# **RESEARCH ARTICLE**

# Numerical simulation and analysis of combustion chamber model design to investigate the effects of number of inlet and concentration of oxidizer mixture on combustion characteristics

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### ABSTRACT

In this research it is found that number of inlets had a significant impact on combustion characteristics specifically emission of CO and unburned hydrocarbons. After the selection of number of inlets MILD investigation had been done on the effect of concentration ( $\gamma$ ) of CO2/O2 on the combustion characteristics. It is found that by increasing the number of inlets decrease the emission level and unburned hydro carbon in outlets. For concentration of oxidizer, we find a value between 0.80-0.85 will be efficient for combustion due to minimum emission levels and unburned hydrocarbons. The research has been carried out in Ansys CFD fluent-> Energico 18.2-> Chemkin->. The model for reaction solves in energico and chemkin to generate results for unburned hydrocarbons and emission of CO.

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Copyright © 2024 by author(s). Applied Chemical Engineering is published by Arts and Science Press Pte. Ltd. This work is licensed under the Creative Commons Attribution-NonCommercial 4.0 International License (CC BY 4.0). https://creativecommons.org/licenses/by/4.0/ *Keywords:* Oxy-fuel combustion; Allam cycle; CO2 capture; Burner; partially premix combustion

## **1. Introduction**

Controlling emissions is an important issue today and attracts the attention of many researchers who want to work in this field. Governments are implementing new laws and regulations to control carbon emissions in order to reduce the effects of global warming. Adoption of new technologies can control greenhouse gas emissions. MILD (Moderate and Intense Low Oxygen Dilution), which is the difference between impingement or flameless oxidation technology, is a new design and technology that provides low pollution and increases the thermal efficiency of the combustion system<sup>[1-3]</sup>. Moderate and Intense Low Oxygen Dilution combustion occurs at low temperatures in the range of 1100-1500 K and is characterized by a flat thermal field and small temperature changes. It is also called flameless because under the right conditions there is no visible flame during oxidation.

Although the concept used in MILD combustion have been known for some time, a better understanding of the flame characteristics in MILD combustion has yet to be discovered. The basic working principle of this technology is the exhaust gas and heat recovery concept. The heat from the exhaust gas is used to increase the temperature of the oxidant stream, and the exhaust gas is used to dilute the oxidant vapor to reduce the oxygen concentration and control the temperature in the combustion chamber. MILD combustion technology allows the use of different oxidants; for example, the oxidant mixture used in this study is O2/CO2. Fluid mixing is widely used in many applications. For premixed combustion, the reactants must be mixed before entering the combustion chamber, The quality of mixture<sup>[4]</sup> and uniformity in velocity<sup>[5,6]</sup> Promotes complete combustion and reduces pollutant emissions. Timely mixing of products based on minimum gas mixture quantity has an important effect on ensuring continuity and high performance in micro combustion devices that power micro devices<sup>[7]</sup>.

For modelling micro mixer combustion system according to Zhen et al.<sup>[8]</sup>, the difference in the length of the air nozzle shows a significant difference in the flame. They found that the flame created by the short nozzle has a central height and a small capacity due to the air/fuel mixture. micro-mixed combustion technology<sup>[9]</sup> is an effective system here. A micromixer (MM) is a combination of multiple tubes which consist fuel injector mixes fuel with oxidizer at a micro level and divide in to multiple flames during combustion. Micro mixer is an emerging technology<sup>[10]</sup> It has been successfully implemented by different power companies such as Honeywell Garrett<sup>[11]</sup>, Mitsubishi Hitachi Power<sup>[12]</sup>, and GE (General Electric)<sup>[13]</sup>. However, MM never used for oxyfuel combustion before. York et al.<sup>[14]</sup> and Asai et al.<sup>[15]</sup> test the combustion of hydrogen-rich fuel in MM burners and demonstrate stable, flashback-free operation of such burners. Funke et al.<sup>[16]</sup> An MM combustion chamber with approximately 1600 flamethrowers was designed for integration into existing gas turbines. They reported that the use of the MM combustion chamber resulted in stable operation during engine acceleration, idling and starting. Dodo et al.<sup>[17]</sup> tested carbon capture conditions of integrated gasification combined cycle (IGCC) and MM air burner were simulated. The syngas fuel analogues used consist of H2, CH4 and N2; HF varies from 40% to 60%, and the three carbon capture efficiencies are 0%, 30% and 50%, respectively. The MM burner operates stably under atmospheric pressure without combustion or combustion. Previously influence of number of inlets on oxidizer and fuel mixer studied by Ahmed Abdelhafez et. Al<sup>[18]</sup> and compare three headend. Headend 1 (HE1) which has 61 jets of 3.175-mm diameter, arranged on a hexagonally, with a uniform jet spacing of 5.5 mm. Headend 2 (HE2) has 37 jets with larger diameter (3.970 mm 25% increase), also arranged hexagonally, with a spacing of 5.5 mm. HE 2 has less jets compared to HE1 in order to maintain almost the same combustor power. Headend 3 (HE3) is similar to HE 2, but with a jet spacing of 7.0 mm (27% increase). The stability of the three heads was determined and optical and temperature measurements were made in the selected flame of each head. The entire study was carried out at a flame speed of 5.2 m/s to maintain the same conditions and pressure. Although there were differences in beam width and spacing between heads, the limit of the three systems was found to be only about 45 K apart. This is a strong statement of the geometric simplicity of gas turbine micromixers and is therefore recommended here as a real replacement (gas/oxidizer/geometry) and very stable device for oxyfuel combustion in zero emission power plants. HE1 is better than HE2 and HE3. It was observed that increasing the flame width (from HE1 to HE2) favored the formation of larger flames in HE2, which were more stable than the smaller flames in HE1 at the low adiabatic flame temperature (AFT) of approximately 1658 K.

