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# NUMERICAL SIMULATION OF COMBUSTION IN A SINGLE ELEMENT $H_2$-$O_2$ CRYOGENIC ENGINE

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## ABSTRACT

The liquid propellant rocket engine combustion chamber represents one of the most difficult engineering flow systems in operation. The ignition of the propellants injected into a rocket combustion chamber and the subsequent propagation and anchoring of the flame is an important design consideration for all types of rockets. Reliable ignition has to be guaranteed and the initiated turbulent diffusion flame has to stabilize without over pressure or blow out. The control of ignition in a rocket engine is a critical problem for combustion chamber design. Delayed ignition may lead to high unsteady chamber pressure that can damage the engine (strong ignition) whereas early ignition may not sustain to reach steady state. Predictivity of the models and numerical tools to analyse the ignition transient has still limitations. In $H_2/O_2$ rocket combustors, the injected propellants are ignited by a stream of hot gas originating from the igniter device. The hot gas has to mix with the injected propellants to initiate combustion in a situation which is characterized by strong spatial inhomogeneties. This paper presents the numerical study of ignition characteristics of $H_2$ & $O_2$ propellant combination in cryogenic combustor. The main objective is to get an insight into the main processes involved in the ignition of cryogenic engines. The pressure, temperature, velocity profile and propellant mass fraction variation along the combustion chamber is addressed. The characteristics of diffusion flame, shear layer combustion, recirculation zone and flame propagation are also addressed. The reaction mechanism is studied using Eddy Dissipation Model/Finite Rate Chemistry. Numerical simulation results were compared with the experimental data.

Key words: IGNITION, NUMERICAL SIMULATION OF COMBUSTION, ROCKET ENGINES

## 1. INTRODUCTION

Understanding ignition processes is extremely important to design reliable combustion devices. Due to non-hypergolic nature of $H_2$-$O_2$ propellant combination, the ignition takes place using separate ignition system i.e. pyrotechnic, pyrogen or spark ignitors. The ignition of cryogenic propellant in coaxial injector consists of atomization, vaporization, mixing and finally initiation of ignition. Due to the fast reaction chemistry of $H_2$-$O_2$, the rate of mixing controls the reaction rate. The initiation of ignition and sustainability of the flame front upto steady state without over pressurisation or blow out is the major challenge for coaxial-shear-diffusion combustion. In turbulent non-premixed configurations such as coaxial flow and bluff body flows, ignition failure is mainly due to incomplete mixing at the spark location. The combustion initiation in rocket engines is usually based on igniter devices. The under expanded hot gas products from igniter are injected into the combustion chamber while the propellant valves are sequentially opened/closed to cause entry of the propellants to the combustion chamber at a adequate mass fraction. Ignition in such configurations is mainly driven by turbulent mixing, convective effects, thermodynamic conditions, interaction between the under expanded igniter jet and propellants jets, chemistry and two phase flow effects. Mayer et al. [1] studied the atomization of a liquid oxygen jet by a surrounding gaseous hydrogen jet and the effect of ignition on atomization processes. Indeed, an ignition delay leads to the evaporation of an important amount of liquid oxygen and thus to the creation of a significant volume of gaseous flammable mixture into the chamber. After ignition the flame spreads over the whole chamber leading to a sharp pressure peak. Once the mixture is burned, diffusion flame anchors at the injector lips.

Ignition was triggered by a spark plug and the experiment showed that after the initiation of the flame kernel, the flame propagated in a partially premixed mode before stabilizing in a diffusion mode. The temporal evolution of the distance of the upstream flame edge from the injector face plate is the main feature to characterize the flame anchoring and flame stabilization process. Here the focus of the study is on the usage of the chemical kinetics models for hydrogen-oxygen combustion. In most cases the assumption of thin flame (infinitely fast chemical reactions) gives reliable results. Hence, there is no actual need to use the detailed kinetic mechanisms in CFD simulations. However, the assumption of thin flame is not completely satisfied in rocket combustion chamber where the turbulence is very high. Due to this reason, the model of the chemical kinetics should be used for the modeling of the combustion in rocket engine which has to be validated and verified with experimental result. Of course chemical reactions drive combustion, but indeed combustion process depends on heat and mass transfer too. Although turbulence model, equations of state, transport coefficients and chemical kinetic mechanism can be validated separately, the resulting physical-chemical model needs the final validation as a whole.

