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Numerical Simulation of Methane/Air Combustion with CO₂ Dilution in A Gas Turbine Combustor

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Abstract: In this paper, a numerical simulation of Methane/Air combustion within a model of gas turbine combustor is presented. The effect of CO₂ as diluent is investigated in primary and secondary zone. Eddy dissipation model for the turbulence and flamelet model for chemistry simulation used. Temperature distribution and NO fraction in flow affected due to decreased amount of O₂ in air flow. Results showed as the fraction of CO₂ increased in air fraction especially in primary zone, the amount of NO reduced significantly and flame length and maximum temperature decreased in combustor.

Keywords: Combustion, Dilution, Gas Turbines, NO_x

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1 Introduction

Nowadays, the optimization of combustion performance and the reduction of pollutant emissions require considerable research efforts from the gas turbine industry. The basic objectives in combustor design are to achieve easy ignition, high combustion efficiency and minimum pollutant emissions. Under such conditions two phenomena are to be controlled or avoided. First, the increase of NO_x emissions due to the high levels of pressure and temperature needs to be restrained. Second, the feedback mechanism caused by the coupling between the flow and the flame may result in instabilities which originate in the periodic formation of inhomogeneous fuel pockets, the periodic shedding of large structures and the amplification of the acoustic waves.

Numerical methods are in that context very attractive alternatives to the expensive experimental set-ups required in such areas of research.

Reynolds Averaged Navier Stocks (RANS) combustion simulation is widely used in academic researches. In other hand the Large Eddy Simulation which are offer numerous potential advantages and by solving for large flow structures while small scale effects are modeled. Eighty percent of eddies scale solved without any modeling and just 20% close to kolmogrov scale modeled. The implications on the numerical predictions are of importance but still need to be illustrated and validated in the context of industrial applications. For information and illustrations of the potential of each method, the reader is referred to results obtained with state-of-the-art RANS[8]- [12]and LES[13]- [18].

This study constitutes a step further toward the full demonstration of RANS for gas turbine engines with flamelet model.multiphase flows. It addresses the problem of dilution jets in an industry-like configuration.

The design of gas turbine combustion chamber is based on combined theoretical and empirical approach and the design of combustion chamber is a less than the exact science. A technical discussion on combustion technology status and needs will show that the classic impediments that have hampered progress towards near stoichiometric combustion still exist. The process of combustor design has taken a new meaning over the past several years as three dimensional codes and other advanced design and validation tools have finally changed the approach from a “cut and burn” technique to a much more analytical process.

Mixing processes are of paramount importance in the combustion and dilution zones. In the primary zone, good mixing is essential for high burning rates and to minimize soot and nitric oxide formation, whereas the attainment of a satisfactory



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temperature distribution (pattern factor) in the exhaust gases is very dependent on the degree of mixing between air and combustion products in the dilution zone. A primary objective of combustor design is to achieve satisfactory mixing within the liner and a stable flow pattern throughout the entire combustor, with no parasitic losses and with minimal length and pressure loss. Successful aerodynamic design demands knowledge of flow recirculation, jet penetration and mixing, and discharge coefficients for all types of air admission holes, including cooling slots.

Good amount of literature is available on modeling of the process of combustion for and hydrocarbon fuels ([11]- [27]). Charles K. Westbrook et al. [28] have reviewed the progress in the field of computational combustion over last 50 years encompassing 3D DNS and LES approaches. They have observed that many commercial CFD codes use unstructured grid which offer the advantage of being more suitable to massively parallel computing environment, as well as an ability to deal with complex geometries.

The paper presents the design of tubular and annular combustion chamber followed by three dimensional simulations in tubular and annular combustor with full film cooling to investigate the velocity profiles, species concentration and temperature distribution within the liner. The fuel under consideration is methane.

The computational approach attempts to strike a reasonable balance to handle the competing aspects of the complicated physical and chemical interactions of the flow and the requirements in resolving the three-dimensional geometrical constraints of the combustor contours, cooling slots, and circular dilution holes. The modeling employs non-orthogonal curvilinear coordinates, second-order accurate discretization, multi-grid iterative solution procedure, the k - turbulence model, and a combustion model comprising of an assumed probability density function flamelet concept. The complicated mixing process can be better understood with more detailed information supplied by the numerical simulation.

Accordingly, in present study an attempt has been made through CFD approach using CFX 12 to analyze the flow patterns within the combustion liner and through different air admission holes, namely, primary zone and dilution zone and wall cooling, and from these the temperature distribution in the liner and at walls as well as the temperature quality at the exit of the combustion chamber is obtained for tubular and annular combustion chambers designed for gas turbine engine.

NO_x emissions were calculated by the use of thermal and prompt models. Computations of NO_x formation rates and NO_x concentrations were carried out using a post-processor based on previously calculated velocities, turbulence,

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temperature, and chemical composition fields. To take into account turbulence fluctuations, a joint two-variable PDF was used in the calculation of the mean NO_x formation rate.

2 Geometry

The can combustor is a feature of the gas turbine engine. Arranged around a central annulus, can combustors are designed to minimize emissions, burn very efficiently and keep wall temperatures as low as possible. The basic geometry is shown below with a section of the outer wall cut away.