Researchers have studied the effects of different nozzle parameters, injection medium, ambient temperature and layout on supersonic injection characteristics to achieve the desired design. However, there are some studies on the effect of nozzles on CO2/O2 oxy-fuel combustion. This study covers the effect of the number of nozzles on CO2/O2 oxy-fuel combustion and provides the necessary oxidant concentration to achieve the lowest CO emissions. For this, Ansys Fluent is used.

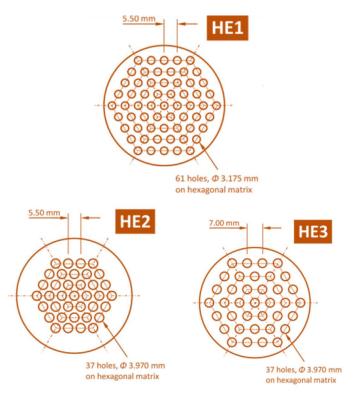


Figure 1. Representing different number of inlets.

# 2. Methodology

The solution is been carried out following 4 steps shows in **Figure 1** starting from Modeling in solid works initial solution in Ansys fluent. Solution of reaction in Energico and Chemkin to solve reaction kinematics.

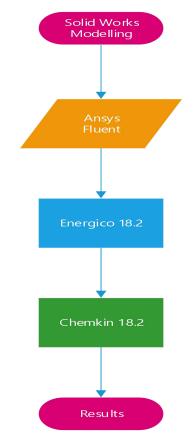


Figure 2. Flow chart showing the process use for numerical simulation.

### 2.1. Mesh

Numerical modeling was carried out in Ansys Workbench using the Fluid Flow (Fluent) software package. To simulate combustion, **Figure 3** shows tetrahedral mesh with maximum and minimum grid size of 0.1 and 3.2 mm shows in **Table 1**.

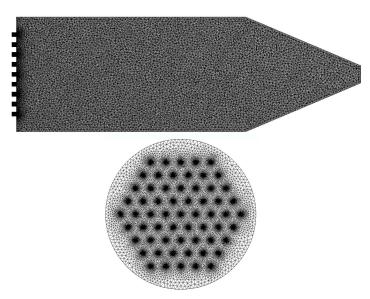


Figure 3. Section of the computational mesh of a combustion chamber with jet burners.

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Grid Size	Values
Minimum Element	0,1 mm
Maximum Element	3,2 mm

### 2.2. Combustion model

RANS k-epsilon turbulence model is chosen with enhance wall treatment. Species transport is partially premix.