Toshimi et al. [2] explains on numerical computation on axisymmetric laminar diffusion flame taking into account the detailed chemical kinetics and multicomponent diffusion. The laminar jet diffusion flame formed in a co-flowing oxidizer and fuel is a fundamental flame type. This flame has attracted much research attention on flame characteristics and its structure.

Guilhem Lacaze et al. [3] presents the comprehensive development of a combustion model for turbulent non-premixed flames at high pressure supercritical condition. In $H_2$-$O_2$ combination rocket engine, combustion is affected by strain, pressure and heat loss processes. Flame sensitivity is studied to define the topology of liquid oxygen- hydrogen flame and sensitivity.

N.J. Brown et al. [4] explains about the experimental studies of lean, near stoichiometric and rich hydrogen oxygen flames to predict the composition and temperature profiles at low pressure combustion.

O. Gurliat et al. [5] depicts that the local flame velocities as well as local convection velocities at the point of ignition are determined by image displacement velocimetry method. Depending on the injection condition of the propellant, some distinct phases of the transient startup process could be observed and are discussed in terms of Weber number & Reynolds number.

## 2. PHYSICS OF IGNITION IN ROCKET ENGINES

Ignition of liquid rocket engines is characterized by high-speed injection jets and very fast chemistry. If the ignition delay is short, reactants will not be sufficiently mixed to react strongly. If the ignition delay is large, the mixed reactants ignite too strongly and generate high and dangerous pressure levels. To obtain the smooth start of the engine, the valve sequencing plays an important role during start transient process.

Three main phenomena controls liquid rocket engine ignition: high velocity jets, auto ignition and $H_2/O_2$ combustion. The ignition of the engine follows a specific sequence. First the system is thermally conditioned with propellants to reach a nominal state & to cool down the injection lines. Purging using gaseous helium (GHe) through Liquid Oxygen (LOX) circuit will prevent entry of H2 to the LOX circuit till the LOX is admitted into the chamber. This is followed by $H_2$ injection and the igniter is triggered after few milliseconds. The igniter produces a high pressure jet leading to a strongly under expanded jet in the chamber. Finally, the oxidiser ($O_2$) is injected and combustion begins.

## 3. MODELLING OF SINGLE ELEMENT CHAMBER

The cryogenic combustor with single element coaxial injector is used for study of the combustion characteristics. The modelling & meshing of the combustor along with coaxial injector is carried out using ANSYS ICEM CFD software. The choice of the software is given adherence to the compatibility of the computer data and the design documentation. The ANSYS CFX solver is used to solve the governing equations. The k-ε model is used for the turbulent modelling and Eddy Dissipation Model (EDM) is used for combustion modeling. The EDM is fast reaction chemistry model with higher Damkohler number. Damkohler number is a non-dimensional parameter defined as the ratio of turbulent mixing to chemical reaction timescale.

Two types of tests (simulations) have been done in this work i.e. Single Element chamber without nozzle segment and Single Element chamber with nozzle segment.

The first test case is a Single Element Co-axial injector chamber without nozzle segment. This configuration is selected to study the flame characteristics of coaxial injector configuration and to understand the energy distribution and species mass fraction along the combustion chamber.

The second case is a Single Element Co-axial injector chamber with nozzle segment. This configuration is used to estimate the performance parameters like chamber pressure and C-star efficiency. All the aero thermo chemical behaviors of the single element combustor were derived from the simulation and the results were compared with experimental data.

The test rig is fueled with gaseous hydrogen and oxygen by a coaxial injector and connected to the atmosphere by an exhaust nozzle. Figure-1 gives the schematic of the single element chamber with coaxial injector.

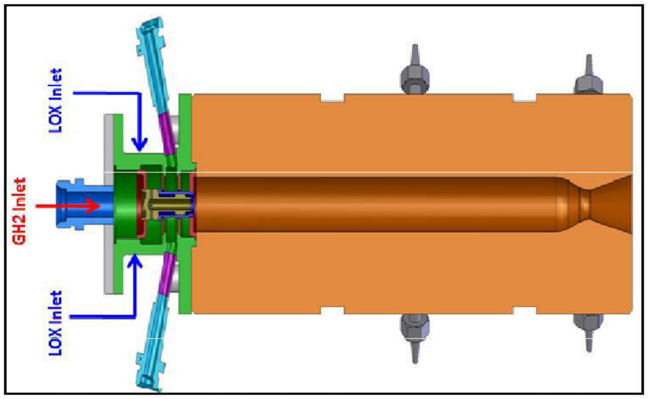

FIGURE 1 : SCHEMATIC OF SINGLE ELEMENT CHAMBER

Flow pattern in a coaxial injector element is given in figure-2.