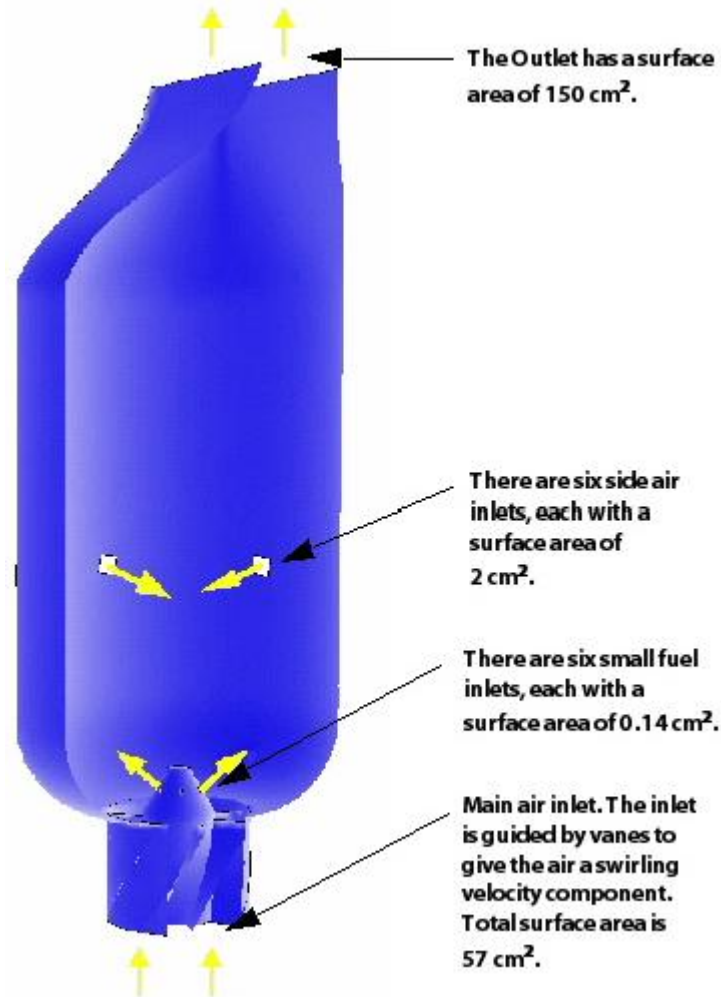


Figure 1- Combustor schematic

Due to the fact that the fuel (methane) and oxidizer (air) undergo “fast” combustion (whereby the combustion rate is dominated by the rate of mixing of the



materials), the Finite Rate Chemistry model is not a suitable combustion model for the combustor in this paper. The Combined EDM/FRC model capability is a superset of the Eddy Dissipation model capability, and has no benefit over the Eddy Dissipation model in this case. In fact, the convergence behavior of the Combined EDM/FRC model may be worse than that of the Eddy Dissipation model.

The Eddy Dissipation model, the Laminar Flamelet model, and the Burning Velocity model are suitable for modeling “fast” combustion. The Burning Velocity model capability is a superset of the Flamelet model capability, with the extra capability of being able to handle premixed fuel/oxidizer. Because the combustor in this tutorial does not use premixed fuel/oxidizer, the extra capability of the Burning Velocity model is not required and therefore it is sufficient to use the Flamelet model.

The Eddy Dissipation model tracks each individual chemical species (except for the constraint material) with its own transport equation. This model is flexible in that you can readily add new materials, such as additional fuels, to the simulation without complications. A limitation of this model is that radical or intermediate species, such as CO, cannot be calculated with adequate accuracy. This may lead to over-prediction of flame temperature, in particular in fuel-rich regions.

The Laminar Flamelet model can simulate the products of incomplete combustion; for this reason, it generally provides a more accurate solution than the Eddy Dissipation model. One drawback of the Flamelet model is that it requires the availability of a flamelet library suited for the required fuel/oxidizer combination over the pressure and temperature ranges of interest.

The NO models used in the two parts of this tutorial are very similar. The only difference is in how the O-radical concentration is obtained for the 'Thermal NO' formation step:

Eddy Dissipation model: The O-radical is not a component of the mixture; instead, its concentration is estimated using the O₂ concentration and temperature.

Flamelet model: The O-radical concentration is calculated from the Flamelet library, where its concentration information is directly available.

3 Mesh Generation

The grid is fully unstructured and composed of tetrahedral. To control the total number of cells and reduce computational cost, mesh refinement is enforced where necessary. More specifically, injection areas, wall regions and jet trajectories must

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be sufficiently resolved to capture the appropriate range of length-scales. To facilitate refinement along the jet The grid is fully unstructured and composed of tetrahedral. To control the total number of cells and reduce computational cost, mesh refinement is enforced where necessary. More specifically, injection areas, wall regions and jet trajectories must be sufficiently resolved to capture the appropriate range of length-scales. To facilitate refinement along the jet.

Tetrahedral grid is used to discretized the geometry and 106651 is the number of nodes.

