Abstract—This study focuses on turbulent combustion interactions in a stagnation point reverse flow (SPRF) combustor. The non-preamixed and premixed combustion cases are modeled by using partially stirred reactor (PaSR) combustion model with one-step global reaction chemistry. Turbulent activities have been examined with large eddy simulation (LES) technique including k-equation subgrid turbulence modelling.

Keywords— LES, SPRF, Turbulent combustion, OpenFOAM, PaSR

I. INTRODUCTION

Combustion control is a challenging issue. Nowadays, investigations on combustion are focused on controlling of the combustion, reducing the emissions of the harmful gases such as NOx and provide flame stability as well. The SPRF combustor is a smart design combustor with a reduced size that promotes internal gas recirculation due to the outflow ports that located in the same geometrical plane as inflow, while the opposing end is a closed plate [1]. This design enables the products to interact with the incoming reactants as they leave the combustor. Therefore, the reactants are diluted with large amounts of the inert gases, which reduces the combustor temperature and this causes lower NOx and CO emissions [1]. Lean combustion enhances the flame stability and prevents quenching as well [2]. The SPRF combustor is numerically investigated with different sub-grid models such as linear eddy models [2, 3] and thickened flame models [2].

The high-accurate direct numerical simulation (DNS) method is still not fast enough in terms of computational time. Unlike DNS, large eddy simulation (LES) resolves only the energy-containing structures and it is computationally less expensive. In addition, instead of modelling all the turbulent structures as in Reynolds-averaged Navier Stokes (RANS), only small-scale structures are modelled in LES. Hence, the modelling error in LES is smaller than RANS [4]. For combustion, mixing of the fuel and oxidizer is a key subject. Therefore, the interaction between turbulence and flame front is the main factor which affects the stability of the flame and combustion efficiency in the combustion chamber [5]. Moreover, LES is more applicable for wide ranges of time and length scales as seen in many combustion applications [6].

The objective of this study is to investigate SPRF combustor numerically by using LES methodology with PaSR combustion model [7] and one-step global chemistry. Both cold flow and reacting flow cases are considered.

First, we will present the results of the non-reactive case in order to show the quality of the grid for reacting simulation. Then, the analyses are extended for premixed and non-premixed cases. Results are compared with experimental data.

II. MATHEMATICAL MODELLING

Non-reacting studies are modeled with incompressible set of Navier-Stokes equations while for the reacting studies, compressible approach is employed.

The LES equations are derived from the Navier-Stokes equations given by a spatial filtering procedure. This procedure involves filtering out the fluctuating, small-scale, high frequency motions and modeling their effect on the slowly varying large eddies. The separation between large and small scales is determined by the grid size, $\Delta$

A Favre spatial top-hat filter is employed to derive LES equations. Thus, any variable ($f$) is decomposed into a resolved ($\tilde{f}$) and a unresolved quantity ($f'$) by using a filter operation, such as $f = \tilde{f} + f'$. The Favre filtering, represented by the symbol $\tilde{f}$ in the following is defined for any variable $f$, by:

$$ f = \frac{\tilde{f}}{\tilde{\rho}} $$

where the over-bar represents spatial filtering.

Assuming that the filter commutes with differentiation, which is strictly true only when the filter width is constant, and applying the filter to the compressible Navier-Stokes equations, the LES equations [6] can be written as:

$$ \frac{\partial \tilde{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\tilde{\rho} \tilde{u}_i) = 0 $$

$$ \frac{\partial \tilde{\rho} \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j}(\tilde{\rho} \tilde{u}_i \tilde{u}_j) = - \frac{\partial \tilde{p}}{\partial x_i} + \frac{\partial}{\partial x_i} \left( \tilde{\tau}_{ij} + \tilde{\tau}_{ij}^{vis} \right) $$

$$ \frac{\partial \tilde{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\tilde{\rho} \tilde{h}) = \frac{\partial \tilde{\rho} \tilde{h}}{\partial t} + \frac{\partial}{\partial x_i} \left( \tilde{\rho} \tilde{u}_i \tilde{h} - \tilde{\rho} \tilde{h} + k \frac{\partial \tilde{h}}{\partial x_i} + \tilde{\omega}_x \right) $$

$$ \frac{\partial \tilde{\rho} \tilde{h}}{\partial t} + \frac{\partial}{\partial x_i} \left( \tilde{\rho} \tilde{u}_i \tilde{h} \right) = \frac{\partial}{\partial x_i} \left( \tilde{\rho} \tilde{u}_i \tilde{h} + \rho \tilde{D}_k \frac{\partial \tilde{h}}{\partial x_i} \right) + \tilde{\omega}_x \quad k = 1..N $$

In the above equations, $\tilde{u}_i$ is the $i$-th filtered velocity component, $\tilde{\rho}$ is the filtered mass density, $\tilde{\tau}_{ij}$ is the filtered stress tensor, and $\tilde{\omega}_x$ is the filtered vorticity.
pressure, $h$ is the filtered enthalpy, $\omega_r$ is the heat release, $\tilde{Y}_k$ is the species mass fraction of the $k^{th}$ species, $\tilde{\omega}_k$ is the species reaction rate of the $k^{th}$ species, $\lambda$ is the thermal conductivity, $D_k$ is the molecular diffusion coefficient of the $k^{th}$ species and it is described by Fick’s law.

