

Experimental and calculated detonation cells in gaseous ethanol-oxygen mixtures

Titouan Fessard, Léa Vilasi, Vincent Rodriguez, Pierre Vidal
Institut Pprime, UPR 3346 CNRS, ENSMA, 86961 Futuroscope-Chasseneuil, France

2 Introduction

Liquid alcohols (e.g., methanol, ethanol) are low-carbon, highly volatile liquid fuels commonly used in industry. Studying the conditions for igniting their detonation is important for preventing accidents during transport or storage. Harnessing their detonation in air or oxygen is also of practical interest as a combustion process in advanced propulsion systems designed to achieve pressure gain for more efficient combustion, such as rotating detonation engines [1–3].

Few studies have been conducted on the detonability of alcohol-oxidizer gas mixtures. Eaton et al. [4] and Diakow [5, 6] studied the width of detonation cells in vaporized methanol/ethanol-oxygen mixtures and compared it to predictions from correlations with calculated lengths of the ZND reaction zone. Diakow et al. [5] and Zevallos et al. [7] investigated the detonation propagation and the deflagration-to-detonation transition (DDT) limits of vaporized ethanol–air mixtures. The propagation of detonation in gaseous mixtures obtained by vaporization of a liquid fuel layer into a gaseous oxidant was addressed by Hieronymus et al. [8, 9] and Dengel et al. [10, 11]. They studied the propagation of detonations in methanol-oxygen liquid-gas systems and showed that the detonation velocity decreases with decreasing pressure and becomes constant after a step corresponding to the pressure-flammability limit of the gas phase. These studies mainly describe detonations occurring directly in the gas phase at the surface of the liquid above the flammability limit. Detonation below this limit occurs throughout the gas phase where the liquid has diffused. Hieronymus et al. [9] found no dependence of detonability on liquid layer thickness. Dengel et al. [10, 11] did not observe any influence of the detonation on the liquid surface as it passes over.

In this work, we experimentally analyze the 3D cellular structure of detonation in gaseous ethanol-oxygen mixtures using side-view and front-view recordings on soot foils. We then calculate the mean cell width as a function of the equivalence ratio and initial pressure width using the predictive model based on graph theory and geometric probabilities by Monnier et al. [12]. Section 2 describes the experimental setup and methodology, Sect. 3 presents and analyzes the results, and Sect. 5 concludes the work.

3 Experimental setup and methodology

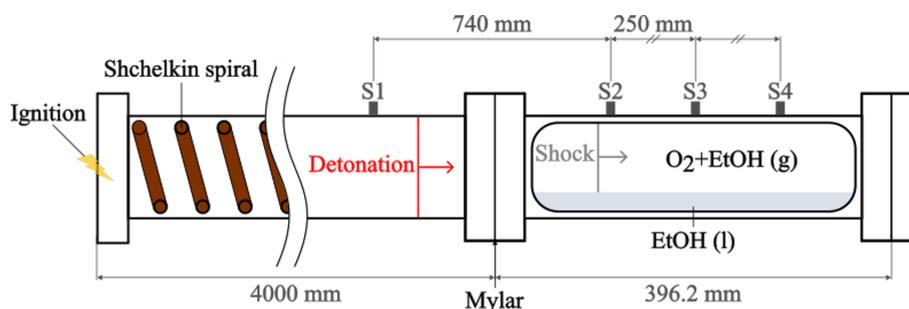


Figure 1: Scheme of the experimental setup.

The setup consisted of two sections, i.e., the booster and the test chamber, with lengths of 4 m and 0.4 m, respectively, and the same square cross-section of $50 \times 50 \text{ mm}^2$. They were separated by an $18 \text{ }\mu\text{m}$ thick plastic film (Mylar). The methodology involved initiating a detonation in the booster section with an electric arc and accelerating the transition to a steady detonation with a Shchelkin spiral. Upon impact, the Mylar foil acted as a piston, generating a shock that may or may not initiate detonation in the gas of the test chamber, depending on its initial characteristics - namely, equivalence ratio, initial pressure, and temperature. The advantage of the shock-to-detonation process over the deflagration-to-detonation transition is that it ensures detonation initiation over shorter distances. The booster gas was either a $\text{H}_2 + \frac{1}{2} \text{O}_2$ or $\text{C}_3\text{H}_8 + 5 \text{O}_2$ mixture at ambient temperature (299 K) and the same initial pressures as the test chamber. The mixtures in the chamber consisted of gaseous ethanol ($\text{C}_2\text{H}_5\text{OH}$) and oxygen (O_2) at varying initial pressures p_0 , equivalence ratios (ER), and ambient temperature. The chamber was filled with gaseous O_2 and a thin layer of liquid $\text{C}_2\text{H}_5\text{OH}$ (1 mm). After a few minutes, the liquid vaporized and diffused into the gaseous O_2 , forming a homogeneous mixture saturated with ethanol. Under these conditions, the equivalence ratio decreased with increasing initial pressure p_0 . The initial pressures p_0 ranged from 15 to 100 kPa. The liquid layer of ethanol above the underside of the chamber served only to generate the gas mixture. The liquid layer remaining after the desired composition has been achieved has no effect on the propagation and structure of the detonation (Sect. 4).