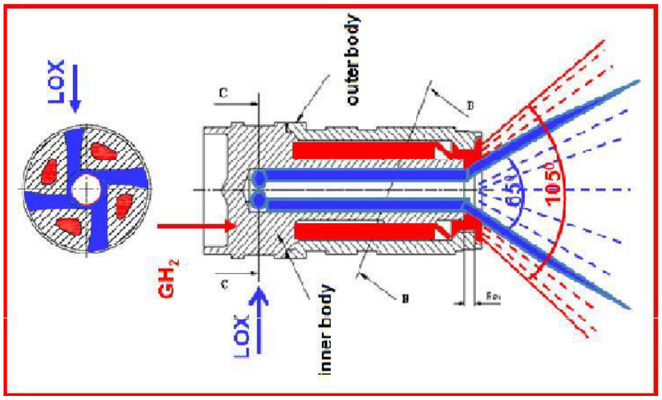

FIGURE 2 : FLOW PATTERN IN COAXIAL INJECTOR

## 4. SIMULATION OF COMBUSTION

In this study, the $H_2$-$O_2$ kinetic scheme with two steps reaction chemistry is formulated. The reacting equations are

$$\mathbf{H_2+O_2 \rightarrow 2OH}$$
$$\mathbf{H2+20H \rightarrow 2H_2O}$$

Different meshes and the models of diffusion and thermal conductivity were tried before getting the final results. A fully unstructured tetrahedral mesh is used for the final simulation. For the present calculation, upwind scheme with physical time scale is used. Forward rate constant for reaction is computed using expanded version of Arrhenius Equation.

The expanded version of the Arrhenius Equation is a

$$\mathrm{k} = AT^{\beta} exp^{\frac{-E}{RT}}$$

where, k : Reaction rate
A : Pre-exponential factor
T : Temperatur
E : Activation Energy
R : Universal gas constant

In Eddy Dissipation Model, the reaction rate;

$$\mathrm{k} \; \alpha \; \frac{\varepsilon}{k}$$

where, ε: Eddy Dissipation rate
$k$ : Turbulent kinetic energy

The formulation solves the fully coupled governing equations of mass, momentum, total energy and species as follows;

### Mass conservation equation:

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho u) = 0$$

**Where**

ρ is the density and
u is the three dimensional velocity vector

### Momentum conservation equation:

$$\frac{\partial}{\partial t}(\rho u) + \nabla.\left[\rho u \ \times \ u + \frac{P}{M2} I\right] = \nabla.\tau$$

where, P : Pressure, M : Mach number, μ : dynamic viscosity and Re : Reynolds number
Viscous stress tensor

$$\tau = \frac{\mu}{Re}[-\frac{2}{3}(\nabla.u)I + (\nabla u + \nabla u^T)]$$

### Energy conservation equation:

$$\frac{\partial}{\partial t}(\rho E) + \nabla.[(\rho E + P)u] \\ = \nabla.[q_E + M^2(\tau.u)] + Q_E$$

where, Total energy: :

$$E = e_s + \frac{M^2}{2}$$

Sensible energy:

$$e_s = \sum_{i=1}^{N} h_i Y_i - \frac{P}{\rho}$$

Enthalpy:

$$h_i = \iint C_{pi}(T, P)dTdP$$

$Q_E$ = Heat release rate due to chemistry

### Species transport equation for $i_{th}$ species:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla.(\rho Y_i u) = \nabla.q_i + \omega_i$$

where, Y : Species mass fraction
q : Mass diffusion
ω : Rate of diffusion

These equations are coupled using a cubic equation of state and appropriate treatments of thermodynamic and transport properties to capture correctly supercritical effects occurring at high pressures.

## 5. RESULTS & DISCUSSION

The simulation is carried out for single element chamber considering two cases i.e. without & with nozzle configuration. Results are summerised below.

