

## SIMULATION OF ROTATING DETONATION ENGINES

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### EXECUTIVE SUMMARY

Rotating detonation engines (RDEs) have received increased attention as possible replacements for conventional gas turbine systems owing to their expected high thermal efficiency. The compression across the detonation wavefront driven by chemical reactions induces additional pressure gain. Although extensive research has been performed by both the experimental and numerical communities to realize these devices, they are limited to hydrogen/air chemistry because of its high detonability and relatively low-complexity kinetic mechanism. To make RDEs more practical and applicable, simulations of the detailed physics with hydrocarbon chemistry need to be conducted. With the allocated time on Blue Waters in 2019, the researcher has performed a series of full-system simulations with ethylene/air chemistry. These simulations reveal that the slow wave propagation observed in experiments is due to a wave aided by the deflagration mode, with wave speeds within 5% of the experimental results.

### RESEARCH CHALLENGE

Although RDEs are increasingly being studied, the concept originates from the 1960s. Recent advancements in materials science and a better understanding of detonative combustion enable the RDE system to be operable. Extensive research has been performed through experiments and simulations to understand and optimize the operation of RDEs [1–3]. However, most of the research has been conducted with hydrogen/air mixtures, while hydrocarbon chemistry is the more practical fuel [2,3]. Several experiments with ethylene/air mixtures reveal that the wave

speed is drastically slower than hydrogen/air mixtures, at nearly 50% of the ideal case [1]. Furthermore, the flame front is thicker than that of hydrogen/air chemistry. To understand the detailed physics of combustion in RDEs, simulations of the full system are necessary.

Full-system RDE simulations with ethylene/air chemistry raise three primary challenges owing to their unique geometry and dynamics. First, the fuel and oxidizer are separately injected using a nonpremixed injection scheme, which requires the use of unstructured grids. Secondly, ethylene/air chemistry is more complex and stiffer than hydrogen/air chemistry. In other words, the number of species being transported will increase the computational cost. Lastly, a finer resolution is necessary to resolve the reaction induced by the shock wave at the wavefront. Since the geometry is complex and three-dimensional, a finer resolution exponentially increases the computational cost. To perform the full-system simulation, a highly scalable solver and a large amount of allocation time on high-performance computing resources are necessary.

### METHODS & CODES

The University of Michigan detonation solver, UMdetFoam, is based on OpenFOAM and Cantera. OpenFOAM provides the finite-volume tools, which are widely used in the turbulent and combustion community. UMdetFoam implements a MUSCL-based Harten–Lax–van Leer-contact scheme for space and second-order Runge–Kutta scheme for time integration. Diffusion terms are discretized by the Kurganov, Noelle, and Petrova method. In order to handle chemistry integration, this finite-volume meth-

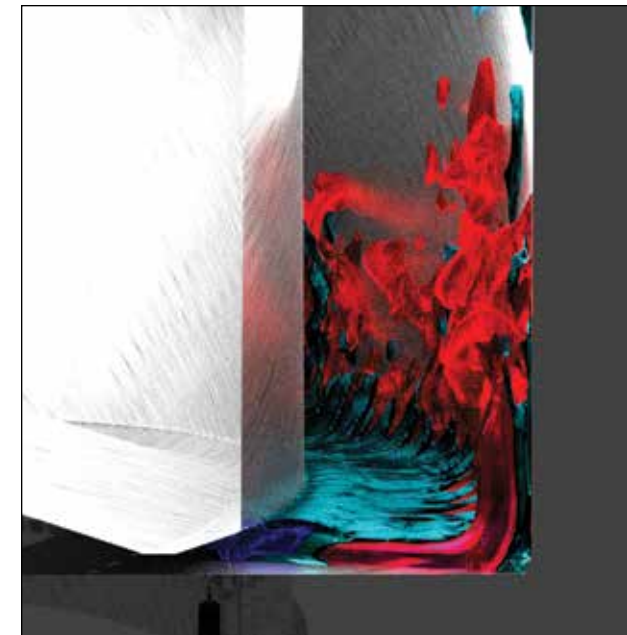


Figure 2: Injection dynamics of the fuel and oxidizer streams within the RDE annulus. The fuel stream is pushed to the outer wall by the oxidizer stream, imposing fuel/oxidizer stratification within the system.

od solver was coupled with Cantera, an open source framework for chemical kinetics, thermodynamics, and transport processes. UMdetFoam has MPI-based parallelism with linear scalability demonstrated up to 60,000 cores, with support for GPUs. For this study, a reduced-order two-step mechanism was employed to reduce the computational cost.

