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COMPUTATIONAL MODELING OF ROTATING DETONATION ENGINES

Allocation: GLCPC/840 Knh
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EXECUTIVE SUMMARY

We have used the Blue Waters supercomputing resource for full-system simulations of rotating detonation engines (RDEs) with an aim of improving the efficiency of power generation and propulsion systems. The RDE system provides pressure-gain combustion, which increases the efficiency of the thermodynamic cycle. A reliable RDE design can increase cycle efficiency by up to 30% compared to a conventional combustor system. Within the RDE, a continuous detonation wave propagates through a fuel–air mixture. Due to the extreme conditions within the device, numerical simulations are particularly useful in understanding the complex flow physics while minimizing the use of expensive experiments. To this end, we developed a massively parallel compressible flow solver, UMdetFOAM, to provide high-fidelity simulation results to better understand RDE dynamics. We used numerical simulations to understand the dynamical features of the flow field, including the nature of detonation processes.

RESEARCH CHALLENGE

The conventional combustor, based on deflagration flame propagation, has been actively studied in the previous century. While this system is mature and reliable, significant improvements in efficiency are unlikely. Thus, pressure-gain combustion—the mode used by RDEs—has recently gained traction as a next-generation combustor system [1]. RDEs use a detonation-based thermodynamic process that allows for increased thermodynamic efficiency over the traditional Brayton cycle combustor, and is seen as a more robust combustor concept than the previously explored pulse detonation engines (PDEs). In RDEs, a continuous detonation wave propagates through a fuel–air mixture to achieve combustion and increase pressure inside the constant volume, mitigating the pressure losses that occur in conventional engines. As opposed to PDEs, the continuous pressure gain associated with RDEs reduces the complexity of coupling the combustor with a downstream turbine system in realistic applications. Advancements in related technologies, such as high-temperature materials science and flow control systems, have led to an increased interest in detonation-based combustion as a viable method for increasing fuel efficiency and reducing the environmental impact of propulsion systems.

Although a series of experiments has been conducted within the community, the detailed flow physics, such as the nonuniformity effect on the detonation structure and the turbulent mixing process, are unknown [1,2]. In order to augment experimental work, high-fidelity computational tools need to be developed to simulate the complex physics within these engines and accelerate the design process. Insights gained from the combination of high-fidelity simulations and experiments can then be used to optimize RDE design.

The focus of this study is the effect of fuel injection design on the robustness of the detonation process. In this context, the RDE configuration presents unique numerical challenges. First, a detailed chemical kinetics capability is required to simulate the nonpremixed injection of fuel and oxidizer. Second, the solver must utilize unstructured grids to mesh the complex injection geometries. Third, the presence of detonation fronts requires numerical tools that reduce dispersive as well as dissipative errors. These challenges need to be overcome to perform reliable simulations of the RDE configuration. The goal of this research lies in developing a compressible flow solver for simulating RDEs with complex geometries, creating detailed models for combustion processes, and using high-performance computing to enable simulation-aided design.

METHODS & CODES

We developed an in-house compressible flow solver, UMdetFOAM, for this research. Open-source platforms such as OpenFOAM [3], for its finite volume method, and Cantera, for its chemistry mechanism readers, are core foundations of the solver. We realized two critical achievements through these platforms: (1) the ability to define unstructured grids in a parallel environment; and (2) the ability to utilize any detailed chemistry mechanism of interest. We performed the discretization of the convective terms and the time integration of the Navier–Stokes equations using a Monotonic Upwind Scheme for Conservation Laws-based Harten–Lax–van Leer–Contact scheme and a second-order Runge–Kutta method, respectively. The chemical source terms are handled explicitly through a detailed multistep mechanism for hydrogen and air with nine species and 19 steps. Additionally, we implemented detailed chemical mechanisms for the combustion of hydrocarbons.

RESULTS & IMPACT

In this study, we simulated the RDE geometry experimentally studied by the Air Force Research Laboratory. The flow configurations, such as the fuel and oxidizer injection pressure, correspond to their experiment.