### 5.1 Simulation without nozzle

Boundary conditions applied for the simulation are $H_2$ & $O_2$ flow rates at the combustor inlets and chamber pressure at the outlet in order to study the combustion characteristics in the chamber. Temperature distribution along the combustor is given in figure-3. Non uniformity in temperature is observed near to the injector face plate which is due to the characteristics of coaxial injector element. Gradual mixing is observed at the downstream segment of the combustor and uniform temperature obtained at the combustor exit.

The signature of diffusion combustion is observed in the coaxial injector configuration in which the ignition takes place in the $H_2/O_2$ shear layer.

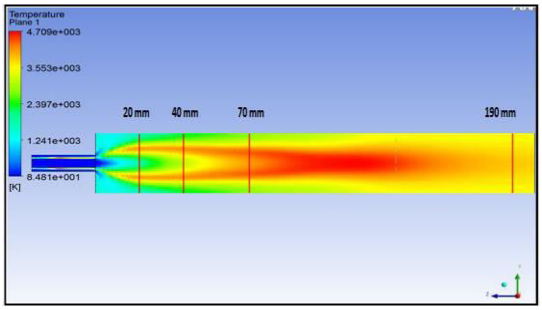

FIGURE 3 : TEMPERATURE PROFILE IN A COAXIAL INJECTOR

As the flame propagates away from the injector face plate, mixing characteristics of the propellants improves resulting in uniform temperature profile. Figure-4 shows the profile of the temperature along the chamber away from the injector face plate.

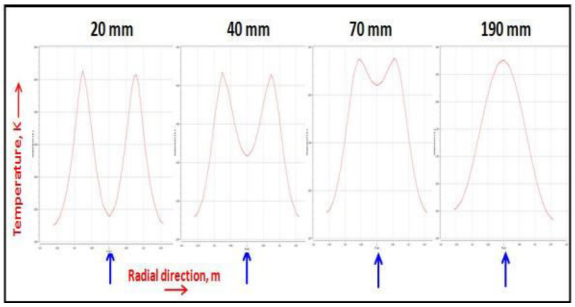

FIGURE 4 : TEMPERATURE PROFILE VARIATION ALONG THE CHAMBER

In the coaxial injector configuration, the propellant mixture mass fraction coexists only in a small region in the chamber which is the characteristics of diffusion flame. Figure-5 gives the propellant mixture mass fraction along the radial direction at an axial distance of 60 mm from the injector face plate.

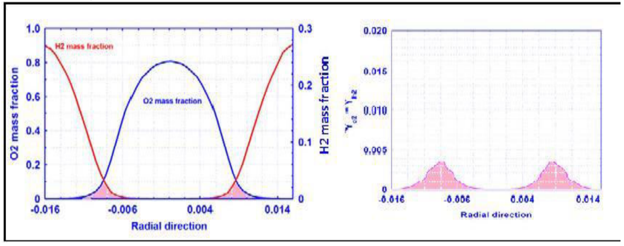

FIGURE 5 : MIXTURE MASS FRACTION ALONG RADIAL DIRECTION

The variation of the $O_2$, $H_2$ and $H_2O$ along the radial direction is compared with typical diffusion flame. In case of confined control volume coaxial injector single element chamber, due to presence of recirculation zone, the combustion product $H_2O$ mass fraction near the wall is more compared to normal diffusion flame. Figure-6 shows the comparison of species distribution in the single element combustor with typical diffusion flame [6].

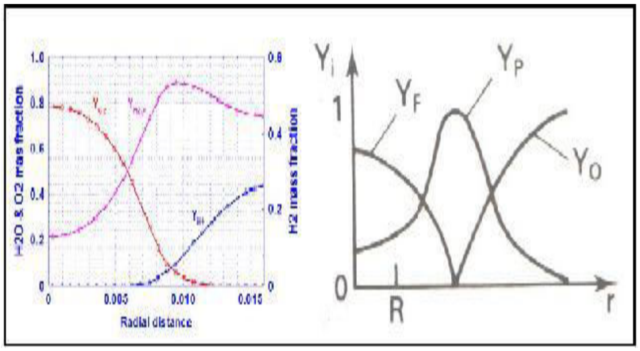

FIGURE 6 : CHARACTERISTICS OF DIFFUSION FLAME

The temperature buildup along the axial direction is given in figure-7 which indicates that near to the face plate, the combustion chamber temperature is more than stoichiometric temperature which is due to non-equilibrium condition during initial ignition transient.

