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Sensitizing Reaction Chemistry in Detonation

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Sensitizing Reaction Chemistry in Detonation

Hai Wang (PI), Professor, Stanford University

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Abstract

The project centered on a rational sensitization of the chemistry effect without notably affecting the unburned mixture properties. The work measured the minimum detonation tube diameter and detonation cell size for a series of fuel-oxidizer-diluent mixtures in which the ignition delay time is altered by doping a trace amount of additive (e.g., ozone). The doping has little to no effect on fluid and mixture thermodynamic properties, including viscosity, conductivity, speed of sound, and adiabatic flame temperature. Additionally, available chemical reaction models were extended to detonation simulations and expanded to include the chemistry of ozone in fuel oxidation. Molecular dynamics studies focused on the interaction of shocks with nano-droplets of *n*-dodecane with the goal of understanding heterogeneous energy transfer in shocks.

Key Objectives

This AFOSR sponsored project has four key objectives:

1) to isolate the chemistry effect from gasdynamic effects on detonation, by measuring the minimum detonation tube diameter and detonation cell size for a series of fuel-oxidizer-diluent mixtures in which the ignition delay time is altered by chemical doping without incurring significant changes in the thermodynamic properties of the burned and unburned mixtures;
2) to expend the applicability of available chemical reaction models for detonation modeling and to include the chemistry of ozone in fuel oxidation;
3) to demonstrate that natural gas is a viable detonation fuel with better detonation properties than methane;
4) to carry out molecular dynamics studies focused on the interaction of shocks with nanoparticles.

Accomplishments

We have completed the project, met the objectives, and exceeded our initial goals. Specifically, in meeting the first objective, we realized the importance of boundary conditions on detonation cell structures and detonation propagation. We have extended the initial plan by developing a geometric model (*detgem*) to closely model this effect, and by collaborating with the Duisberg group (Prof. A. Kempf) and the UConn group (Profs. X. Zhao and A. Poludnenko) in the area of direct numerical simulations of detonations in spatial confinement, both using realistic reaction chemistry. Overall, the project led to important advances in our basic understanding of detonation waves, their structures, and the energy transfer mechanisms.

Key highlights include:

The effect of ignition promoters on H_2-O_2 detonation structure was evaluated with one-dimensional ZND calculations and experimental detonation cell measurements. Test conditions include a sweep of ozone concentration (up to 3000 PPM by mol), initial pressure (up to 30 kPa), equivalence ratio (0.4 to 1.5), Ar and N_2 dilution (up to 50%), and CF_3I concentration (up to 3000 PPM). The ZND calculations demonstrate that ozone addition reduces induction length without affecting heat release length or thermodynamic properties such as Chapman-Jouquet (CJ) speed, allowing for a unique evaluation of the effect of ignition delay on detonation structure. Experimentally, ozone addition acts to reduce characteristic cell size (by up to 40%). Within the conditions tested, measured cell width is found to better correlate with total reaction length, defined as induction length plus exothermic length, instead of induction length alone used in existing correlations. The results confirm that the detonation structure is controlled largely by chemical length scales. Also studied is the addition of CF_3I, which is traditionally used as a fire suppressant. Although at high concentrations CF_3I displays a radical scavenging function, at the concentrations considered in the current work, CF_3I also acts as an ignition promotor due to the production of the I atom, which promotes chain branching during ignition. Finally, the ozone and CF_3I additives were found to have, at most, a minor effect on cell regularity. This work was carried out to meet objectives 1 and 2 of the project, and was published as Refs. 1 and 2.

A geometric model with a low computational complexity capable of simulating detonation behavior in physical systems is proposed. In support of the geometric model development, a series of cylindrical 1D simulations with a variable size initiation kernel are performed in hydrogen-oxygen

mixtures. From these 1D simulations a detonation cell stabilization mechanism is identified. The stabilization mechanism is predicated on the size of the gap between the pressure and temperature fronts at the point where the average pressure front velocity along one cell length is equal to the CJ velocity. This gap, in a multidimensional detonation, is the ignition kernel of a subsequent blast, and dictates the formation of the subsequent cell. Serial analysis of blasts in this context leads to a unique stable blast kernel size for any mixture, which, within the uncertainty of the initial kernel state, can predict the experimental cell length for mixtures considered in this study. Using a tabulation of the 1D simulations as an input, a formulation and sample results of the geometric model are shown. The geometric model can reproduce both qualitative and quantitative features of experimental detonation cellular structure. This work was carried out to meet objectives 1 and 2 of the project, and was published as Refs. 3.