The filtered LES equations contain terms representing the effects of the unresolved subgrid scales on the resolved large scale motions that need to be modelled: the subgrid-scale stress tensor $\tau^{sgs}_{ij}$, the subgrid enthalpy flux $\tilde{p}\tilde{u}_i\tilde{h} - \tilde{p}\tilde{u}_i\tilde{h}$, and the subgrid convective mass flux $\tilde{p}\tilde{u}_i\tilde{Y}_k - \tilde{p}\tilde{u}_i\tilde{Y}_k$.

**A. Turbulence Modelling**

Using eddy viscosity approximation, the subgrid-scale stress tensor $\tau^{sgs}_{ij}$ is approximated as follows,

$$\tau^{sgs}_{ij} = -2\nu^{sgs}_{ij}S_{ij}^{\text{rs}} + \frac{2}{3}k^{sgs}S_{ij}^\kappa$$

where $\nu^{sgs}$ is the subgrid-scale viscosity, $S_{ij}^{\text{rs}}$ is the resolved-scale strain rate tensor defined as,

$$S_{ij}^{\text{rs}} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} - \frac{\partial \tilde{u}_j}{\partial x_i} \right)$$

One equation eddy model, also known as the k-equation model [8] relates the subgrid-scale kinetic energy to the flow field as;

$$k^{sgs} = \frac{1}{2} (\tilde{u}_i\tilde{u}_i - \tilde{u}_i\tilde{u}_i)$$

The subgrid-scale eddy viscosity $\nu^{sgs}$ is computed using $k^{sgs}$,

$$\nu^{sgs} = C_v \sqrt{k^{sgs}}$$

Here, $C_v$ is a model coefficient and determined as 0.07. The equation of motion of the subgrid-scale kinetic energy is given by [9],

$$\frac{\partial (\rho k^{sgs})}{\partial t} + \frac{\partial (\rho \omega k^{sgs})}{\partial x} = \frac{\partial}{\partial x} \left[ \rho (\nu^{sgs}) \frac{\partial k^{sgs}}{\partial x} \right]$$

Here, the production term $P^{sgs}$ is defined as,

$$P^{sgs} = -\tau^{ij}_{sgs} \frac{\partial \rho}{\partial x}$$

and the dissipation term $D^{sgs}$ is modeled as

$$D^{sgs} = C_e \frac{k^{3/2}}{2}$$

where $C_e$ is another model coefficient, which is unity.

**B. Combustion Modelling & Chemistry**

The gradient diffusion assumption is applied for the unclosed terms in the species and the energy equation.

$$\tilde{p}\tilde{u}_i\tilde{Y}_k - \tilde{p}\tilde{u}_i\tilde{Y}_k = \frac{\mu}{Sc} \frac{\partial \tilde{Y}_k}{\partial x}$$

$$\tilde{p}\tilde{u}_i\tilde{h} - \tilde{p}\tilde{u}_i\tilde{h} = \frac{\mu}{Pr} \frac{\partial \tilde{h}}{\partial x}$$

Here, $Sc$ and $Pr$ are Schmidt and Prandtl numbers, and considered as unity in this study.

For the turbulence and chemistry interaction Partially Stirred Reactor (PaSR) model [7] is employed. In this approach, a computational cell is split into two different zones. In one zone all reactions occur, while there are no reactions in the other zone. Hence, it allows to neglect any fluctuations while calculating the chemical source terms. The reaction rate of this computational cell is determined by the fraction of the reactor in this cell. Reactive volume fraction $\kappa$ is calculated as

$$\kappa = \frac{\tau_r + \tau_c}{\tau_r + \tau_c + \tau_{mix}}$$

Here, $\tau_r$, $\tau_c$ and $\tau_{mix}$ represent the residence time, chemical reaction time and mixing time, respectively. Overall the species reaction rate $\tilde{\omega}_k$ and the homogenous reaction rate $\omega_k$ of the computational cell have the following relationship [10],

$$\frac{c^1 - c^0}{\delta t} = \tilde{\omega}_k = \omega_k$$

Here, $c^0$ is the initial and $c^1$ is the final averaged concentration in the reaction zone.