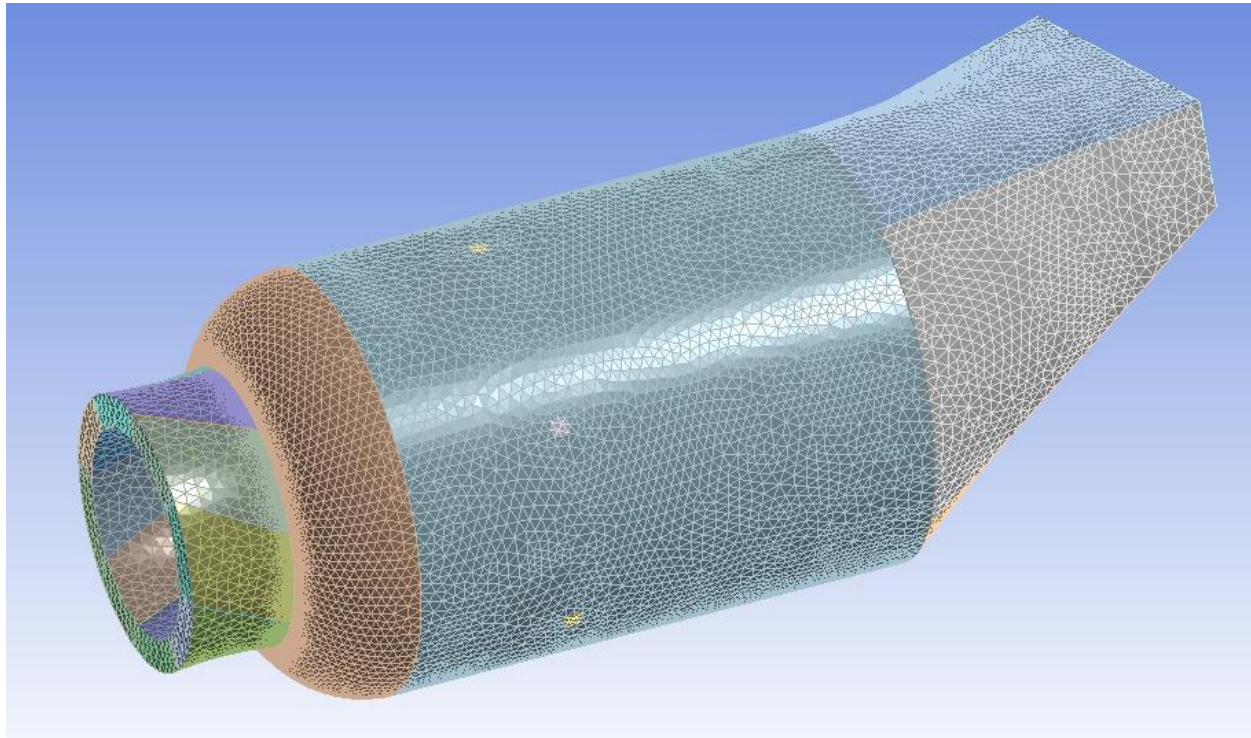


Figure 2- generated grid for combustor model

To study the independence of the results with respect to the grid size, a several grids used in reference case. It is seen the temperature distribution and The species fraction remain constant by increasing the grid over 106651 nodes. The near wall grids conformed and mesh density over whole geometry are the parameters which improved in mesh study.



Table 1- Grid independency study

Case	Grid #1	Grid #2	Grid #3
Temperature	1330.05 [K]	1331.05[K]	1331.14 [K]
HO2 Mass Fraction	0.0601247	0.0602047	0.0602053
CO2 Mass Fraction	0.0732185	0.0735185	0.0735195
NO Mass Fraction	1.68052e-006	1.58052e-006	1.50052e-006

In Table 1, three grids result presented, 50231, 106651 and 210467 are nodes of grids respectively. It is concluded the changes in parameters listed above is under 1% so the grid #2 is the basic mesh in the numerical cases.

4 Governing Equations

The governing equations including the continuity, momentum, energy and species conservation are as followed:

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = S_m \quad (1)$$

Momentum equation (with respect to i direction):

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \quad (2)$$

where

$$\tau_{ij} = \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] - \frac{2}{3} \frac{\partial u_l}{\partial x_l} \delta_{ij} \quad (3)$$

The energy equation is (with respect to i direction):

$$\frac{\partial}{\partial t} (\rho E) + \frac{\partial}{\partial x_i} (u_i (\rho E + p)) = \frac{\partial}{\partial x_i} \left(k_{eff} \frac{\partial T}{\partial x_i} - \sum_{j'} h_{j'} J_{j'} + u_j (\tau_{ij})_{eff} \right) + S_h \quad (4)$$

where

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$$h_j = \int_{T_{ref}}^T c_{p,j} dT \quad h = \sum_j m_j h_j \quad E = h - \frac{p}{\rho} + \frac{u_i^2}{2} \quad (5)$$

The species conservation equation is:

$$\frac{\partial \rho}{\partial t} (\rho m_i) + \frac{\partial}{\partial x_i} (\rho u_i m_i) = - \frac{\partial}{\partial x_i} J_{i,i} + R_i + S_i \quad (6)$$

where

$$J_{i,i} = - \left(\rho D_{i,m} + \frac{\mu_t}{Sc_t} \right) \frac{\partial m_i}{\partial x_i} \quad (7)$$

And:

$$R_i = M_i \sum_{k=1}^{N_R} v'_{i,k} M_i AB \rho \frac{\epsilon}{k} \frac{\sum_p m_p}{\sum_j v''_{j,k} M_j} \quad (8)$$

In the above equations, S_m is the mass added to the continuous phase, Sh includes heat of chemical reaction and Si is the rate of creation by addition from the dispersed phase.

The turbulence model was chosen to be k- . The constants of the k- model are taken from [1]The interactionbetween turbulence and chemical reactions has been considered byusing the eddy dissipation method [2] and [3].

The simple reaction (stoichiometric) between H₂ and O₂ is considered as the chemical reaction. The governing equations are solved based on a finite volume approach.

5 Numerical scheme

An algebraic multi-grid method is applied to the coupled linearized discrete equations arising from an implicit pressure based finite volume discretization system of equations. The whole methodology is modeled by using CFX solver.

Each simulation normally takes about 9 CPU hours.



The solution convergence is judged according to the residuals of governing equations. The results reported in this paper are based on the criteria that the residual of each equation should be smaller than 1.0×10^{-6} .

Table 2- Fluid model characteristics

Fluid Models	Material	Methane Air Mixture
	Reference Pressure	1 [atm]
	Heat Transfer	Thermal Energy
	Combustion	Eddy Dissipation
	EDM Coeff. B	0.5
	Thermal Radiation	P 1
	Component Models > N2	Constraint
	Option	Reacting Mixture
	Material Group	Gas Phase Combustion
	Reactions	Methane Air Single Step Reaction

5.1 Boundary conditions

Three inlet conditions and one outlet shown in Figure 3.

Boundary and initial conditions dealing with a fully compressible flow solver, For clarity, the set of BC's used in the RANS is listed in Table 3, Table 4 and Table 5.

