IGNITION BEHAVIOR OF SUPERCRITICAL LIQUID FUEL IN COMBUSTION SYSTEM

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Abstract

In systems that involve super-critical liquid fuel combustion, the temperature of the propellants is in the sub-critical state when they are injected into the combustion chamber. However, during the process of combustion, the system experiences a shift in its state of thermodynamics from subcritical to supercritical. The present study predicts the ignition behavior for super-critical liquid fuel combustion through the techniques of computational fluid dynamics (CFD). Simulations are carried out for a single shear coaxial injector’s test case of the combustion chamber. For super-critical combustion, the present research uses kerosene as a fuel and gaseous oxygen as the oxidizer. Simulations are carried out at a steady state for various values of rich flammability limit (RFL). The real gas model, Soave-Redlich-Kwong (SRK) is used for performing simulations in the present study. On the other hand, for the various values of rich flammability limit (RFL), transient simulations are carried out for ideal gas. It has been observed that the simulations performed for steady-state closely approximate the experimental data in comparison to transient simulations. It is also observed that the inherent stability issues involved in transient simulations emphasize the use of an ideal gas model for its computation.

Keywords: CFD; Ignition transients; Kerosene oxygen combustion; Real gas; Shear coaxial injector; SRK model

I. Introduction

The processes involving supercritical thermodynamic conditions are of great technological interest in propulsion applications [XVI]. In liquid fuel combustion, propellants are usually mixed and burnt in conditions, where temperature and pressure are in the supercritical state. In the supercritical conditions, a dark distinction exists among Moheez Ur Rahim et al
the phases of liquid and gaseous state, however, the properties of fluid and thermodynamics for the phases of liquid and gases are existing together [XIX] [XVII]. When propellants are injected, they are in the sub-critical state before ignition but at the time of ignition, there is an increase in both the pressure and temperature which causes the thermodynamic state to change from sub-critical to super-critical. Improper design of starting controls may accumulate propellants that are not burnt in the combustion chamber. These propellants upon ignition may explode, sometimes resulting in severe damage to the combustion chamber [IX]. There is an utmost requirement for adjustment of control activities to operate at the same time to start ignition procedure and to convey a smooth and solid push for developing desired characteristics. There are numerous issues linked with non – linear mass flow and heat exchange qualities. For instance, qualities relating to the filling cryogenic propellants in unconditioned engine systems, variations in mass flow, surges in pressure, changing of phase, instabilities in combustion, hammer effects in the lines of feed, turbopumps working extensively more than its designed conditions, and so forth. These reasons encourage, simulation of ignition behaviour for being an essential factor in reducing the cost of experimental tests. [VI].

To successfully design and fine-tune the system, it is essential to develop software tools that can be utilized for analyzing the system. Most of the time, the process of ignition in a combustion system with liquid fuel has non-linear interactions among multiple components of the engine. The phenomena associated with these interactions can be flow resistance, operation of off-design turbo-pump, transfer of heat, phase change, and the combustion process. In addition, it should always be noted that the products and physical properties of the liquid propellants obtained because of the combustion in such a framework will change quite rapidly. Thus, it will be a challenging task to develop tools that can predict the behaviour of combustion in dynamic systems having such complexities

Several tools are developed for simulating the transient behaviour of the combustion system. As in 2000, [XII] developed a tool to study transient engine systems based on disassembly methods. It is assumed that the module had an independent physical function and demonstration which is mathematical in nature. Also, there exists a parameter interface of uniform exchange among every module and the physical unit can be used to subdivide the system further into several modules. In 2000, [I] had a successful attempt of developing a “dynamic simulator for liquid-propellant rocket engines”. The tool was named CRESP-LP. Also, [X] developed the code and performed various analyses to study transient behaviour in the combustion system. In Russia, a wide range of investigations has been performed on the transient behaviour of systems. These examinations have generated a database that assisted in the testing of an extensive range of liquid engines which were developed. Problems of transient behaviour in engines for liquid fuel combustion have also been studied in [XVIII] and [II]. In [V], the researcher has presented in great detail the analysis of transient behaviour by using a simple ordinary differential equations approach complemented with experimental-based empirical equations. The experimental–based empirical equations are used in situations, where the only use of the ordinary differential equations is not adequate for depicting the occurring phenomena. CNES (Centre National d’Etudes Spatiales) also known as National Centre for Space Studies in Europe has dedicated a library developed in the platform of AMESim for the modeling and simulation of dynamics of the system [XV]. The platform portrays various

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The experiments are not only costly and time-consuming but are sometimes difficult to carry out as they require a controlled environment for their prompt and successful execution. This article focuses on the use of CFD as a reliable tool to simulate and predict the behaviour of ignition for combustion system of supercritical liquid fuel, as it is economical as well as robust in the initial design phase.