Optical oxygen probes (Pyroscience PreSens Oxygen Dipping Probe PSt3) were used to measure the oxygen concentration in the test mixture. The detonation velocities and pressures in the booster and the test chamber were measured using four Kistler 603CAB pressure transducers (Fig. 1, S1-3, $1 \text{ }\mu\text{s}$ response time, 300 kHz natural frequency), each coupled to a Kistler 5018A charge amplifier (200 kHz bandwidth). The cellular structure of the detonation was characterized using side-view and front-view soot-coated foils. The side-view foils covered the entire length of the sidewall of the test chamber and, together with the velocity measurements, provided a criterion for detonation stability based on nearly constant cell geometric properties. The front-view foils were perpendicular to the direction of detonation

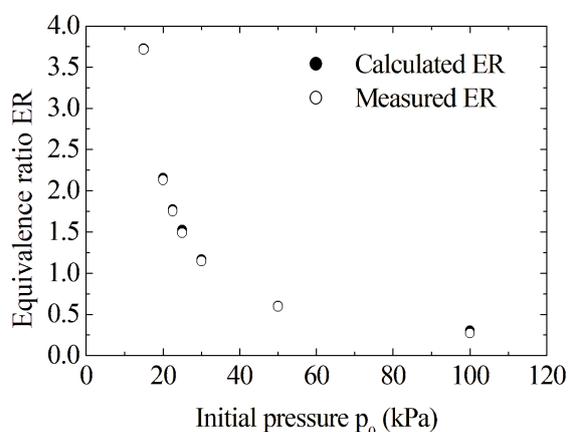


Figure 2: Calculated and measured equivalence ratios (ER) of EtOH-oxygen mixtures relative to the initial pressure p_0 in the chamber.

propagation and covered the entire cross section of the chamber.

We measured the composition of the ethanol-oxygen mixture in the chamber using oxygen probes at an initial temperature of 299.15 ± 1 K. No significant variations in the mixture composition were observed with respect to the longitudinal or transverse position of the measurements. Ethanol diffuses into the oxygen as a function of temperature and pressure, and the composition stabilizes after 3-5 minutes under our experimental conditions. This period represents the minimum delay required after injection to ignite the detonation in the booster gas. Figure 2 shows the measured and theoretically estimated equivalence ratios (ER), assuming the gas mixture is saturated with ethanol.

4 Results and analysis

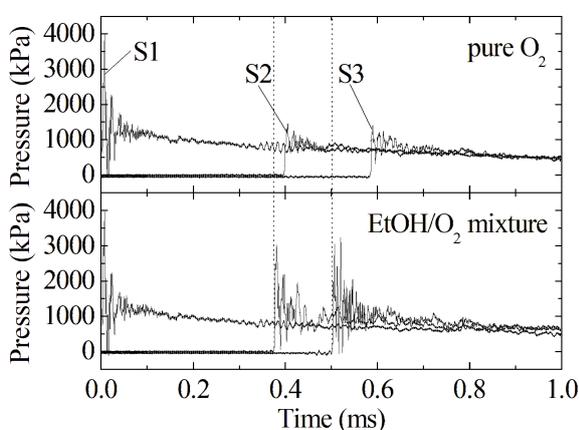


Figure 3: Pressure signals with $p_0=50$ kPa. Top: shock in O_2 . Bottom: detonation in EtOH/ O_2 mixture at ER=0.59.

evidenced by larger cells of nearly uniform size and orientation relative to the tube axis. The front view in Figure 5 shows the cell patterns during the steady propagation phase at the end of the test section. The edges of these patterns correspond to the positions of the transverse waves that bound the cells at the instant of the head-on impact with the soot-coated foil. These recordings show that the detonation propagates steadily through the assumed uniform distribution of EtOH in oxygen. The liquid layer appears to have no visible effect on the detonation cells, as they all have approximately the same characteristics regardless of their vertical positioning.