Non-premixed and premixed cases are performed using one-step global mechanism [11]. Methane oxidation step is applied as follows:

$$CH_4 + \frac{3}{2}[O_2 + 3.76N_2] \rightarrow CO_2 + 2[H_2O + 3.76N_2]$$

The reaction rate is defined by the Arrhenius law,

$$k = A e^{-\frac{E_a}{RT}} C_0^{0.8}$$

Here, $E_a$ is the energy of activation, $R$ is the universal gas constant, $A$ and $b$ are experimental parameters.

**III. NUMERICAL MODELLING**

Simulations are carried out by using the open source CFD package OpenFOAM [12]. Reacting cases are simulated by the PIMPLE algorithm which is a combination of PISO (Pressure Implicit with Splitting of Operator) and SIMPLE (Semi- Implicit Method for Pressure-Linked Equations) algorithms. For non-reacting studies, only PISO algorithm is employed. Second order, central difference numerical schemes are applied to convective and viscous terms. The time advancement is discretised by a second order, backward difference scheme. The one equation eddy model is implemented as a subgrid model. The numerical stability is sustained by setting the Courant number 0.3 for reacting and 1 for non-reacting studies. Adaptive time stepping technique is applied and physical time step is observed as $2 \times 10^{-7}$ for reacting and $1 \times 10^{-6}$ for non-reacting simulations.

Statistical accumulations are chosen to be 8 flow-through times and they are carried out after an initial transient. The accumulations of statistics are taken at each time step, and the simulations are run until the second order statistics have converged.
IV. DESCRIPTION OF CASES

A. Geometry

The combustion chamber on which the work carried out is represented schematically in Fig. 1 along with a snapshot of the flame during experiments. The SPRF design consists of a cylinder, 308mm in length and 70mm in diameter, where inflow and outflow ports are mounted on the top of the cylinder. The bottom of the chamber is closed. The burner itself consists of a central jet with a diameter of 4 mm, surrounded by an annular air inlet.

One of the most challenging issues about the SPRF geometry is to provide the proper inlet boundary conditions. Since pressure losses and recirculation zone occur at the inlet nozzle exit sections, these nozzle sections are not included in computational grids.

The grid resolution effect on the flow statistics has been investigated providing both radial and azimuthal refinements. The number of grid points for the streamwise, radial and azimuthal directions are listed in Table 1. The non-reacting, cold flow study is taken into consideration while evaluating these structured type meshes.

B. Computational Grid

The computational domain which is depicted in Fig. 2 covers all geometric characteristics of the SPRF combustor. To prevent discontinuities and high skewness values on streamwise axis, butterfly grid methodology as shown in Fig. 3, which scattered the grid elements on axis, is followed.

C. Studies

Three main studies have been carried out as it can be seen from Table 2. In this table, flow rates are in $m^3/s$ and temperature is in $K$. In order to provide a consistent comparison with experiments, the same mass flow rates of the experiments are taken into consideration, while determining the inlet velocities. Fluctuating velocities are imposed directly from the inlet nozzle exit section. The central fuel jet is assumed to be shut off for non-reacting and premixed cases. The pre-heating effect is included by setting the temperature to the values given in the table. Atmospheric pressure is applied to the outflow region with a partially reflecting condition that allows the pressure waves from downstream to enter the computational domain. The no-slip and adiabatic condition are prescribed to the solid wall boundaries.

V. RESULTS & DISCUSSION

In this section, we will first present the non-reacting cold flow results along with the experimental data to show the effect of grid resolution on turbulent statistics and spectra. Then, for the chosen grid, these analyses will be expanded for the premixed and non-premixed reacting cases. Furthermore, CO$_2$, CH$_4$ and temperature variations along the centreline of the
A. Non-reacting Results

Figure 4 shows the variation of the mean axial velocity along the centerline of the combustor for the non-reacting cold flow simulations as summarized in Table 1. Results are compared with the experimental data [2]. The exit plane of the injector corresponds to $x = 0$. Due to the cylindrical cavity in front of the central tube, the velocity of the jet slows down which then results in a recirculation bubble in this region. Downstream of this region annular jet merges and it reaches to 70 m/s peak velocity. Further downstream jet slows down and the mean axial velocity decays.

![Mean axial velocity along the centerline](image1)

The variations of the mean velocity in the radial direction are analysed at three axial locations: $x = 57, 113, 187$ mm. Figure 5 presents the comparison between LES and experimental data of the mean axial velocity at these axial locations. Computations appear to be more symmetrical than the experiments, which is likely due to the misalignment of the inner tube within the annular injector [13]. The shear layer existence due to the reverse flow feature and the stagnation point effect can be observed clearly from these radial velocity profiles.

