International Conference on Numerical Combustion
Rome, Italy, October 14-17, 2025
www.icnc2025.com

Transition from Single to Double Cellular Structures in Confined Hydrogen-Nitrogen Oxide Detonations

Behrang Shirvani[1]*, Brian Maxwell[1] Remy Mevel[2]
* behrang.shirvani@uottawa.ca
[1] Department of Mechanical Engineering, University of Ottawa, 161 Louis Pasteur, Ottawa, K1N 6N5, Canada
[2] School of Aeronautics and Astronautics, Zhejiang University, Hangzhou, China

Detonation waves in hydrogen–nitrogen oxide mixtures (i.e. H_2-NO_2/N_2O_4) can exhibit a double cellular structure under certain conditions, believed to be attributed to a two-stage heat release process with different amplitudes and timescales [1]. This study presents new insights into the behavior of these detonations through two-dimensional (2D) numerical simulations with detailed chemistry, and where momentum losses have been taken into account using a simple flow-divergence model [2,3]. Although previous experiments on H_2-NO_2/N_2O_4 detonations have confirmed the existence of this double structure at high pressures, its disappearance at lower pressures has remained an open question [4-8]. Our simulations confirm that at ambient pressures, at 100 kPa, a well-defined double cellular detonation structure persists. However, at lower pressures, 25 kPa, a significant velocity deficit occurs when momentum losses are present, and a transition to a single, irregular cellular structure is observed. At present, preliminary results of our investigation have revealed that when losses due to flow divergence are omitted at low pressures, the double cellular structure is restored. This finding highlights the sensitivity of detonation structure to hydrodynamic losses. The results support previous speculation that the transition from double to single cellular structures is not solely a function of pressure but also depends on the hydrodynamic losses [9]. In this sense, it is likely that losses cause elongation of the cellular structure in such a way that only the fine structures are captured by simulation at low pressures with losses, while the large structures extend beyond the physical domain simulated. Future work will focus on increasing numerical resolution better to capture the coupling between chemical kinetics and hydrodynamics. Also, we aim to better understand how the inner structures are formed, in order to detail the dynamics of the double cellular structure.

References

[1] Joubert F, Desbordes D, Presles HN. Detonation cellular structure in NO_2/N_2O_4-fuel gaseous mixtures. Combustion and Flame. 2008;152(4):482-95.
[2] Smith J, Schmitt C, Xiao Q, Maxwell B. On the nature of transverse waves in marginal hydrogen detonation simulations using boundary layer loss modeling and detailed chemistry. Combustion and Flame. 2024;268:113598.
[3] Xiao Q, Weng C. Unified dynamics of hydrogen–oxygen–diluent detonations in narrow confinements. Fuel. 2023;334:126661.
[4] Luche J, Desbordes D, Presles HN. Détonation de mélanges H_2-NO_2/N_2O_4-Ar. Comptes Rendus Mécanique. 2006;334(5):323-7.
[5] Guilly V, Khasainov B, Presles HN, Desbordes D. Simulation numérique des détonations à double structure cellulaire. Comptes Rendus Mecanique. 2006;334(11):679-85.
[6] Sugiyama Y, Matsuo A. On the characteristics of two-dimensional double cellular detonations with two successive reactions model. Proceedings of the Combustion Institute. 2011;33(2):2227-33.
[7] Davidenko D, Mével R, Dupré G. Numerical study of the detonation structure in rich H_2-NO_2/N_2O_4 and very lean H 2− N 2 O mixtures. Shock Waves. 2011;21:85-99.
[8] Desbordes D, Presles HN, Joubert F, Douala CG. Etude de la détonation de mélanges pauvres H_2-NO_2/N_2O_4. Comptes rendus. Mécanique. 2004;332(12):993-9.
[9] Virot F, Khasainov B, Desbordes D, Presles HN. Two-cell detonation: losses effects on cellular structure and propagation in rich H_2-NO_2/N_2O_4-Ar mixtures. Shock Waves. 2010;20(6):457-65.