In this study, a  $k-\epsilon$  two-equation turbulence model is used. The turbulent kinetic energy equation k is expressed

as follows:

Conservation law for turbulent kinetic energy:

$$\frac{\partial k}{\partial t} + \overline{u} \cdot \nabla k = P - \varepsilon + \nabla \left[ \left( \nu + \frac{\nu_t}{\sigma_k} \right) \nabla k \right]$$

The equation of dissipation rate  $\varepsilon$  is given as follows:

$$\frac{\partial \varepsilon}{\partial t} + \overline{u} \cdot \nabla \varepsilon = C_{1\varepsilon} \frac{\varepsilon}{k} P - C_{2\varepsilon} \frac{\varepsilon^2}{k} + \nabla \left[ \left( \nu + \frac{\nu_t}{\sigma_{\varepsilon}} \right) \nabla \varepsilon \right]$$

Where k – turbulent kinetic energy,  $\varepsilon$  - rate of dissipation of turbulent kinetic energy, P – generation of turbulent kinetic energy,  $v_t$  – Turbulent viscosity

Turbulent viscosity:

$$v_t = C_v \frac{k^2}{\varepsilon}$$

Сν=0.09, σk=1, σε=1.3, С1ε=1.44 и С2ε=1.92

Combustion was modeled with the thin flamelet model by using a partially premixed option in ANSYS FLUENT which can be modified for premixed flame by setting the inlet mixture fraction to a constant value (fuel-to-mixture ratio). In order to indicate that the inlet mixture is a combustible mixture the mixture fraction variance is set 0 by virtue of constant equivalence ratio. Flamelet kinematics and mechanism is import from the directory GRI mech and UOS.

### 2.3. Model combustor setup

Figure 4 shows boundary condition for simulation and performing grid independence test.

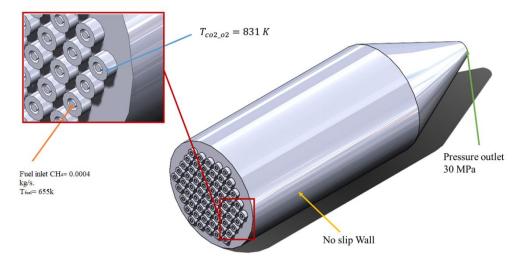


Figure 4. Model used for simulation and its boundary conditions.

The oxidizer inlet mass flow rate is set to be varied depending on the concentration CO2 and O2. For this condition following formula is been considered and oxidizer concentration is denoted by  $\gamma$ 

$$\gamma = \frac{G_{co2}}{G_{co2} + G_{o2}}$$

To find mass flow rate O2 is constant at 0.00176 kg/s. Mass flow rate of CO2 varies with different gamma and as it is partial premix model need to add with mass flow rate of O2.

$$G_{oxidizer=G_{co2}+G_{o2}}$$

### 2.4. Grid independence Test

Grid independence test has been done with different maximum element size and its influence on temperature. It can be seen that after 0.32 cm (i.e. 3.2mm) the change in temperature is negligible although in general with different grid size there is negligible error. However, 3.2 mm is considered most effective solving turbulence model.

Figure 5 shows grid independence test which has been carried using boundary

condition  $\gamma CO2=0.7$  where  $G_{oxidizer=0.005867 kg/s}$ 

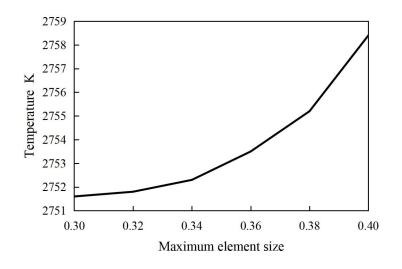


Figure 5. Grid independence test.

### 2.5. Computational domain and boundary condition

The research has been carried out with different inlet diameter and found most effective diameter with minimum underburned hydro carbon and CO emission. Table 2 mention all the diameter studied were carried out before.

N⁰	Fuel supply diameter, mm	Fuel supply speed, m/s	Hydraulic diameter of supply of mixture of oxidizer and diluent	Supply speed of the mixture of oxidizer and diluent, m/s
1. (1,5;2,5;8,5)	1,5	0,05	6	0,03
2. (1,5;2,5;5,25)	1,5	0,05	2,75	0,15
3. (1,5;2,5;5)	1,5	0,05	2,5	0,18
4. (1,5;2,5;4,6)	1,5	0,05	2,1	0,25
5. (1;2,5;4,5)	1,5	0,05	2	0,28

Table 2. Different diameter for inlets of combustion chamber.