Table 3- Fuel inlet boundary

Boundary Details	Normal Speed	40 [m s ⁻¹]
	Static Temperature	300 [K]
	Component Details	CH ₄
	Mole Fraction	1

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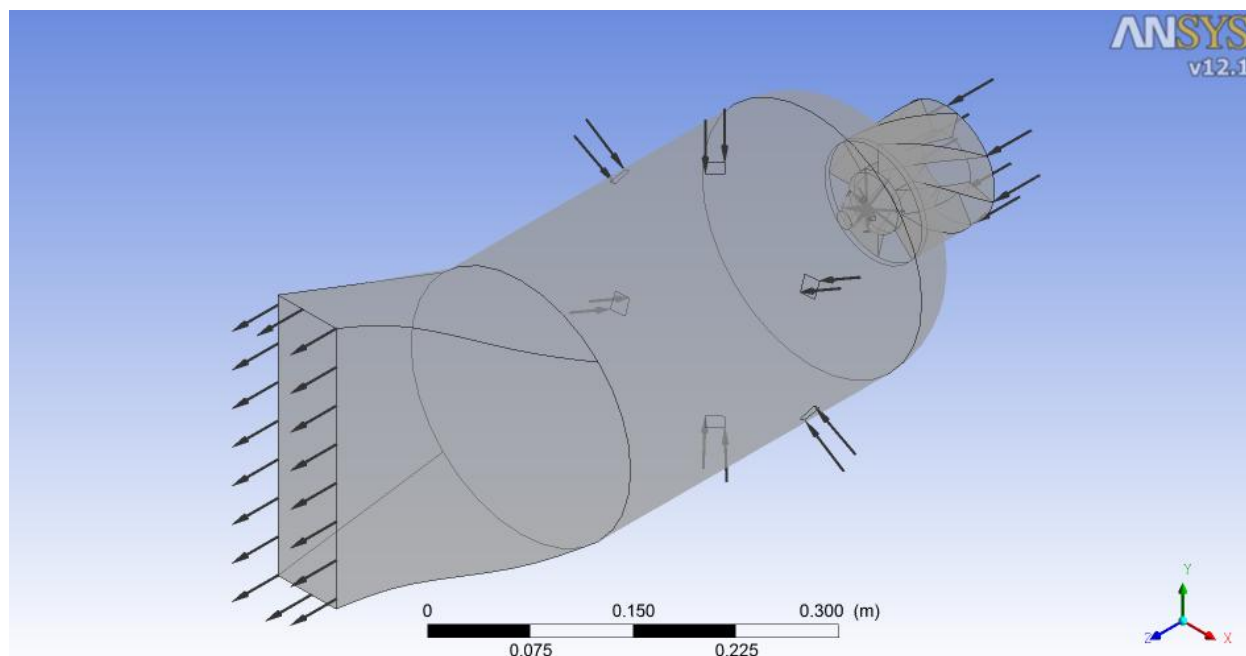


Figure 3- Boundary conditions specified on combustor model

Table 4- Main oxidizer injector

Boundary Details	Normal Speed	10 [m s ⁻¹]
	Static Temperature	300 [K]
	Component Details	O ₂
	O ₂ Mole Fraction	0.21
	N ₂ Mole Fraction	0.79

Table 5- Dilution Oxidizer Injector

Boundary Details	Normal Speed	6 [m s ⁻¹]
	Static Temperature	300 [K]
	Component Details	O ₂
	O ₂ Mole Fraction	0.21
	N ₂ Mole Fraction	0.79

The mass fraction of CO₂ in air inlet (main and dilution oxidizer injectors) varies in cases. Six different cases studied. CO₂ as diluent added to oxidizer injector and



mole fraction 0.10, 0.15 and 0.20 varies to investigate the effects in main and dilution injectors.

6 Results

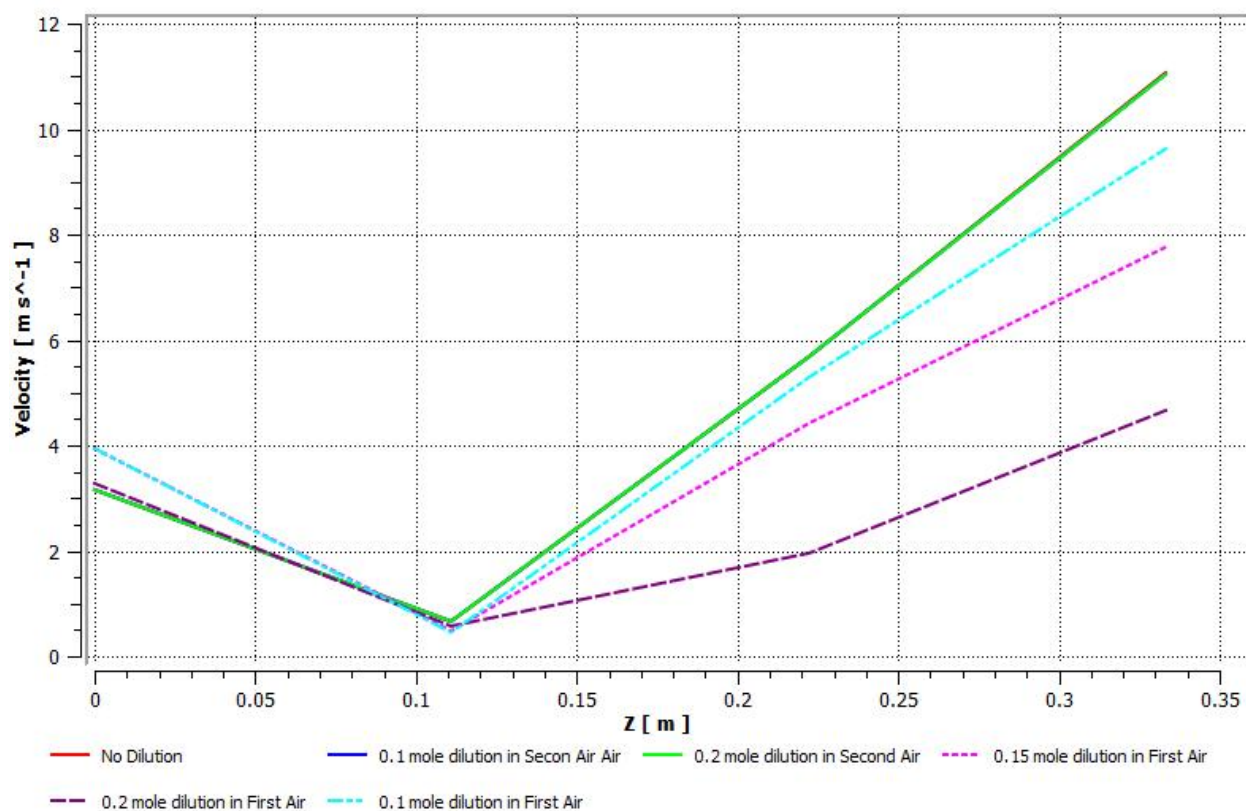


Figure 4- Velocity profiles in six different cases

The critical study of flame structure reveals that the present design offers narrow flame with maximum temperature in primary zone being of the order of 1300^K. H. The intense mixing and formation of re-circulation zone at the core of primary zone are responsible for short and narrow flame structure as is observed through flow visualization (Figure 8) in present study.

