detonation front of hydrocarbon oxygen and nitrogen mixtures at elevated initial pressures. Combustion and flame. 1986 Apr 1;64(1):113-23.

[6] Westbrook CK, Urtiew PA. Chemical kinetic prediction of critical parameters in gaseous detonations. InSymposium (International) on Combustion 1982 Jan 1 (Vol. 19, No. 1, pp. 615-623). Elsevier.

[7] Murray SB, Lee JH. The influence of yielding confinement on large-scale ethylene-air detonations. Prog. Astronaut. Aeronaut. 1984;94:80-103.

[8] Khokhlov A, Austin J, Pintgen F, Shepherd J. Numerical study of the detonation wave structure in ethylene-oxygen mixtures. In42nd AIAA Aerospace Sciences Meeting and Exhibit 2004 Jan 5 (p. 792).

[9] Gottiparthi K, Genin F, Srinivasan S, Menon S. Simulation of cellular detonation structures in ethylene-oxygen mixtures. In47th AIAA Aerospace Sciences Meeting including The New Horizons Forum and Aerospace Exposition 2009 (p. 437).

[10] Araki T, Yoshida K, Morii Y, Tsuboi N, Hayashi AK. Numerical analyses on ethylene/oxygen detonation with multistep chemical reaction mechanisms: Grid resolution and chemical reaction model. Combustion Science and Technology. 2016 Mar 3;188(3):346-69.

[11] Poludnenko AY, Oran ES. The interaction of high-speed turbulence with flames: Global properties and internal flame structure. Combustion and Flame. 2010 May 1;157(5):995-1011.

[12] Poludnenko, Alexei Y., and Elaine S. Oran. "The interaction of high-speed turbulence with flames: Turbulent flame speed." Combustion and flame 158, no. 2 (2011): 301-326

[13] Xu C, Poludnenko AY, Zhao X, Wang H, Lu T. Structure of strongly turbulent premixed n-dodecane–air flames: Direct numerical simulations and chemical explosive mode analysis. Combustion and Flame. 2019 Nov 1;209:27-40.

[14] Kozak Y, Dammati SS, Bravo LG, Hamlington PE, Poludnenko AY. WENO interpolation for Lagrangian particles in highly compressible flow regimes. Journal of Computational Physics. 2020 Feb 1;402:109054.

[15] Dammati SS, Kozak Y, Rising C, Reyes J, Ahmed KA, Poludnenko AY. Numerical investigation of the accuracy of particle image velocimetry technique in gas-phase detonations. Proceedings of the Combustion Institute. 2021 Jan 1;38(3):3671-81.

[16] Gardiner TA, Stone JM. An unsplit Godunov method for ideal MHD via constrained transport. Journal of Computational Physics. 2005 May 20;205(2):509-39.

[17] Simon S, Mandal JC. A cure for numerical shock instability in HLLC Riemann solver using antidiffusion control. Computers & Fluids. 2018 Sep 30;174:144-66.

[18] Strang G. On the construction and comparison of difference schemes. SIAM journal on numerical analysis. 1968 Sep;5(3):506-17.

[19] Tao Y, Smith GP, Wang H. Critical kinetic uncertainties in modeling hydrogen/carbon monoxide, methane, methanol, formaldehyde, and ethylene combustion. Comb. Flame. 2018;195:18-29.

[20] G. Smith, Y. Tao, and H. Wang, Foundational Fuel Chemistry Model Version 1.0 (FFCM-1), 2016, http://web.stanford.edu/group/haiwanglab/FFCM1/pages/FFCM1.html

[21] Gamezo VN, Vasil'ev AA, Khokhlov AM, Oran ES. Fine cellular structures produced by marginal detonations. Proceedings of the Combustion Institute. 2000 Jan 1;28(1):611-7.

[22] Taylor BD, Kessler DA, Gamezo VN, Oran ES. Numerical simulations of hydrogen detonations with detailed chemical kinetics. Proc. Combust. Inst. 2013 Jan 1;34(2):2009-16.

[23] SDToolbox - Numerical Tools for Shock and Detonation Wave Modeling, Explosion Dynamics Laboratory, Contributors: S. Browne, J. Ziegler, N. Bitter, B. Schmidt, J. Lawson and J. E. Shepherd, GALCIT Technical Report FM2018.001 Revised January 2021, http://shepherd.caltech.edu/EDL/PublicResources/sdt/