![Axial velocity profiles at axial locations x=57,113 and 187 mm](image2)

In summary all three grid studies showed almost similar trend for the mean axial velocity. As a result of the grid refinement, the momentum transfer from the axial direction to the radial and azimuthal directions can be better predicted in regions especially where the flow returns. It can be seen from Fig. 5 that Grid2 and Grid3 provided slightly better resolution for reversed mean velocities with respect to Grid1. Fig. 6 also shows the effect of the grid refinement within the concept of turbulent fluctuations. All three grids show similar trend. Besides the radial and centreline comparisons of the mean and rms profiles of the non-reacting studies, the computed energy spectrum of “Grid1” is also represented in Fig. 7 for different probe locations probe1, probe2 and probe3, which are 22, 35 and 35 mm far from the inlet section respectively. Kolmogorov’s -5/3 law is preserved more than one decade for all three probes. From all these analyses, one can conclude that “Grid1” is capable of representing necessary flow mechanics of SPRF geometry when the computation time of LES calculation is taken into consideration. Reacting studies are evaluated with “Grid1”.

![FFT of the axial turbulent kinetic energy from 3 probe locations within Grid1](image3)
B. Reacting Results

Figure 8 compares the measured mean axial velocity and the computed mean axial velocity for premixed (PO LES) and non-premixed (NPO LES) simulations. Results are compared with the experimental data [14]. The presence of the recirculation bubble in the region downstream of the inlet appears at the region where the velocity slows down in the computations especially for the premixed operation. However, the recirculation bubble cannot be seen in experiments. In experiments, the mentioned cavity is infinitely long, while in this study geometrical cavity is not really considered due to the numerical stability issues. Due to this cavity modelling approach, peak velocity of the premixed operation is predicted, while the non-premixed peak velocity is well predicted. Downstream of this region the velocity decay tendency merges before the stagnation zone for premixed and non-premixed operations.

The comparison of the computed mean axial velocities and experiments for the reacting cases is depicted in Fig. 9. There is a slight over-prediction for non-premixed cases close to the injector, especially at \( x = 57 \) and 113 mm. The magnitude of the reverse flow velocities is also overpredicted near the combustor walls. This over-prediction can be related to the velocity change due to the reversed burnt products’ heat release.

Figure 10 presents the rms velocity profiles at selected axial locations for the reacting cases. Turbulence combustion interaction seems well captured except the asymmetry from the experiments, which is mentioned earlier. It should be noted that the existence of high rms values far from the inlet is an indication of the turbulence generation due to heat release.

Figure 11 shows the comparison of the computed and the experimental data of the CO2 mole fraction along the centerline. Trends are truly predicted by the computations. In the non-premixed mode, the CO2 concentration tends to increase until the stagnation zone while the CO2 concentration does not change in the premixed mode after \( x = 175 \) mm. This shows that the flame in the non-premixed mode located further downstream in the combustor.

The measured and the computed temperature along the centreline of the combustor is presented in Fig. 12. There exist some discrepancies close to the injector. However, the general trend of the temperature profile is truly captured for premixed and non-premixed cases. It can be seen that larger heat release is obtained in experiments. This is directly related to reactant temperatures, which are not measured correctly only preheating effect is provided.
Figure 13 compares the fuel mole fraction along the centerline for the premixed case. Although the general trend for the fuel consumption is under-predicted, the computed fuel consumption point, which is approximately at $x = 170$ mm matches with the experimental data. Hence, there is no incomplete combustion.

The averaged heat release results can also give an idea about the flame mechanics of the individual cases. The computed averaged heat release contours and the experimental averaged heat release results obtained with the chemiluminescence technique [13] are presented in Figs. 14 and 15 for non-premixed and premixed operations, respectively.

The lifted non-premixed flame can be seen in Fig. 14. This has been considered as the effect of the air jet that surrounds the fuel from hot product reverse flow. Because of the shielding effect of the coaxial air flow, fuel and air have time to mix before hot products are entrained.

In the premixed operation the flame is attached to the inlet region as shown in Fig. 15. The reversing hot products at the stagnation zone meet with the reactants within shear layer region. As a result, the incoming reactant temperature tends to increase. This can be clearly seen in Fig. 16 which presents the velocity contours and vectors near the shear layer region close to the inlet. In both operating conditions, the recirculation of the hot products stabilizes the flame. Hence, this mechanism also explains how stable combustion process is provided in such a lean condition.

VI. CONCLUSIONS AND FUTURE WORK

The main purpose of this study is to investigate and analyze the SPRF combustor with LES using an open source flow solver. Although a simple chemical mechanism and combustion modelling approach is considered, the turbulent combustion in this unique combustor is well resolved and LES results are validated with experimental data.

Results show that LES k-equation turbulence modelling approach is a very powerful tool for resolving such a complex flow field and the flame structure.

The recirculation of the hot products stabilizes the flame, hence this design can operate under very lean conditions in non-premixed and premixed conditions.

In order to provide comparable results for this type of industrial burner, different combustion models and reaction mechanisms will be considered in future studies.
REFERENCES