Detonation properties of methane and natural gas were studied using ZND simulations and detonation limit experiments. The experiments were performed in two tube sizes, 32 mm and 6.4 mm in inner diameter over a range of initial pressures (between 3.4 kPa and 35 kPa) and with stoichiometric fuel- oxygen compositions. The fuels considered are high purity methane, high purity methane with dopant ozone, a real natural gas, and a family of natural gas surrogates. The natural gas surrogates were developed based on North American natural gas composition variations and designed to capture the expected mean and variance of fundamental combustion properties of natural gases. All natural gases tested in this work show a substantially smaller detonation induction length (about 40%) and a lower detonation pressure limit (30% in terms of limiting pressure) than high purity methane. The ozonated methane at 3000 PPMv of ozone doping performed similarly to the natural gases. Overall, the results suggest that in methane-based mixtures, a smaller induction length correlates with a more predictable detonation behavior as evidenced by a lower detonation pressure limit. As such, natural gases are expected to have a wider operating range when used as a fuel for detonation-based engines. As importantly, induction length calculation results reveal that the variability in detonation and combustion behaviors resultant from composition variability is expected to be similar between natural gases and commercial methane. Finally, the results suggest that for safety-related studies, neat methane is a poor surrogate for studying natural gas explosions. This work was carried out to meet objectives 2 and 3 of the project, and was published as Ref. 4.

Three-dimensional (3D) detonation simulations solving the compressible Navier-Stokes equations with detailed chemistry are performed in both square channel and round tube geometries. The simulations are compared with each other and with two-dimensional (2D) channel simulations and round tube experiments of identical mixture and conditions (stoichiometric hydrogen oxygen with 3000 PPMv ozone at 300 K and 15 kPa) with the goal of understanding the effect of confinement and boundaries on detonation structure. Results show that 3D detonations propagate with highly inhomogeneous blast dynamics, where blasts emerge not only from intersections of two transverse waves (similar to 2D propagation) but also from intersections of many transverse waves (unique to 3D detonations in the confinements tested). Intersections of many transverse waves lead to extreme thermodynamic states and highly overdriven wave velocities, well in excess of those seen in the ZND model and in 2D simulations. 3D simulations in the square channel show highly regular blast latticing, smaller detonation cells, and highly oscillatory velocities when compared to the round tube simulations. Round tube simulations show more spatially non-uniform blast dynamics. The conclusions reached in the current work are found irrespective of numerical grid resolution. This work was carried out to meet objectives 1 and 2 of the project, and was published as Ref. 5.

In corroboration with Dr. Fotia's group at AFRL, detonation propagation dynamics in curved channels were investigated using both experimental and geometric modeling approaches. Quasi-two-dimensional curved channels with a range of channel widths and curve radii were tested. Experimentally, three propagation modes were observed: a stable propagation mode featuring flat detonation front and steady near-CJ propagation, a unstable mode with varying frontal structure and velocity oscillations, and failure to propagate. The observed propagation modes can be organized into a regime map, with the channel width to cell width ratio and inner radius to outer radius ratio being the two independent dimensionless variables. Data from both this study and literature show that for a given channel width to cell width ratio, there exists a critical inner-to-outer radius ratio that sets apart the stable and unstable propagation modes. This is because of the competition between the focusing effect of the outer concave boundary (with respect to detonation wave) and the diverging effect of the inner convex boundary. With increasing channel-to-cell width ratios, the critical inner-to-outer radius ratio decreases. Detonation failure is most likely found in the region of small channel-to-cell width ratios. Geometric modeling results and their trends are in agreement with experimental observations. In addition, geometric modeling is able to test geometries that were not accessible through experiments and validate the overall trends. Lastly, despite a good agreement among different experimental studies using cell width as the detonation structure length scale, the actual cell sizes are subject to specific initial and boundary conditions. As a result, quantities involving cell sizes may have uncertainties up to a few factors. This work was carried out to meet objectives 1 and 2 of the project, and was published as Ref. 6.