### RESULTS & IMPACT

In this study, the ethylene/air RDE facility at the Air Force Research Laboratory was simulated. The channel width was 22.86 mm, and the dimensionless area ratio between the oxidizer inlet and the detonation chamber was 0.059.

The full-system simulation enabled extraction of extensive data on the physics in the combustion facility. Fig. 1 shows the general behavior of the system. The pressure wave propagates in the azimuthal direction, aided by the reaction. The wavefront of this RDE is thicker than that of hydrogen/air, as reported in the 2018 *Blue Waters Annual Report*. Furthermore, oblique shock waves are not created with ethylene/air mixtures, and the product gases appear at some distance from the chamber bottom. This wave standoff behavior is also observed in the experiment. Analysis suggests that the wave is not in the detonation mode but is in a deflagration mode strong enough to sustain the wave. The incomplete mixing and low detonability of the mixture cause this deflagration-dominant mode of operation. The simulation captures the slow wave speed within 5% of the experimental data, which is almost 50% of the ideal condition. The fuel and oxidizer injection behavior are extracted from the simulation as well. The fuel stream is pushed to the outer wall by the oxidizer stream, as

shown in Fig. 2. In other words, the mixing is not enhanced near the chamber bottom, causing the standoff of the flame.

The simulation also shows that the injection velocity was almost constant during RDE operation because the wave is too weak to affect the injection dynamics. This result can help researchers to optimize the design of RDEs and to understand the effect of low detonability and fuel-oxidizer stratification on the wave structure. Design improvements resulting from high-fidelity simulations and experiments bring RDE systems closer to realization.

### WHY BLUE WATERS

The Blue Waters high-performance computing resource greatly accelerated this research for three primary reasons: (1) users are provided with a large number of cores to run cases and exploit the parallelizability of the solver, which is necessary to simulate full-system RDEs; (2) the working directory allows users to store the large amounts of data (50 TB) generated by numerical simulations without concerns over exceeding a storage quota; and (3) helpful support staff are available to professionally and promptly reply to user questions and concerns. In this study, nearly 10,000 cores were parallelized to perform full-system RDE simulations. The computing resources allowed the project to quickly implement, test, and deploy computational tools and to achieve the desired results.

### PUBLICATIONS & DATA SETS

T. Sato and V. Raman, Detonation structure in ethylene/air-based non-premixed rotating detonation engine, submitted to *J. Propul. Power*, 2019.

S. Prakash, R. Fiévet, V. Raman, J. Burr, and K. H. Yu, “Analysis of the detonation wave structure in a linearized rotating detonation engine,” *AIAA Journal Special Issue on Continuous Detonation and its Applications* (in press), 2019, doi: 10.2514/1.J058156.

S. Prakash and V. Raman, “Detonation wave propagation through stratified fuel-air mixtures,” submitted to *Shock Waves*, 2019.

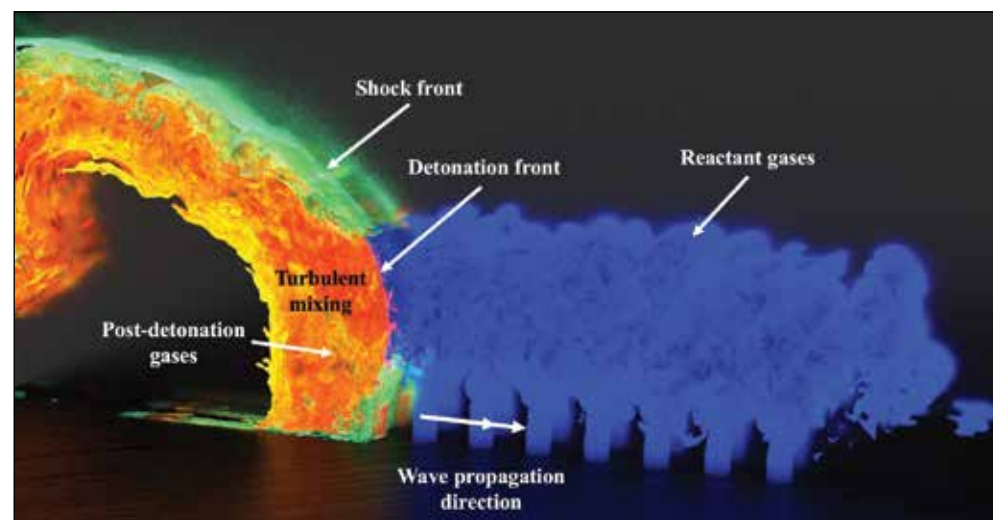


Figure 1: General behavior of the detonation wave through a linear array of injectors. A detonation wave propagates to the right, consuming an inflow mixture of premixed hydrogen/air reactant gases.