Similar trends for velocity It is important to note that the pressure drop across the combustion chamber is around 10% of the inlet pressure which is quite tune with the published results for tubular combustion chamber.

In Figure 5, Figure 6 and Figure 7, 10 cases are demonstrated. Case 1 corresponds to no dilution case, case number 2 -4, 5-7, 8-10 related to dilution at primary, secondary (dilution) and both zones respectively.

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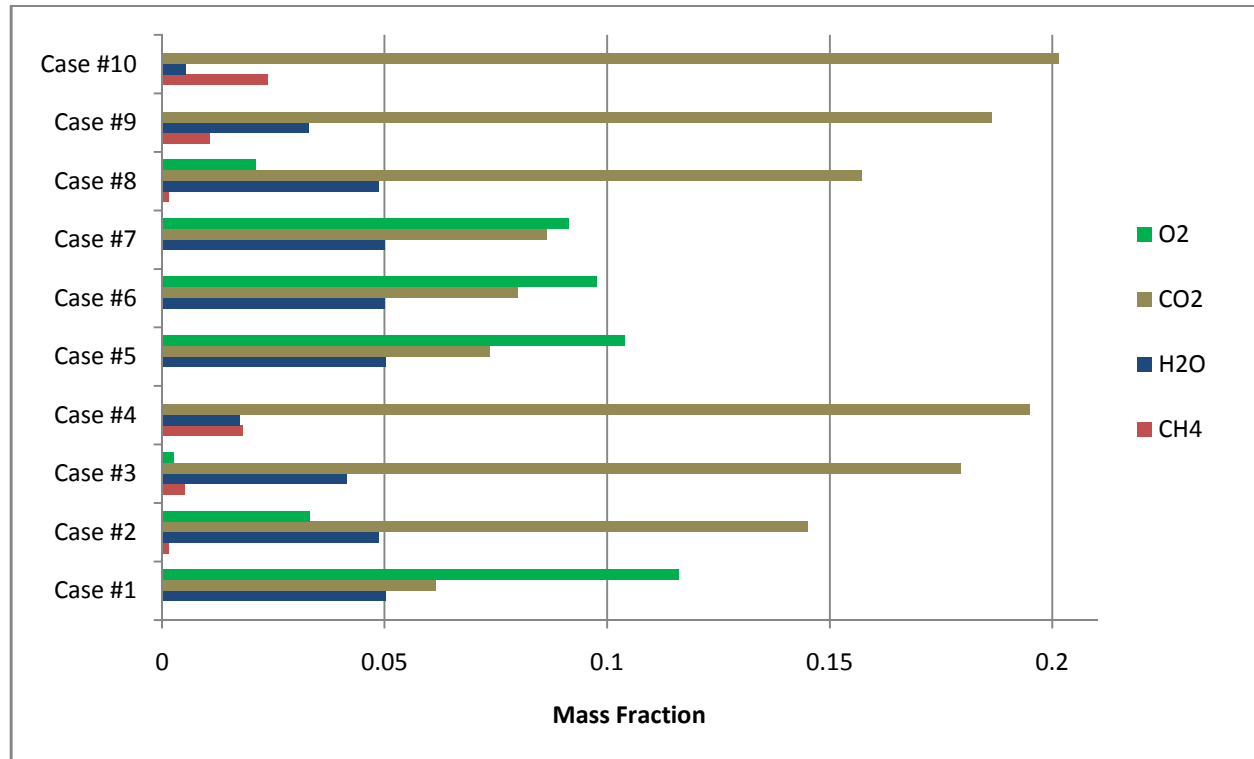


Figure 5- Mass fraction in outlet

The fluid flow in the tube can be mainly divided into back flow zone, mixing zone and trailing fluid zone. This fluid flow texture ensures the proper flow field in the combustor and affects the air distribution through different air admission holes. High levels of radial and tangential turbulence were observed in the central core region throughout the combustor. High losses are encountered in the dump region and where the jets bend towards the outer and inner annuli. The design of these zones needs to be taken utmost care to reduce the losses in the combustor. The flow behavior in the combustor, including the flow back zones, eddies, and their size and intensity, will apparently control the combustion behavior and then the performance of the engine. High velocity from primary and dilution air admission holes of the order of 10 m/s is witnessed.

The formation of counter rotating vortices from the second row of primary zone ensures cutoff of flame.