The dependence of detonation cell regularity on mixture gasdynamic and chemical kinetic properties are investigated through hydrogen-oxygen detonations with different diluent and ozone addition. A total of seven mixtures are specifically designed such that the post-shock specific heat ratio γ_{VN}, representing the gasdynamic effect, and the effective activation energy ϵ_i, representing the chemistry effect, can be varied independently among these mixtures. Both experiments and two-dimensional (2D) Navier-Stokes simulations are performed. For the ranges of γ_{VN} and ϵ_i considered, γ_{VN} is found to moderately affect cell regularity. For mixtures of relatively large γ_{VN} ($\geq$1.3), detonation cells become slightly irregular with decreasing γ_{VN}. A clear increase in cell irregularity is found when γ_{VN} is small (<1.3). In contrast, the impact of ϵ_i on cell regularity is more notable: mixtures of large ϵ_i produce significantly more irregular cells, corresponding to frequent appearances of transverse detonation structures that dominate the global burning behavior. Finally, ozone is qualitatively and quantitatively shown to regulate the detonation structures in both simulations and experiments tested in this study, and results suggest that trace additives that alter the ϵ_i of a mixture can likely be used to tune the mixture for a desired regularity. This work was carried out to meet objectives 1 and 2 of the project, and was published as Ref. 7.

A detonation cellular stability theory based on dynamics of reactive decaying blasts is proposed, elucidated, and examined through detailed analysis of two-dimensional (2D) numerical simulations of hydrogen-oxygen detonations. Different from previous blast-based theories, the proposed stability theory resolves the transient process of decoupling between shock and reaction fronts in decaying blasts, and correlates the size of unburnt pockets behind decaying shock fronts and that of the subsequent blast kernels. Simulations of hydrogen-oxygen detonations with and without dopant concentrations of ozone are performed and analyzed. Ozone is known to reduce ignition delay times without altering the thermodynamic properties of the base mixture, thus enabling the investigation of the impact of ignition kinetics on detonation cellular stability. The cell size reduction, observed in the simulations in the ozonated mixture, is well described by the proposed stability theory and in

agreement with recent experimental cell measurements reported in Crane *et al.* [1]. It thus suggests the necessity of detailed chemical kinetic models in detonation simulations to accurately capture the blast decay behavior and predict detonation cell size. The inclusion of diffusive physics, i.e., solving the Navier-Stokes equations instead of the Euler equations is seen to marginally affect the detonation cellular stability (minimal detonation cell size change) but reduces the propagation speed due to boundary losses. Two channel heights, 6 mm and 24 mm, are tested and the cell size increase due to mode-locking is also explained by the stability theory. In addition, a detailed grid convergence study is performed, which examines both the kinetic and macroscopic structural features as a function of grid resolution. This work was carried out to meet objectives 1 and 2 of the project, and was published as Ref. 8.

The deflagration-to-detonation transition (DDT) process inside reactant-product mixing layers is studied using one-dimensional transient simulations of stoichiometric hydrogen-air mixtures. Such processes are seen to be responsible for the multi-front detonation propagation in rotating detonation engines (RDEs). For a given mixture, two modes of combustion dynamics, detonation and deflagrative flame, are observed at different mixing layer lengths. A critical mixing layer length can be identified for detonation formation using the Zeldovich theory, where the local characteristic velocity – the inverse of spatial gradient of ignition delay time – is equal to the theoretical Chapman-Jouguet (CJ) speed. As the mixing layer is comprised of mostly diluted or partially reacted mixtures, detonation formation is not possible in regions of relatively high burnt mixture content even if the Zeldovich criterion is met. The impact of initial pressure and addition of ignition promoter on the DDT process are also investigated. At higher initial pressures, the critical mixing layer length becomes smaller, in agreement with the experimental observation that the multi-front operation mode occurs more favorably at elevated pressures. Ignition promoting additives such as ozone do not affect the DDT behavior, as the reduction in ignition delay time does not change the location of critical characteristic velocity. Knowing the critical mixing layer length scales, the occurrence of multi-front RDE operation can be estimated by comparing the residence time of a single detonation front in RDEs to the developing time of the mixing layer. This work was carried out to meet objectives 1 and 2 of the project, and was published as Ref. 15.

A diverse computational toolset is needed to understand and design devices which use detonation. State-of-the-art detonation simulations are highly resolved and are thus expensive and challenging to set up. We developed a model, *detgem*, which leverages the underlying physics of cellular structure to predict detonation propagation at a cost many orders of magnitude lower than conventional simulations. In this model, we empirically develop the transverse wave mechanism in *detgem* based on experimental and computational results of detonations bounded by an inert gas layer. We then demonstrate that *detgem* can predict cellular detonation propagation in a range of useful geometries: detonation in semi-bounded channels, detonations in a range of channel widths, and detonations in U-bends. All of the expected detonation physics are observed in the model results. The model is then used to study the effect of curvature in detonation propagation. Highly curved channels cause triple point focusing on the outer wall, but they act as a triple point sink on the inner wall, which eventually leads to detonation destabilization and failure, with propagation length inversely proportional to curvature. This work was carried out to meet objectives 1 and 2 of the project, and was published as Ref. 16.