II. Description of Test Case

In this study, simulations are performed using CFD for shear coaxial injector within the combustor geometry of windowed subscale with kerosene and gaseous oxygen as a liquid fuel and oxidizer respectively [III]. Details related to the model, available experimental data, grid generation, and imposed boundary conditions are discussed below.

Problem Description

The shear coaxial injector was used in an experimental setup for a high-pressure combustion experiment [VII]. The only two parts of the assembly of the injector are the outer body and the center post. For determining the drops in pressure at liquid and gas injector metering orifices are used in the propellant inlet ports of the injector [III]. Overall length and inner diameter from the plate of the injector to the nozzle’s throat are 182 mm and 22 mm, respectively [III]. To observe the flow in the combustion flow field of high-pressure having spray of kerosene/gaseous oxygen, a windowed combustor is designed. The body of the combustor has three modules for flame visualization, adjusting combustor length, exhaust nozzle, and channel for cooling water as upstream, middle, and downstream modules respectively. To ignite the propellant spray, an induction coil of high voltage i.e., 11kV along with a motorcycle spark plug (NGKCR8EIX) is used. The technique of shadowgraph visualization in the experiment test was used for observing transient ignition. The luminosity of the flame of kerosene is very high, because of the emitting particles of carbon [III]. To exclude light sources of higher intensity, it was required to have the light emission of flame from the shadowgraph image [III]. A light-emitting diode of high power i.e., 27 Watts was used in the experimental test as a source of light, which is 2100 lumens. Light is made parallel using Plano–Convex lens having
300 mm of focal length. The parallel light passes through the window of two quartz by the flow field of combustion and is then focused on the Charge Coupled Device (CCD) arrays of Photron APX – RS high-speed camera. A custom–made Multipoint Control Unit (MCU) controller is used for controlling the sequence of ignition. Because of the difference in the time of filling for the volume between the injector and valve, oxidizer and fuel are simultaneously injected, however, the opening signal valve for the oxidizer is transmitted 500 ms faster than that of the fuel [VII]. Fig. 1 shows the combustor of the shear coaxial injector with subscale windows simulated in the study.

Fig. 1. The combustor of the shear co-axial injector with subscale windows [VII]

Configuration of Test Case

This study considers the geometry of the subscale windowed combustor of the test case [VII]. Fig. 2 shows the detail of geometry of the test case used i.e. subscale windowed combustor. This is a 2D axisymmetric geometry.

Fig. 2. Detail of the geometry for subscale windowed combustor (whole), shear coaxial injector, and nozzle

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Grid Generation

Modeling and mesh generation of shear coaxial type injector inside subscale windowed combustor geometry of the test case [16] for the liquid fuel (kerosene) and the oxidizer (gaseous oxygen) is carried out. A structured grid is generated for the present study. 2D-axisymmetric simulations are performed. The grid used for 2D-axisymmetry computations is shown in Fig. 3.

![Grid at (a) shear coaxial injector region (b) near combustion chamber inlet (c) injector-combustion chamber interface region (d) combustion chamber nozzle interface and (e) throat and a diverging portion of the nozzle](image)

**Fig. 3.** Grid at (a) shear coaxial injector region (b) near combustion chamber inlet (c) injector-combustion chamber interface region (d) combustion chamber nozzle interface and (e) throat and a diverging portion of the nozzle

Boundary Conditions

Boundary condition details are presented in Fig. 4. Steady and transient simulations are carried out. The boundary condition used for steady-state simulations are given in Table 1, on the other hand, the information regarding the transient simulations is shown in Table 2. Data in Table 2 is extracted manually from [VII]. Injection pressure and temperature are identical for simulation of both the cases of transient and steady-state.