Figure 6 shows the distributions of the measured detonation cell widths for initial pressures of 20 and 100 kPa. These distributions were obtained with $\mathcal{O}(100)$ cell width measurements. They have a sufficiently sharp shape to make the most represented value a statistically significant mean. These are 4.1 mm and 10 mm for $p_0 = 20$ and 100 kPa, respectively. We recall (Sect. 3) that vaporization leads to equivalence ratios that decrease with increasing initial pressure, which accounts for the larger mean cell width at 100 kPa. The soot recordings, such as those in Figs. 4 and 5, show that the cell widths remain essentially constant across the height of the chamber. They also show a large number of cells at the detonation front, i.e., the cell widths are small relative to the transverse dimension of the chamber, regardless of the initial pressure.

Non-excessive irregularity, steady propagation, and a sufficiently large number of cells suggest that the

The pressure signals were used to characterize detonation initiation and propagation. Pressure transducer S1 was located in the booster section, while S2 and S3 were located in the test chamber. Figure 3 compares the pressure history records without (top) and with (bottom) the EtOH liquid layer in the chamber for a shock transmitted to the chamber from a stoichiometric C_3H_8 / O_2 detonation in the booster.

Figures 4 and 5 show side-view and front-view soot recordings for $p_0 = 20$ kPa, with detonation cells indicating detonation propagation. Detonation initiation is observed in the lower left of the recording in Figure 4 as an overdriven detonation propagating transversely to the tube axis. This is indicated by the transverse orientation of very small detonation cells that progressively increase in size. Steady propagation is then achieved, as

cell structure is independent of the channel geometry under our conditions. These cell widths are thus suitable for prediction based on the model of Monnier et al. [12], which combines graph theory, geometric probabilities, and ZND properties derived from detailed chemical kinetic mechanisms. Table 1 compares the measured and calculated mean widths and shows excellent agreement with Konnov's kinetic mechanism [13].

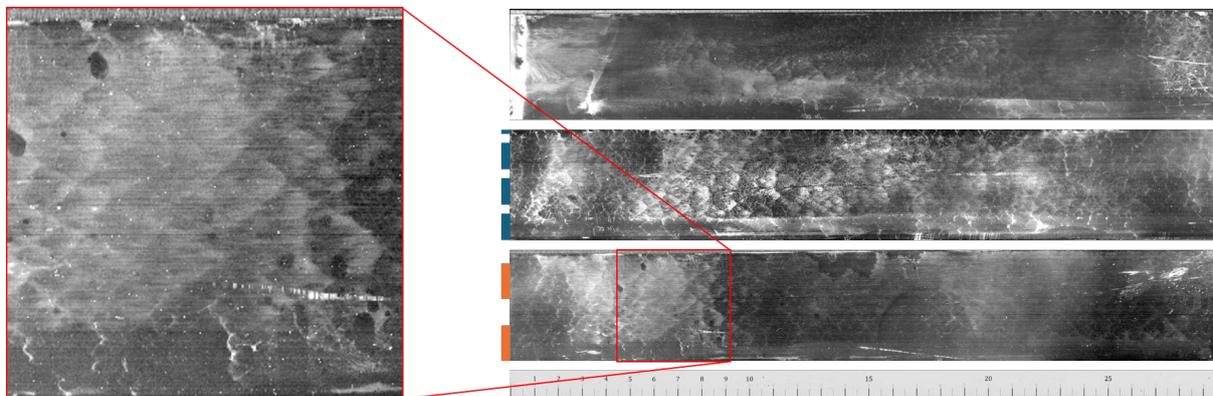


Figure 4: Side-view soot recording of the detonation cellular structure in the EtOH-oxygen mixture at ER=2.12 and $p_0=20$ kPa. The detonation propagates from left to right, lower plates continuing upper ones.