To meet objective 4, we carried out a series of molecular dynamics (MD) simulations for shock interactions with nanodroplets of *n*-dodecane. Fig. 1 shows two sample cases of the droplet time

histories, including drag induced motion and fragmentation/evaporation upon shock interaction. The simulations were carried out for an *n*-dodecane droplet 10 nm in diameter in nitrogen at the pre-shock pressure of 1 bar and post-shock pressure of 28 bar and 1344 K (panel a), and pre-shock pressure of 35 bar and post-shock pressure of 980 bar and 1344 K (panel b). The *n*-dodecane molecules are labeled in red, and N_2 molecules are labeled in green. The post shock conditions correspond to the transition regime with the Knudsen number Kn = 1.1 for panel (a) and the continuum regime with Kn = 0.03 in panel (b). The results suggest that in the transition regime (0:1 < Kn < 10), shock impact causes the droplet to undergo a process that can be best described as surface evaporation (Fig 1a). In the continuum regime (post-shock Kn < 0.1), however, the droplet dynamics is decidedly different. After shock passage, the droplet swells and fragments, in a behavior that is closer to micro-explosion than to surface evaporation (Fig 1b). For this reason, existing d^2 law predicts the droplet evaporation rates in shock waves poorly. Development of the energy transfer mechanism and models of droplet fragmentation is ongoing, and the work is to be submitted for publication in the near future (Ref. 9).

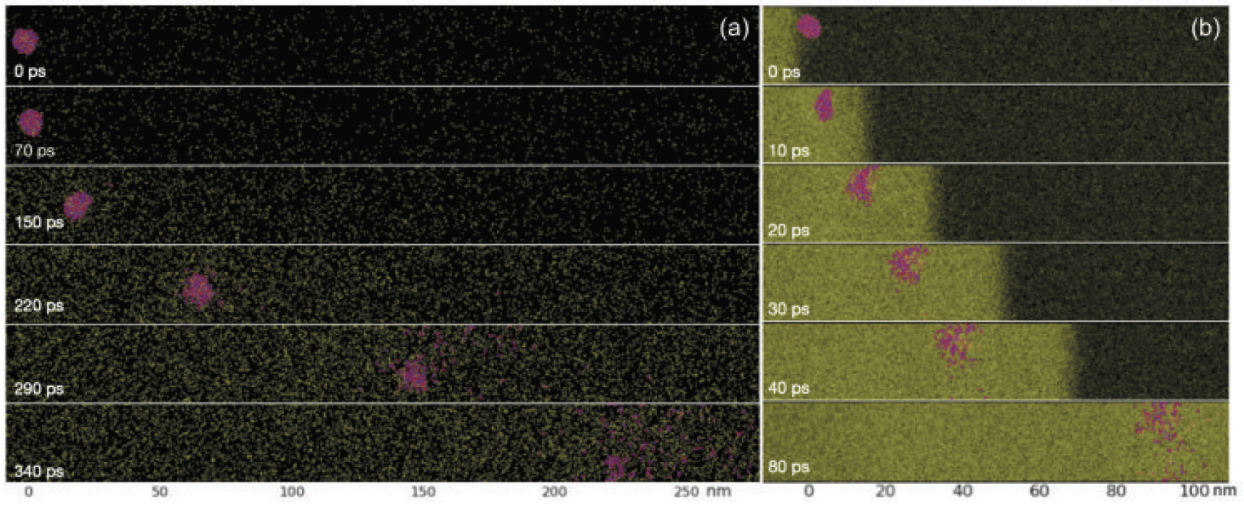

Figure 1. Sample molecular dynamics results of shock interactions with a nanodroplet of *n*-dodecane 10 nm in diameter in nitrogen.

USAF/USSF/DoD/Academia/Industry Relationship or Collaboration Highlights

- A collaboration was initiated between Stanford University and University of Connecticut with the goal of using direct numerical simulation to better accomplish and to exceed the research goals. Biweekly meetings have been held to coordinate the research.
- A collaboration was initiated between Stanford University and AFRL (Dr. M. L. Fotia) with a focus on understanding detonation propagation kinetics and dynamics in bend channels.
- A collaboration was initiated between Stanford University and AFRL (Dr. S. A. Schumaker) with a focus on detonation measurements focusing on detonation cell dynamics.
- New research directions include a more general description of the detonation cell cycle dynamics, especially concerning the mechanisms of energy transfer within a cell, and a transition to droplet and spray detonation.