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Table 1: Boundary condition values used for steady-state simulations

| Boundary conditions                  | Values   |
|-------------------------------------|----------|
| Kerosene mass flow rate             | 13.6 g/s |
| Oxygen mass flow rate               | 34.4 g/s |
| Fuel (Kerosene) temperature at inlet| 291 K    |
| Oxidizer (oxygen) temperature at inlet| 291 K   |

Table 2: Fuel and oxidizer mass flow rate used for transient simulations

| Time | Mass Flow Rate (g/s) |
|------|---------------------|
|      | Oxygen  | Kerosene |
| 0    | 0       | 0        |
| 0.05 | 0.172   | 0.0068   |
| 0.1  | 0.0344  | 0.0136   |
| 0.2  | 0.0344  | 0.0136   |
| 0.3  | 0.0344  | 0.0136   |
| 0.4  | 0.0344  | 0.0136   |
| 0.5  | 0.0344  | 0.0136   |

Solver Setup

Setup of solver for both transient and steady-state simulation are discussed below:

Steady-state simulations

For steady-state simulations, the pressure-based solver is preferred over the density-based solver, this is because the pressure-based solver employs an algorithm that belongs to methods of the general class called the projection method. For 2D axisymmetric geometry, absolute velocity formulation is used. Since the test case problem involves heat transfer, the energy equation is enabled as well.

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For the turbulent flow, viscous SST k-omega model is used instead of laminar assumption. As test case flow is compressible, compressibility effects are enabled as well. For pdf table creation, a chemical equilibrium for state relation is used in the chemistry model. Non-adiabatic energy treatment is used because of heat transfer. 8 bar equilibrium operating pressure value is used as the mean flow pressure. Rich Flammability Limit (RFL) is set from 0.4 to 1 with an interval of 0.2. A minimum temperature of 250K is used in table parameters. Soave-Redlich-Kwong (SRK) real gas model is used. The value of hydraulic diameter is 0.0015m whereas a temperature of 291K is considered for mass flow inlet of kerosene and oxygen. For pressure-velocity coupling scheme of PISO is used.

**Transient simulations**

The solver setup for transient simulations is quite like steady-state simulations. Various procedures are performed like the steady-state simulations. The procedure used which is different from that of the steady-state simulation is discussed briefly in this section. Due to lack of high computational power and time, the fuel-rich flammability limit is set to 0.44 which is approximately twice of the stoichiometric ratio. Stability issues emphasis the use of ideal gas in the density option for the pdf mixture. Values are taken as profile (Table 2) for mass flow inlet of kerosene and oxygen instead of constant value because of transient phenomena.

The first-order implicit transient formulation is used in solution methods. Under relaxation, factor values are used as is shown in Table 3. For attaining stability, small values of under relaxation are used. Especially very small under relaxation values are used for density. 0.001 seconds is set as a time step size, whereas simulations are run for 300-time steps and are set to a maximum of 2000 iteration per step. Relative convergence criteria are used, and its values are set to 0.055 for all model equations. Simulations took approximately four (04) days to complete on a system with configuration i.e., Intel(R) Core (TM) i5 5300U CPU @ 2.30 GHz, 8 GB RAM.

**Table 3:** Under relaxation values used for transient simulations

| Under Relaxation Factor        | Value |
|-------------------------------|-------|
| Pressure                      | 0.1   |
| Density                       | 0.001 |
| Body forces                   | 0.5   |
| Momentum                      | 0.3   |
| Turbulent kinetic energy      | 0.3   |
| Specific dissipation rate     | 0.3   |
| Turbulent viscosity           | 0.3   |
| Energy                        | 0.3   |
| Temperature                   | 0.3   |
| Mean mixture fraction         | 0.3   |
| Mixture fraction variance     | 0.3   |

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Numerical simulations for supercritical combustion of kerosene and gaseous oxygen have been performed in the present study. Computation are carried out for the transient and steady-state. The total rate of mass flow and ratio of oxidizer to fuel is considered as 48 g/s and 2.53 respectively for the selected test case. Computed results are validated and analyzed in the following sections.

Steady-State Simulations

For simulating supercritical kerosene/gaseous-oxygen combustion, a model of non-premixed combustion is used. Chemical non-equilibrium is modeled by utilizing the rich flammability limit (RFL). Simulations are carried out for different values of RFL (Rich Flammability Limit) to compute the absolute pressure of the chamber. Computed pressure is compared with an experimental chamber pressure of 28.1 bars for steady-state simulations as are provided in [III]. RFL value at 0.4, gives better outcomes as compared to other RFL values despite this value being two times the stoichiometric mixture fraction as shown in Fig. 5. The difference between experimental chamber pressure and the present computation value of RFL at 0.4 is only 2 bars, which is 7% of 28.1 (experimental chamber pressure).