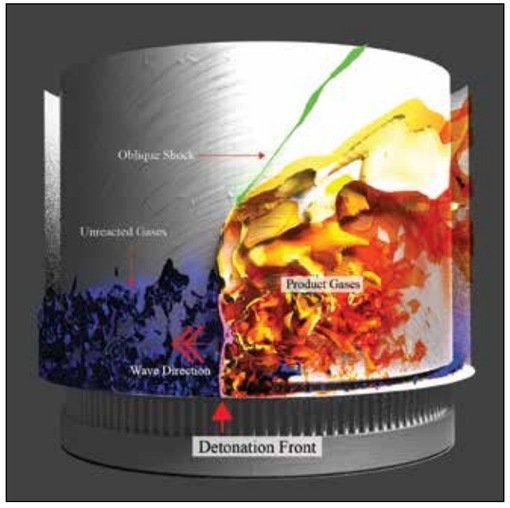

Figure 1: Structure of detonating flow inside an RDE. A detonation wave propagates in the azimuthal direction by consuming unreacted fuel–air mixture. (Purple: detonation front; green: oblique shockwave; blue: unreacted fuel gases; red and orange: detonation product species.)

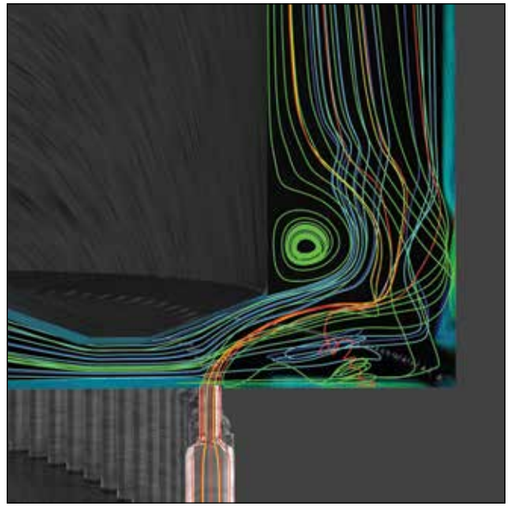

Figure 2: Fluid stream trace near the injection system illustrating the complex flow patterns that induce turbulent mixing. Two streams of the oxidizer gases from the left and the fuel gases from the bottom are mixing in the detonation chamber.

This research confirms that stable detonations present within the RDE configuration are consistent with experimental observations. For example, the wave speed is slower than the premixed theoretical values due to the flow nonuniformity effect. With regard to the injection recovery process, the fuel injector recovers faster than the oxidizer, but both recover to only 75% of the initial profile within a quarter cycle of a detonation wave. Furthermore, the use of detailed chemical kinetics provides a complete view of the highly three-dimensional detonation structure.

Because meshes created by CAD (Computer-Aided Design) data can be directly simulated, our solver can dramatically accelerate the optimization process for engineering design. Further, the above result shows that the detailed RDE dynamics, and the nonuniformity effect on the detonation structure, can be extracted by simulating the complex injection system. This helps the RDE community better understand the physics and optimize this type of combustion system. In conjunction with experimental work, we generated high-fidelity data to assist in the realization of the next-generation combustor.

WHY BLUE WATERS

The Blue Waters high-performance computing resource greatly accelerated our research studies because we could use several thousand computing nodes and exploit the parallelizability of our solver, which is necessary to simulate large systems. Second, the working directory allowed us to manage and store the large amounts of data generated by numerical simulations without concerns over exceeding a storage quota. Finally, multiple job queues catered to our requirements and deadlines. The computing resources allowed us to implement, test, and deploy computational tools quickly and achieve the results we desired. In addition, the project staff were readily available to assist in the implementation of our numerical tools.

PUBLICATIONS & DATA SETS

Sato, T., S. Voelkel, and V. Raman, Detailed Chemical Kinetics Based Simulation of Detonation-Containing Flows. *The ASME Turbo Expo* (Oslo, Norway, June 11–15, 2018).