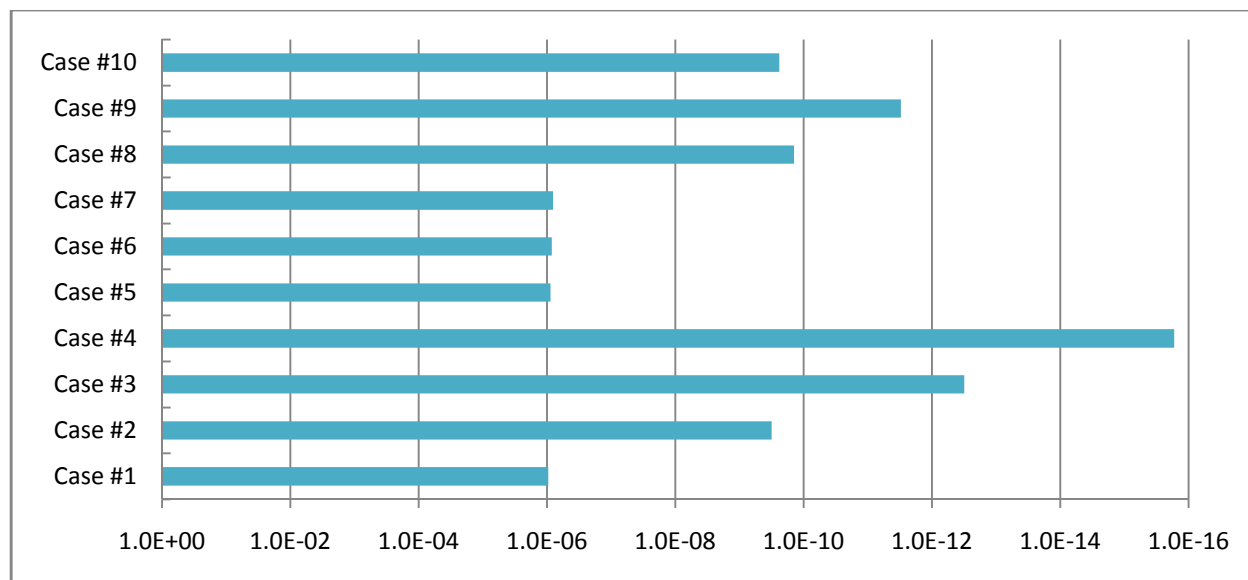


Figure 6- NO mass fraction in outlet

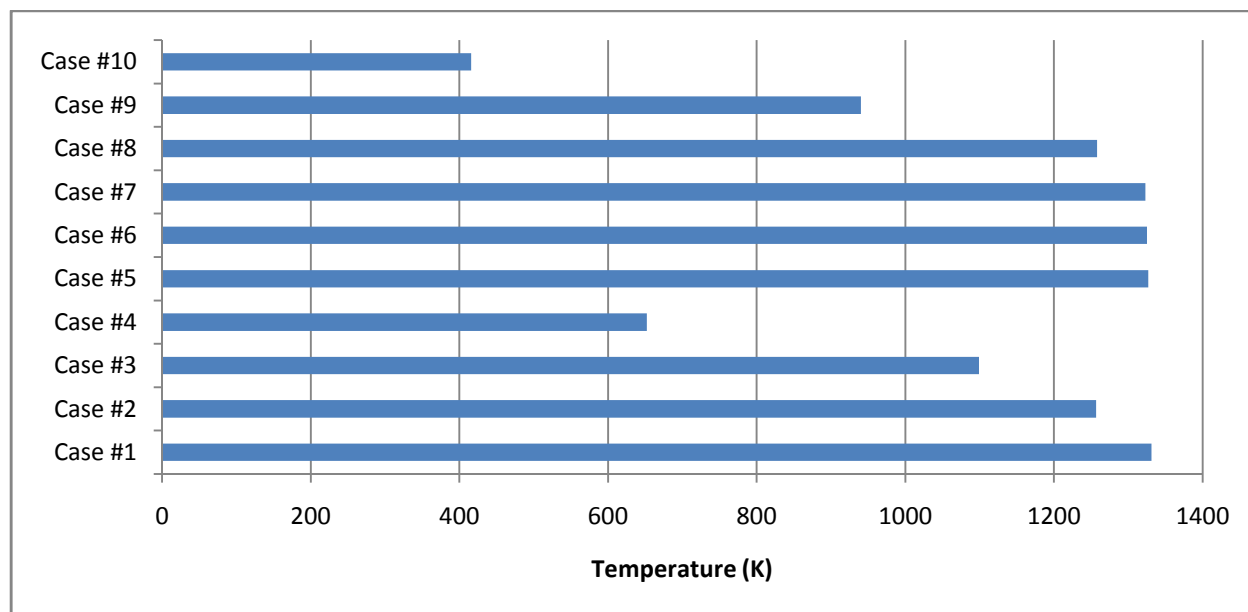


Figure 7- Temperature level at outlet

It is shown in Figure 6 that the NO mass fraction in case number are minimum, which the dilution is 0.15 mole fraction for CO₂. However temperature profile (Figure 8) and averaged temperature in outlet are similar to NO formation.

Apparently CO₂ dilution decreases the amount of pollutant but the reduction in temperature in case #4 and #10 in which the primary zone has 0.01 mole fraction (N₂ mole fraction in all cases is constant to 0.79) is lower than other cases.

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Turbine inlet temperature (TIT) is the most important parameter in gas turbine engine performance. Except material limitation as the TIT increased the efficiency of whole cycle falls up so the basic goal in dilution aspect should be keeping TIT (combustor outlet temperature) constant to has the constant efficiency.

The case # has the best pollutant in outlet but as the dilution is 0.15 CO_2 the temperature reduction is not order of other cases such as .it is very worthy while the NO fraction decreased by diluting the temperature (important parameter in gas turbine engine) remains approximately constant.

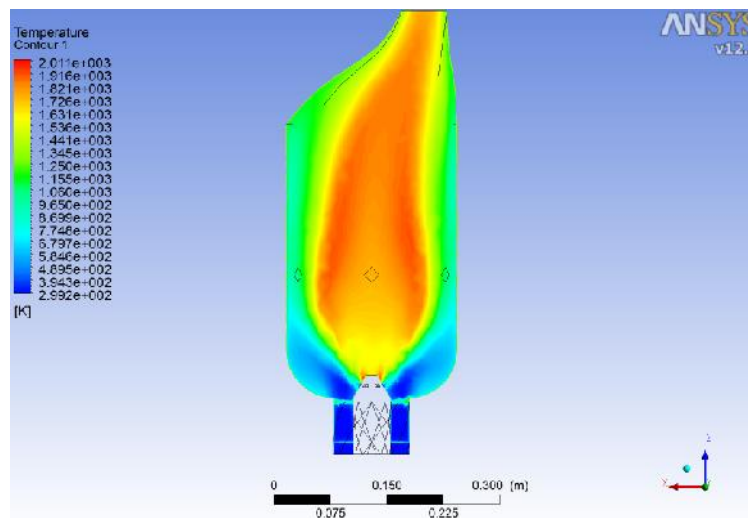


Figure 8- Temperature profile in combustion chamber without dilution at stoichiometric ratio