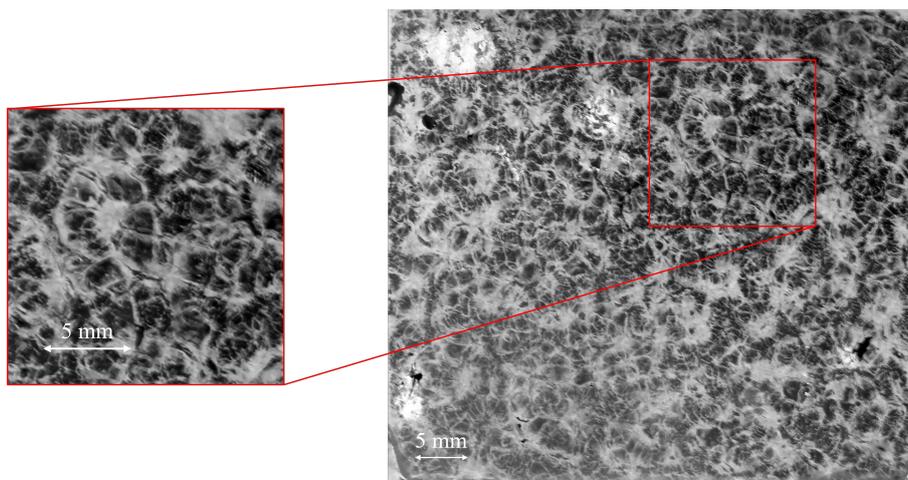


Figure 5: Front-view soot recording of the detonation cellular structure in the EtOH-oxygen mixture at ER=2.12 and $p_0=20$ kPa.

Table 1: Measured (λ_x) and calculated (λ_c) [12] cell mean widths for EtOH-oxygen mixtures.

p_0 (kPa)	ER	λ_x (mm)	λ_c (mm)	Chemical mechanism
20	2.13	4.1 ± 1.3	5.1	Konnov [13]
			11.6	SanDiego [14]
100	0.27	10 ± 1.8	10.5	Konnov [13]
			17.1	SanDiego [14]

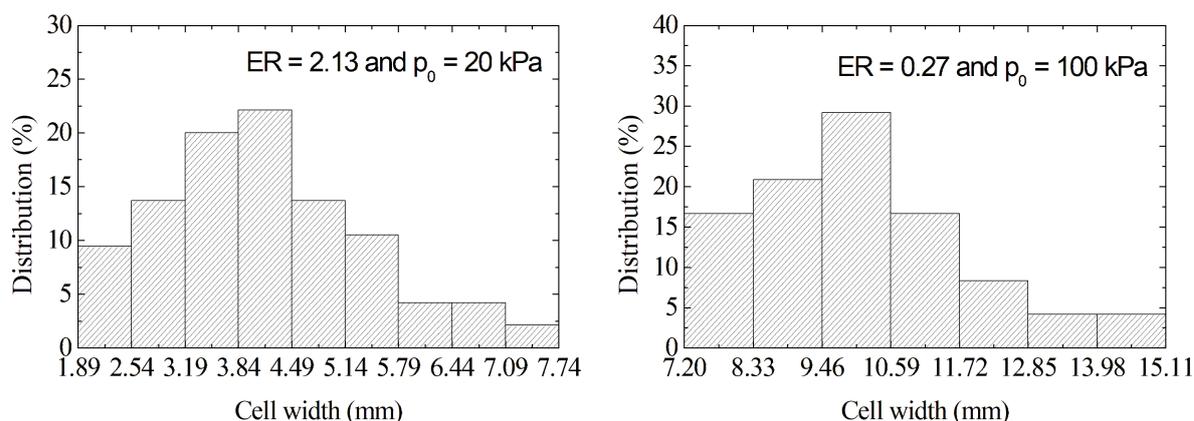


Figure 6: Cell width distributions for EtOH-O₂ mixtures with (Left) ER = 2.13 and $p_0 = 20$ kPa, and (Right) ER = 0.27 and $p_0 = 100$ kPa.

5 Conclusion

This study demonstrates the possibility of detonation in ethanol-oxygen mixtures from direct observation of the cellular structure of the detonation reaction zone. Homogeneous ethanol-oxygen gas mixtures were generated by diffusion from a layer of liquid ethanol initially placed under an atmosphere of gaseous oxygen. The initiation, propagation, and cellular structure of the detonation were analyzed using pressure transducers and side-view and front-view soot recordings. Steady detonation propagation in ethanol-oxygen gas mixtures was achieved for several equivalence ratios ranging from 0.27 to 2.13. Calculated mean detonation cell widths – based on graph theory, geometric probabilities, and ZND properties from Konnov’s chemical mechanism – were found to be in good agreement with the measurements, further confirming that detonation effectively propagated in the saturated ethanol-oxygen gas. Ongoing studies address the effect of varying the equivalence ratio at fixed initial pressures.

Acknowledgements: This work was supported by the French Research National Agency (ANR) under the project ANR-21-CE05-0002-01.