- A MURI proposal with Stanford being the lead institution was submitted to ONR focusing on the latter aspect of detonation science.

Participants

Name: Hai Wang
Total Number of Months: 60
Project Role: PI
Researcher Identifier: ORCID 0000-0001-6507-5503
Contribution to Project: Prof. Wang coordinated and planned the research.
State, U.S. territory, and/or country of residence: California, USA
Collaborated with individual in foreign country: Yes
Country(ies) of foreign collaborator: Germany
Travelled to foreign country: Yes
If traveled to foreign country(ies), duration of stay: 2 months

Name: Xian Shi
Total Number of Months: 60
Project Role: Postdoc
Contribution to Project: Dr. Shi conducted and coordinated daily experimental and modeling work.
State, U.S. territory, and/or country of residence: California, USA
Collaborated with individual in foreign country: Yes
Country(ies) of foreign collaborator: Germany
Travelled to foreign country: No.

Name: Jackson Crane
Total Number of Months: 55
Project Role: Ph.D. student
Contribution to Project: Mr. Crane participates in all aspects of the research, including conference presentation
State, U.S. territory, and/or country of residence: California, USA
Collaborated with individual in foreign country: Yes
Country(ies) of foreign collaborator: Germany
Travelled to foreign country: No.

Name: Yue Zhang
Total Number of Months: 3
Project Role: Ph.D. student
Contribution to Project: Mr. Zhang provided the reaction models for detonation modeling.
State, U.S. territory, and/or country of residence: California, USA
Collaborated with individual in foreign country: No

Name: Nikolaos Kateris
Total Number of Months: 6
Project Role: Ph.D. student
Contribution to Project: Mr. Kateris carried out molecular dynamics simulations for shock interactions with *n*-dodecane nanodroplets.

State, U.S. territory, and/or country of residence: California, USA
Collaborated with individual in foreign country: No

Human Resource Development

Jackson Crane, a Ph.D. student on the project, graduated and received his Ph.D. degree from Stanford in 2021. He is currently a postdoctoral fellow at Queens University (Canada) and will become a faculty member in a major Canadian university starting in Fall of 2022.

Xian Shi, a postdoc on the project, was appointed as a Tenure Track Assistant Professor at University of California, Irvine. He is to start the position in January, 2022.

Publications and Presentations:

1. Crane, J., Shi, X., Singh, A., Tao, Y., Wang, H. "Isolating the effect of reaction length on detonation structure: hydrogen-oxygen detonation promoted by ozone," *Combustion and Flame* 200, pp. 44-52 (2019).
2. Shi, X., Crane, J., Wang, H. "Detonation and its limit in small tubes with ozone sensitization," *Proceedings of the Combustion Institute*, 38, 3547-3554 (2021).
3. Crane, J., Xhi, X., Lipkowicza, J. T., Kempt, A. M., Wang, H. "Geometric modeling and analysis of detonation cellular stability," *Proceedings of the Combustion Institute* 38, 3585-3593 (2021).
4. Crane, J., Xian, S., Xu, R., Wang, H. "Natural gas versus methane: ignition kinetics and detonation limit behavior in small tubes." *Combustion and Flame* **237** (2022) 111719.
5. Crane, J., Lipkowicz, J. T., Shi, X., Wlokas, I., Kempf, A. M., Wang, H. "Three-dimensional detonation structure and its response to confinement," *Proceedings of the Combustion Institute*, submitted, 2021.
6. Shi, X., Hencel, R. J., Crane, J., Fotia, M. L., Wang, H. "Geometric stability of detonation propagation in curved channels," *Proceedings of the Combustion Institute*, submitted, 2021.
7. Meagher, P. A., Shi, X., Santos, J. P., Muraleedharan, N. K., Crane, J., Poludnenko, A. Y., Wang, H., Zhao, X. "Isolating gasdynamic and chemical effects on the detonation cellular structure: a combined experimental and computational study," *Proceedings of the Combustion Institute*, submitted, 2021.
8. Lipkowicz, J. T., Crane, J., Shi, X., Wang, H., Wlokas, I., Kempf, A. M. "Kinetics-resolved detonation cellular stability with ozonated mixtures," *Journal of Fluid Mechanics*, in final preparation.
9. Kateris, N., Wang, H. "Shock-initiated fragmentation of *n*-dodecane nano-droplet: a molecular dynamics study," manuscript in preparation.
10. Shi, X., Crane, J., Wang, H. "Extension of detonation limits using ozone as an additive," 11th US National Combustion Meeting, Pasadena, CA, March 24-27, 2019.
11. Crane, J., Shi, X., Wang, H. "Effect of boundary conditions on detonation simulations: A geometric model study," 11th US National Combustion Meeting, Pasadena, CA, March 24-27, 2019.
12. Crane, J., Shi, X., Wang, H. "A comparison of methane and natural gas detonation limit behaviors," AIAA Scitech 2020 Forum, paper AIAA 2020-0445, Orlando, Florida, January 11-15, 2020.
13. Shi, X., Crane, J., Wang, H. "Detonation limit behaviors of methane and natural gas," 2020 Spring Meeting of the Western States Section of The Combustion Institute, Stanford, California, March 22-24, 2020 (canceled).
14. Crane, J., Shi, X., Wang, H. "Geometric modeling of detonation cellular propagation," 2020 Spring Meeting of the Western States Section of The Combustion Institute, Stanford, California, March 22-24, 2020 (canceled).
15. Shi, X., Crane, J., Wang, H. "Deflagration-to-detonation transition inside reactant-product mixing layers," 2021 AIAA SciTech Forum, Jan. 11-15 & Jan 19-21 2021 (virtual meeting).
16. Crane, J., Shi, X., Wang, H. "Detonation geometric model (*detgem*) as a test bed for propagation dynamics in engineering geometries," 2021 AIAA SciTech Forum, Jan. 11-15 & Jan 19-21, 2021 (virtual meeting).
17. Dammati, S. S., Meagher, P., Poludnenko, A., Zhao, X., Shi, X., Crane, J., Rui, X., Wang, H. "Dynamics of gas-phase detonations in ethylene-air mixtures," 12th U. S. National Combustion Meeting, College Station, Texas, May 24–26, 2021.

18. Meagher, P., Dammati, S. S., Zhao, X., Poludnenko, A., Shi, X., Crane, J., Wang, H. "Effects of grid resolution and boundary conditions on 2D simulations of single headed hydrogen detonations," 12th U. S. National Combustion Meeting, College Station, Texas, May 24–26, 2021.
19. Shi, X., Hencel, R., Crane, J., Fotia, M. L., Wang, H. "Detonation propagation in curved channels: A geometric modeling case study," 2022 Spring Meeting of the Western States Section of The Combustion Institute, Stanford, California, March 21-22, 2022.
20. Shi, X., Meagher, P. A., Santos, J. P., Muraleedharan, N. K., Crane, J., Poludnenko, A., Zhaoi, X., Wang, H. "Isolating gasdynamic and chemical effects on detonation cellular structure and regularity," 2022 Spring Meeting of the Western States Section of The Combustion Institute, Stanford, California, March 21-22, 2022.
21. Dammati, S. S., Poludnenko, A., Xu, R. Shi, X., Wang, H. "Dynamics and properties of 2D vs. 3D ethylene-air detonations," 28th International Colloquium on the Dynamics of Explosions and Reactive Systems (ICDERS), Naples, Italy, June19-24, 2022.
22. Meagher, P., Shi, X., Crane, J., Zhao, X., Wang, H. "Forward jetting phenomenon in detonations," 28th International Colloquium on the Dynamics of Explosions and Reactive Systems (ICDERS), Naples, Italy, June19-24, 2022.
23. Shi, X., Meagher, P., Crane, J., Dammati, S. S., Zhao, X., Poludnenko, A., Wang, H. "On cellular multiplicity of detonations in confined channels," Meagher, P., Shi, X., Crane, J., Zhao, X., Wang, H. "Forward jetting phenomenon in detonations," 28th International Colloquium on the Dynamics of Explosions and Reactive Systems (ICDERS), Naples, Italy, June 19-24, 2022.
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25. Meagher, P., Shi, X., Zhao, X., Dammati, S. S., Poludnenko, A., Wang, H. "Cell structure and global heat release in 2D and 3D JP10-air detonations in narrow channels," 28th International Colloquium on the Dynamics of Explosions and Reactive Systems (ICDERS), Naples, Italy, June19-24, 2022.