The flow from the pre-diffuser inlet to the combustor exit can be mainly divided into three zones, namely back flow zone, mixing zone and trailing flow zone. In the first zone or back flow zone the air leaves the swirl cone to the dome at high swirling velocity. After that, the swirling mixture of the air and fuel flows forward and entraps the air in the center area of the liner, and at the same time, the downstream air refills the region. As a result, a counter-rotating vortex pair (CRVP) forms in the central region of combustor liner. Corresponding to a pair of large eddies in this zone, there should be two symmetrical small eddies in the corners of the liner. In the downstream area of the back flow zone, the outside mixture further mixes with the fresh air injected from the dilution holes distributed on the liner wall. The injection flows retard the revolution of the mixed gas and restrain the anterior reverse flow zone. As a result, the back flow zone is cut off by the first pair of the dilution holes and the combustion should mainly occur in the backflow zone under very hot condition, i.e., primary zone. Although a small amount of the mixed

gas is inhaled into the primary zone, most gas flows downstream and mixes with the cold air from the second pair of the dilution holes. This makes the flow in the combustor more uniform.

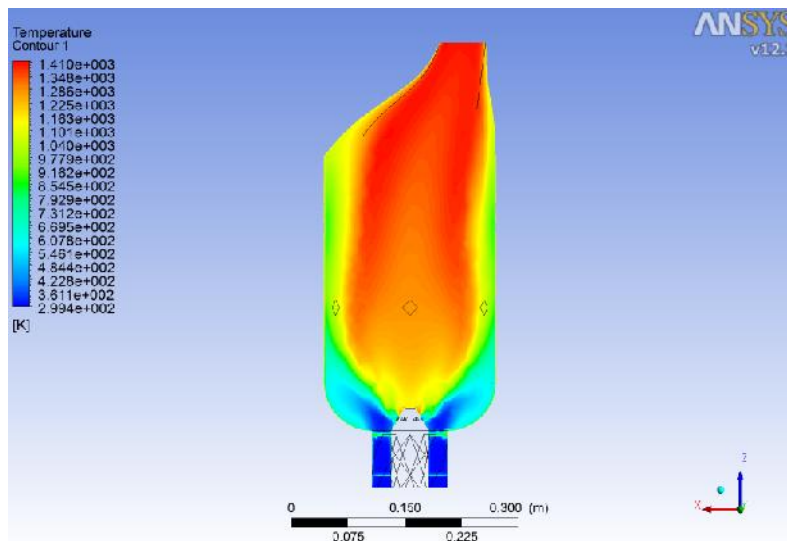


Figure 9- Temperature profile in combustion chamber with 0.10 mole fraction CO₂ in First air zone

Decreasing dilution in the combustion chamber (comparison between Figure 9 and Figure 10) reduces the flame width and maximum temperature. The effect of secondary air inlet is more significant in higher amount of CO₂ dilution.

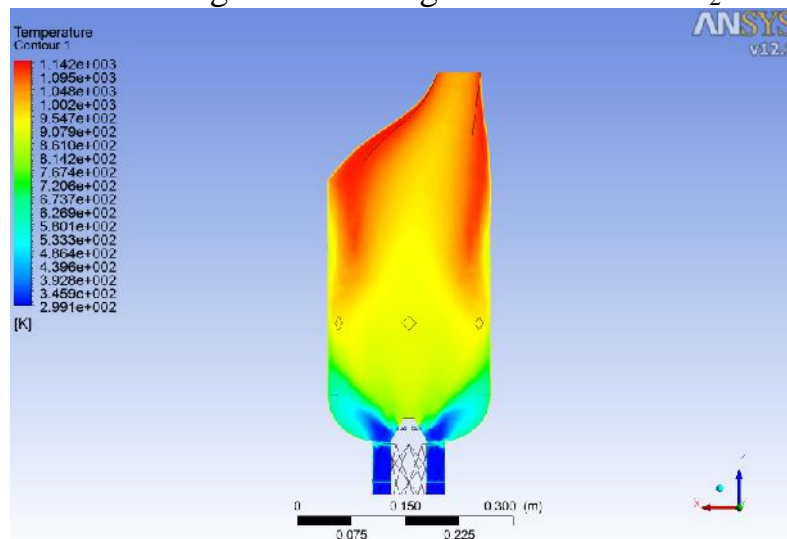


Figure 10- Temperature profile in combustion chamber with 0.15 mole fraction CO₂ in First air zone

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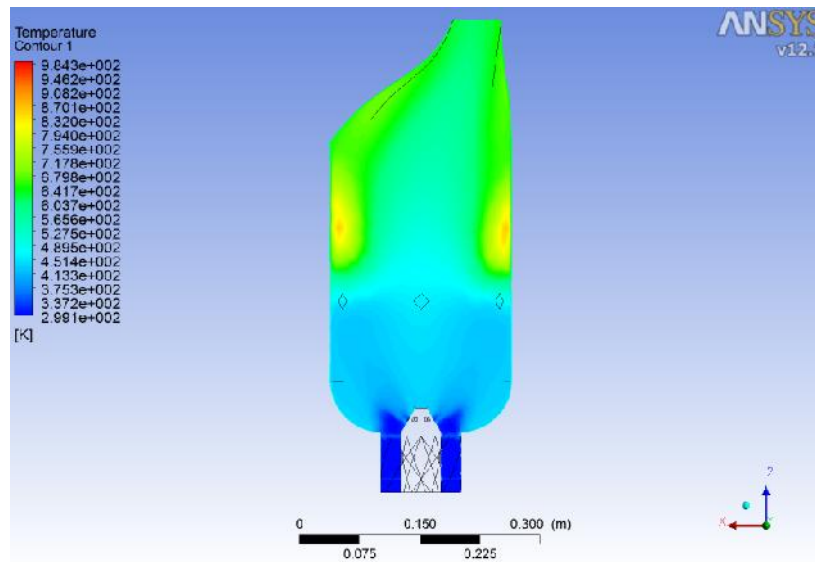