References

- [1] J. Li, Y. Lei, S. Yao, J. Yu, J. Li, and W. Zhang, “Investigation of multi-stage evaporation and wave multiplicity of two-phase rotating detonation waves fueled by ethanol,” *Acta Astronautica*, vol. 213, pp. 418–430, 2023. doi : <https://doi.org/10.1016/j.actaastro.2023.08.037>.
- [2] K. Ishihara, K. Yoneyama, T. Sato, H. Watanabe, N. Itouyama, A. Kawasaki, K. Matsuoka, J. Kasahara, A. Matsuo, and I. Funaki, “Visualization and performance evaluation of a liquid-ethanol cylindrical rotating detonation combustor,” *Transactions of the Japan Society for Aeronautical and Space Sciences*, vol. 66, no. 2, pp. 46–58, 2023. doi : <https://doi.org/10.2322/tjsass.66.46>.
- [3] S. Yao, X. Tang, and W. Zhang, “Structure of a heterogeneous two-phase rotating detonation wave with ethanol–hydrogen–air mixture,” *Physics of Fluids*, vol. 35, no. 3, 2023. doi : <https://doi.org/10.1063/5.0144920>.
- [4] R. Eaton, B. Zhang, J. M. Bergthorson, and H. D. Ng, “Measurement and chemical kinetic model predictions of detonation cell size in methanol–oxygen mixtures,” *Shock Waves*, vol. 22, pp. 173–178, 2012. doi : <https://doi.org/10.1007/s00193-012-0359-x>.

- [5] P. A. Diakow, Detonation characteristics of dimethyl ether, methanol and ethanol air mixtures. PhD thesis, Queen's University (Canada), 2012.
- [6] P. Diakow, M. Cross, and G. Ciccarelli, "Detonation characteristics of dimethyl ether and ethanol-air mixtures," Shock Waves, vol. 25, pp. 231–238, 2015. doi : <https://doi.org/10.1007/s00193-015-0554-7>.
- [7] A. A. M. Zevallos, G. Ciccarelli, and J. A. Carvalho Jr, "Ddt limits of ethanol-air in an obstacles-filled tube," Combustion Science and Technology, 2018. doi : <https://doi.org/10.1080/00102202.2018.1477770>.
- [8] H. Hieronymus, P. Henschen, M. Hofmann, J. Bender, R. Wendler, J. Steinbach, and B. Plewinsky, "Hazards of surface explosions," pp. 897–908, 2001. doi : <https://doi.org/10.1016/B978-044450699-3/50010-0>.
- [9] H. Hieronymus, M. Hofmann, J. Bender, P. Henschen, R. Wendler, B. Plewinsky, and J. Steinbach, "Characterisation of surface explosions," Archivum combustionis, vol. 21, no. 2, pp. 117–125, 2001.
- [10] J. Dengel, R. Wendler, W. Denzer, J. Buchholz, M. Beckmann-Kluge, J. Steinbach, B. Plewinsky, and H. Hieronymus, "Explosions near the surface of organic liquids," Process safety and environmental protection, vol. 83, no. 5, pp. 452–458, 2005. doi : <https://doi.org/10.1205/psep.04199>.
- [11] J. Dengel and H. Hieronymus, "Einfluss der flüssigen phase auf detonationen im zweiphasigen system methanol/sauerstoff," Chemie Ingenieur Technik, vol. 78, no. 1-2, pp. 134–138, 2006. doi : <https://doi.org/10.1002/cite.200500053>.
- [12] V. Monnier, P. Vidal, V. Rodriguez, and R. Zitoun, "From graph theory and geometric probabilities to a representative width for three-dimensional detonation cells," Combustion and Flame, vol. 256, p. 112996, 2023. doi : <https://doi.org/10.1016/j.combustflame.2023.112996>.
- [13] F. Coppens, J. De Ruyck, and A. Konnov, "The effects of composition on burning velocity and nitric oxide formation in laminar premixed flames of $ch_4 + h_2 + o_2 + n_2$," Combustion and Flame, vol. 149, no. 4, pp. 409–417, 2007. doi : <https://www.sciencedirect.com/science/article/pii/S0010218007000636>.
- [14] Chemical-Kinetic Mechanisms for Combustion Applications, San Diego Mechanism web page, Mechanical and Aerospace Engineering (Combustion Research), University of California at San Diego (2016), Last accessed January 2025, 2016. url : <https://web.eng.ucsd.edu/mae/groups/combustion/mechanism.html>.