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Large-eddy/Reynolds-averaged Navier–Stokes simulation of cavity-stabilized ethylene combustion

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ABSTRACT

In this study, a hybrid large-eddy/Reynolds-averaged Navier–Stokes (LES/RANS) method is used to simulate ethylene combustion inside a cavity flameholder. The cavity flameholder considered is Configuration E of University of Virginia's Scramjet Combustion Facility, which consists of a Mach 2 inlet nozzle, a constant-area isolator, a combustor, and an extender, through which the exhaust gases are vented to the atmosphere. To increase the fuel-residence time, a cavity is fitted along the upper wall inside the combustor section of the flameholder. The configuration has the capability of injecting ethylene through a series of ports located upstream of and inside the cavity along the upper wall the combustor. In the simulations, ethylene combustion is modeled using a 22-species ethylene oxidation mechanism. Also, a synthetic eddy method is used to introduce turbulence at the inflow plane of the flameholder. For an equivalence ratio of 0.15, a cavity stabilized flame is predicted. Predictions are compared with lineof-sight temperature, water column-density, water mole-fraction, CO column-density, and $CO₂$ column-density measurements at three stations within and downstream of the cavity. Agreement with experiment is generally good within the cavity. Downstream of the cavity, the simulations predict higher temperatures near the wall. Analysis of the flame structure predicted by the LES/RANS method indicates that the flame propagates into a stoichiometric to fuel-rich mixture near the cavity. Flame angles captured in the simulation are in close agreement with those predicted through classical premixed turbulent flame-speed estimates. Further downstream, the flame structure is non-premixed in character, and near complete conversion of CO to $CO₂$ is observed by the time the flame reaches the combustor exit.

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1. Introduction

The Hypersonic Technology (HyTech) program [\[1\],](#page--1-0) initiated in 1995, was intended to develop a hydrocarbon-fueled scramjet engine for military, transport, and space flight (air-breathing stage) purposes. The X-51A Scramjet Engine Demonstrator (SED), which was developed as part of the HyTech program, uses ethylene for initial ignition and later makes a transition to the hydrocarbon based JP-7 fuel. The X-51A SED performed its first fully successful 240 s flight test on 14 August 2012, increasing the interest in developing hydrocarbon-fueled scramjet engines. Hydrocarbon fuels are preferred over hydrogen due to their high density (which means lower fuel tank volume), ease of handling, and increased safety $[2,1]$. However, the ignition delay times for long chain hydrocarbons are large, meaning that they pose significant challenges when used as fuel in scramjets, where the fuel-residence

⇑ Corresponding author. E-mail address: apotturi@metacomptech.com (A.S. Potturi). times are often less than a millisecond. These challenges include, but are not limited to, ignition of the fuel (which means formation of sufficient number of free radicals to initiate the chain reactions) and flameholding.

The use of cavity flameholders as a way to increase the fuel-residence times and fuel–air mixing has been described by Tishkoff et al. [\[3\].](#page--1-0) They were first used in a joint French/Russian venture, where a hydrogen fueled dual-mode scramjet was tested $[4]$. Later experiments $[5-7]$ showed that use of a cavity after the ramp injector significantly improves the combustion efficiency of hydrocarbon fuels in scramjets. A detailed description of various cavity flameholder designs and their performances is given in Ben-Yakar and Hanson [\[8\]](#page--1-0).

Flight tests can be performed to directly test and study a particular scramjet engine design. In the past, flight tests for scramjet engines were performed using rocket engines to provide initial acceleration to hypersonic speeds. Future designs are looking at combined cycle propulsion systems, which make a transition from turbojet engines to ramjets to scramjets, depending on the vehicle

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speed. In either case, this need for other forms of propulsion systems means that flight tests are expensive and require complex coordination of transitions between different propulsion systems.

An alternative to flight tests are ground based experiments using high-speed wind tunnels. Because of the flow regimes in which the scramjet engines operate, it is extremely difficult and expensive to reproduce the flow conditions for substantial amounts of time and without any contamination in the flow field. Further difficulties in taking measurements without causing any intrusion to the flow make the choice of experimentally studying high-speed combustion processes even less attractive. Due to these technical challenges, it is currently not possible to assess the performance of a scramjet engine over its operational envelope using experimental methods alone.

Given these limitations to flight tests and experimental facilities, using Computational Fluid Dynamics (CFD) techniques as tools to aid in the design of hypersonic vehicles has become an attractive choice. While experiments are used to validate various physical models used in CFD, major design decisions are based on simulations. Over the past few decades, owing to the exponential increase in processor speed and memory capacity, CFD has become an affordable tool for studying complex flows, more so with the advent of parallel computing.

The computational methods used in CFD heavily rely on several models used to represent various physical processes. So, it is essential that the quality and reliability of these models be tested and that their shortcomings are well understood. The present study is part of an effort aimed at better understanding the performance and shortcomings of existing models for high-speed combustion. In the present work, reactive flow within an ethylene-fueled combustor equipped with a cavity for flame stabilization is simulated using North Carolina State University's hybrid LES/RANS solver, REACTMB, which was previously used to simulate high-speed flows with hydrogen-air combustion $[9-15]$. A 22-species $[16,17]$ reaction mechanism is used to model ethylene combustion. Also, to introduce turbulence at the inflow of the flameholder, the synthetic eddy method of Jarrin et al. [\[18\]](#page--1-0) is used. The cavity flameholder considered is Configuration E of the University of Virginia's Scramjet Combustion Facility (UVa's SCF).

2. University of Virginia's Scramjet Combustion Facility

The University of Virginia's Scramjet Combustion Facility (UVa's SCF) is a dual-mode ramjet/scramjet combustor capable of simulating flight conditions at Mach 5 enthalpy. It consists of a Mach 2 inlet nozzle, a constant-area isolator, a combustor, and an extender, through which the exhaust gases are vented to the atmosphere. A schematic overview of the facility is shown in Fig. 1. For more details regarding UVa's SCF, the reader is referred to Fulton et al. [\[19\].](#page--1-0)

2.1. Configuration E

In Configuration E of the UVa's SCF, ethylene is used as fuel. To increase the fuel-residence time, Configuration E is fitted with a cavity on the upper wall of the combustor section. Ethylene can be injected through a series of ports (three rows of ports upstream of the cavity and one row of ports inside the cavity, with each row consisting of five fuel-injecting ports) located along the upper wall of the combustor section. For the case considered in the present study, ethylene is injected through the most upstream row of injectors. The locations of these injection ports and the overall design of Configuration E are shown in [Fig. 2.](#page--1-0)

Mean freestream and stagnation values for the Mach 2 nozzle and combustor are shown in [Table 1](#page--1-0). To achieve an equivalence ratio of 0.15 (mass flow rates of ethylene and air are 1.87 gm/s and 182.75 gm/s, respectively), ethylene is injected at the following stagnation conditions: 973296.3 Pa and 298.0 K. For this equivalence ratio, experimental data is available in the form of Line-of-Sight (LOS) measurements of species mole-fractions, column-densities, and temperatures, obtained using Tunable Diode Laser Absorption Spectroscopy (TDLAS) at three different stations [\[21\]](#page--1-0). The locations of these stations are shown in [Fig. 3,](#page--1-0) and the available experimental data at each of these stations is shown in

Fig. 1. Schematic overview of the UVa's SCF [\[20\]](#page--1-0).

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