Pressure contour inside the combustion chamber and nozzle are shown in Fig. 6. Constant pressure is observed inside the chamber while pressure decrease in nozzle depicts those results are showing physical behaviour qualitatively.
Fig. 6. Pressure (Pascal) contour

Fig. 7 and Fig. 8 present, temperature and density contours. The peak temperature is offset from the axis because of the oxygen entering from an annular portion. Vaporization of kerosene in super-critical combustion is extremely fast and can be visible in the contours of the density. After some distance from the injector, both the kerosene and gaseous oxygen are burnt, however, kerosene is present in a very small amount near the section of the nozzle. The central line of the combustion is mostly crowded by the species on the other hand oxygen is majorly present near the wall of the chamber. In this case, the pressure of the chamber is under-predicted but overall results are very satisfactory. Results are demonstrating the suitability of CFD for predicting combustion of complex problems with acceptable accuracy. Results can be improved if a detailed chemical kinetics mechanism is included.

Fig. 7. Static temperature (K) contour

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Transient Simulations

Transient simulations are also performed for fuel injection into the combustion chamber to 300 ms. Transient inlet mass flow rate profile of kerosene and oxygen is used, as given in Table 2 and presented in Fig. 9. Pressure is built-up within the combustion chamber is computed and is also compared with the experimental data.

The result computed with CFD techniques, and the data obtained from the experiment for the pressure built up during the transient ignition in the combustion chamber is presented in Fig. 10. Although trends are similar, CFD not only under-predicts the steady-state pressure but also implies that the built-up pressure is very progressive. Steady-state chamber pressure in transient simulations is 24.6 bars which is less than not only the pressure of the experiment but also the steady-state results. In this test case, kerosene is found within the supercritical condition, depicting the real gas model being more appropriate for its modeling. Generally, the real gas model of SRK is used for steady-state simulations but because of the inherent stability issues in transient simulations, an ideal gas model for kerosene may be used for its computation.
It is assumed that the increase in error is the consequence of inappropriate modeling. As the predicted chamber pressure built up gradually as compared to the data obtained experimentally, however, it may lack experimental details. The profile of mass flow rate for both the fuel and the oxidizer is used in the present study to extract from [VII]. It is assumed that kerosene and oxygen are injected simultaneously. During computation, both the fuel and oxidizer reach the mass flow rates of their steady-state after 100ms. However, the actual sequence of time and duration for both the kerosene and oxygen is not clear.

It is clearly depicted in the results that after few milliseconds entire combustion chamber is filled with combustion gases of high-temperature. Computed peak temperatures are found to be approximately the same i.e., 3500K for the simulation performed for transient and steady-state. Although there are differences in the numerical computations and experimental results, the results obtained in the present study are very encouraging for the performed simulations.

IV. Conclusions

CFD techniques are used to simulate the combustion of gaseous oxygen and kerosene in the supercritical state. It is being observed that simulations of steady-state are in good approximation to the experimental data. Options for using combustion models of advanced nature are restricted because of the issues instability and inherent complexities. More improved results can be obtained by using actual boundary conditions, the detailed mechanism of chemical kinetics, and improved modeling. However, the results of the present study are encouraging and quite promising for using CFD for modeling and simulating the ignition transient combustion of the super-critical fuel.

Conflict of Interest:

There was no relevant conflict of interest regarding this paper.
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XV. R. Rhote-Vaney, V. Thomas and A. Lekeux, "Transient Modeling of Cryogenic Rocket Engines a Modular Approach," in *4th International Conference on Launcher Technology, Space Launcher Liquid Propulsion*, 2002.

XVI. S. A. Inam, M. Hussain and M. M. Baig, "Numerical Simulation of Liquid Fuel Injection in Combustion Chamber," *Arabian Journal for Science and Engineering*, 2019.

XVII. Smith JJ, "High Pressure LOx/H2 Combustion & Flame Dynamics Preliminary Results," in *40th AIAA/ASME/SAE/ASEE Ji. Propuls. Conf. Exhib.: AIAA*, 2004.

XVIII. V. Kalnin and V. Sherstiannikov, Hydrodynamic Modelling of the Starting Process in Liquid-Propellant Engines (vol.8) Page number 231-242, Acta Astronautica, 1981, pp. 231-242.

XIX. Y. Cengel and M. Boles, *Thermodynamics: An Engineering Approach*. 5th ed. McGraw-Hill College (ISBN 0-07-288495-9), 2005.