Figure 11- Temperature profile in combustion chamber with 0.2 mole CO₂ dilution in first air zone

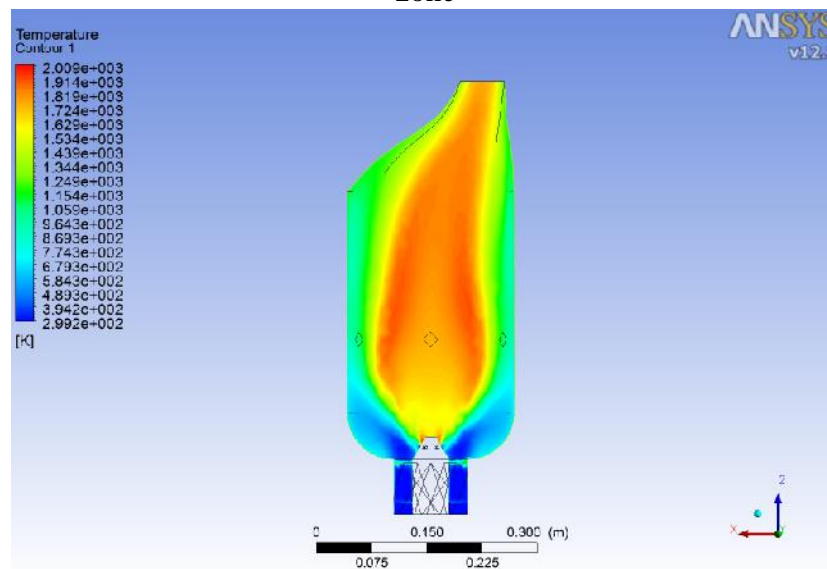


Figure 12- Temperature profile in combustion chamber 0.1 mole fraction of CO₂ in second air zone

Temperature profile in cases without dilution and dilution (Figure 8 with Figure 12 through Figure 14) in secondary zone has similar contour. It is due to low mass flow rate in secondary zone.

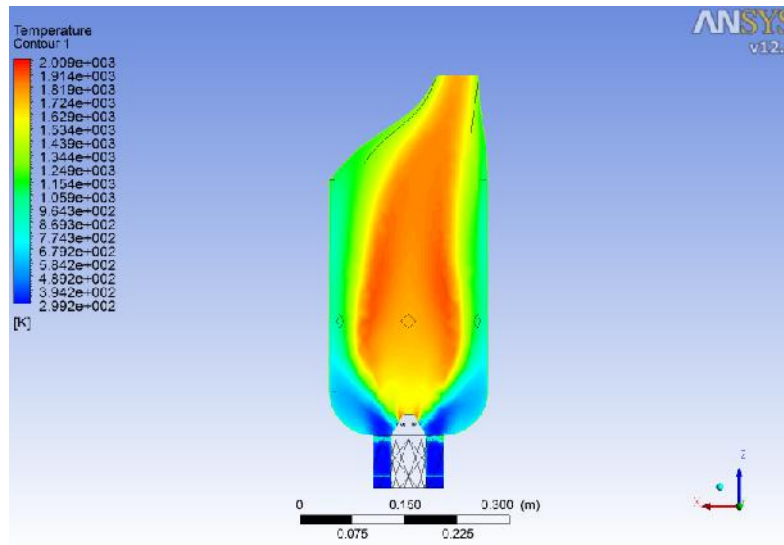


Figure 13- Temperature profile in combustion chamber with 0.15 mole fraction CO₂ in second air zone

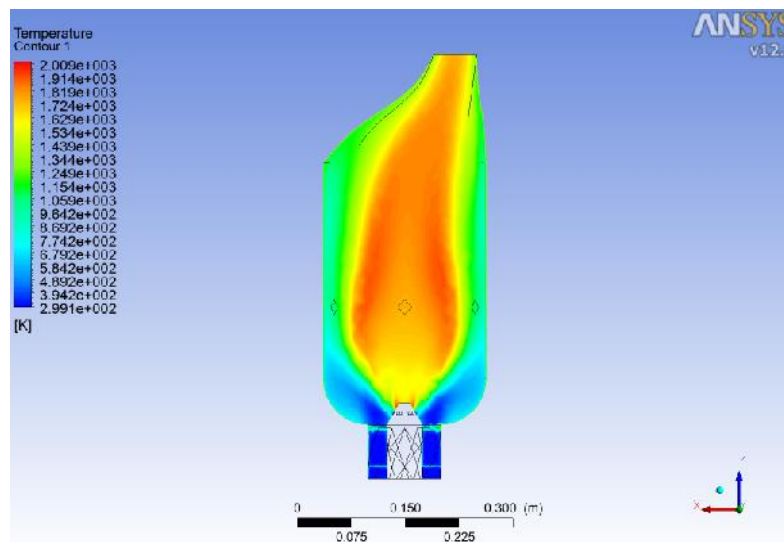


Figure 14- Temperature profile in combustion chamber with 0.2 mole fraction CO₂ in second air zone

7 Conclusion

In the present study, a numerical approach to investigate CO₂ dilution effect in a gas turbine combustor is presented. A model combustor with two section and 6 dilution holes are the basis of the study. 10 different cases which diluent fraction varies are perspective. The temperature profile across the combustion chamber and

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species fraction are the parameters which described in detailed. Several wealthy observations and conclusions are obtained:

- Dilution in secondary zone has no significant effect on flame length in the combustor but the amount of NO as pollutant is lower than other cases.
- Temperature profile decreases higher as the diluent increases. In the case #5 (CO₂ mole fraction at 0.15 in secondary zone) the maximum temperature in outlet is equal to the case without dilution.
- Flame width in the primary dilution has bigger size rather than the dilution in secondary zone and this effect higher averaged temperature in whole combustor.

Nomenclature

P	Pressure
EDM	Eddy Viscosity Method
Z	Axial length
T	Temperature
TIT	Turbine Inlet Temperature
	Equivalence ratio



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