FIGURE 7 : TEMPERATURE PROFILE ALONG THE AXIAL DIRECTION

### 5.2 Simulation with nozzle

The single element coaxial injector chamber is simulated by incorporating the propellant flow rate as the inlet boundary condition and sea level condition at outlet is specified. The pressure, temperature, velocity profiles and species mass fraction variation are compared with the case without nozzle configuration which are comparable.

The diffusion characteristics of the flame along with the recirculation zones are also observed and the chamber pressure is estimated. The estimated chamber pressure is compared with the experimental data for multiple points along the radial direction which shows a variation of 4.6%. Figure-8 gives the comparison of simulated chamber pressure with experimental data. Simulations were carried out with both the propellants in gaseous state. But in actual case LOX may be in saturated condition and some of the particles may be escaping from the domain without reaction. This may be the reason for the lower chamber pressure obtained in the experiment as compared to CFD simulation.

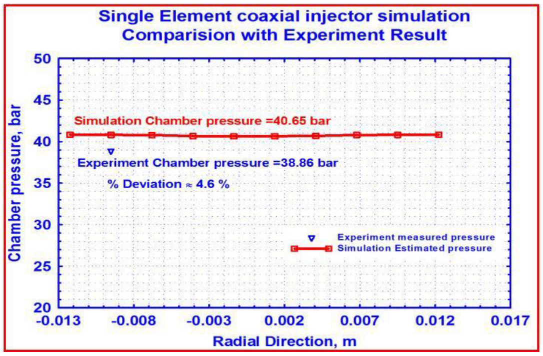

FIGURE 8 : COMPARISON OF SIMULATION RESULT WITH EXPERIMENTAL DATA

The signature of temperature buildup and species mass fraction along the axial direction is comparable with that without nozzle configuration. Figure-9 shows the variation of temperature along the axial direction.

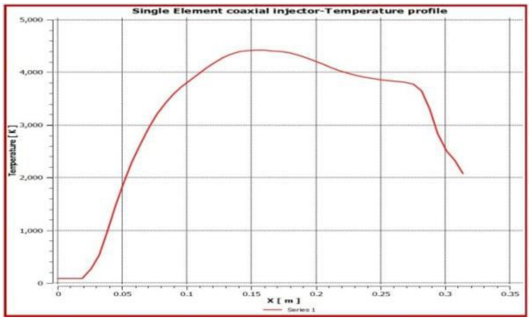

FIGURE 9: TEMPERATURE PROFILE ALONG AXIAL DIRECTION

Figure-10 shows the comparison of temperature and $H_2O$ mass fraction along the radial direction at different axial locations from the injector face plate. It shows lot of non-uniformity very near to injector face plate and uniform temperature at an axial distance of 160 mm away from the injector face plate. As the mixing improves along the chamber axis away from the injector face plate, the mass fraction of $H_2O$ is following the similar trend of temperature.

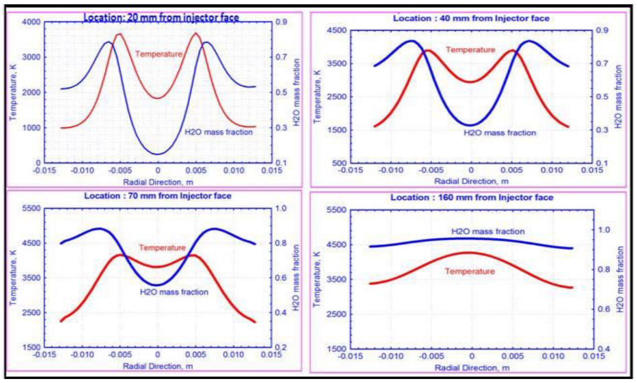

FIGURE 10 : VARIATION OF TEMPERATURE WITH $H_2O$ MASS FRACTION

## 6. CONCLUSION

CFD simulation is carried out on a coaxial single element $H_2$-$O_2$ combustor and the aero-thermo-chemical behavior of the combustor has been predicted. Results indicate that flame is diffusive in nature near to the injector face plate and premixed in nature near to the combustor exit. Also it is observed that the flame anchored at the injector exit and reaction occurred along the periphery of $O_2$ jet. Non uniformity in temperature, velocity and species is observed near to the injector face plate. Mixing characteristics of the single element combustor is also captured in the simulation.

Results of the simulation result have good agreement with experimental observations, showing that simulation captures the right mechanisms of flame ignition, propagation and stabilization.

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