As a result of modeling all selected structures, the dependence of the amount of carbon monoxide at the exit from the combustion chamber and the ratio of dynamic pressures of the components was constructed, presented in **Figure 2**. **Figure 3** shows the dependence of the amount of unburned hydrocarbons on the ratio of the dynamic pressures of the components. The dynamic head ratio is calculated using the following formula:

$$\frac{\rho_{ch4}\omega_{ch4}^2}{\rho_{co2\_o2}\omega_{co2\_o2}^2}$$

Where  $\rho$ = Density and  $\omega$  = Velocity

**Figure 6** and **7** shows Increase in dynamic pressure and diameter of inlet amount of emission level and unburned hydrocarbons also increase. Based on these results type 1 is being choose to perform all the simulation and analysis because type 1 has the minimum value of CO emission and unburned hydrocarbons.

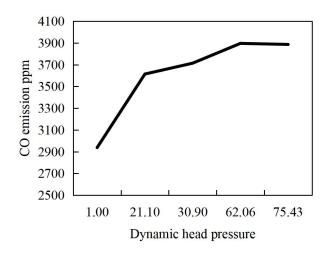


Figure 6. Dependence of the amount of carbon monoxide on the ratio of dynamic pressures of the components.

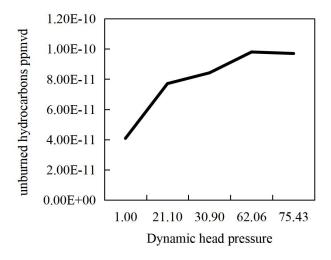


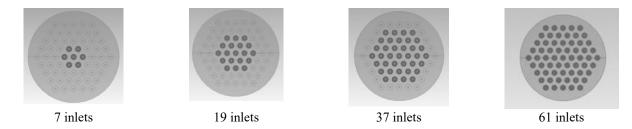
Figure 7. Dependence of the number of unburned hydrocarbons on the ratio of dynamic pressures of the components.

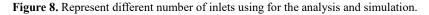
# 3. Result and calculation

#### 3.1. Simulation with different number of inlets

Inlet will be chosen hexagonally and decrease one row in each simulation shown in **Figure 8**. For this the boundary condition are.

The following boundary conditions were adopted: mass flow rates are supplied to the inputs of the components, with initial parameters providing the necessary conditions in the combustion chamber (Gch4 = 0.0004 kg/s, Tch4 = 655 K, Pch4 = 30 MPa; Gco2\_o2 = 0.00898 kg/s, Tco2\_o2=831 K, Pco2\_o2=30 MPa). All mass flow rates are calculated based on the power condition of the carbon dioxide combustion chamber of 15 kW.

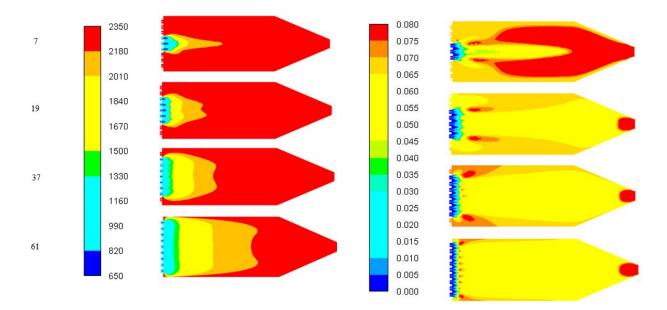




### 3.2. Contours with different number of inlets

In **Figure 9** it is shown that with 61 inlets temperature near the inlet wall is less compared to 7,19 and 37 where temperature near the wall is maximum. Turbulent flame speed with 7 inlets is better uniform compared to 19,37 and 61 when numerically simulated.

In order to create uniformity in turbulent flame speed, numerical simulation is performed with different concentration of oxidizer blend.



a) Temperature (K) with different number of inlets 7,19,37 and b) Turbulent flame speed (m/s) with different number of inlets 7,19,37 and 61

Figure 9. Representing contours with comparing with different number of inlets.

Results of different numbers of inlet.

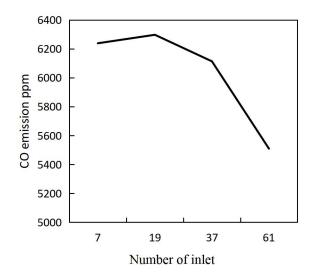


Figure 10. CO emission at outlet with different number of inlets.

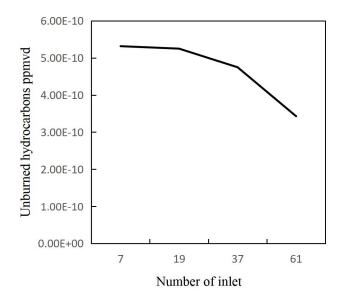


Figure 11. Unburned hydrocarbons at outlet with different number of inlets.

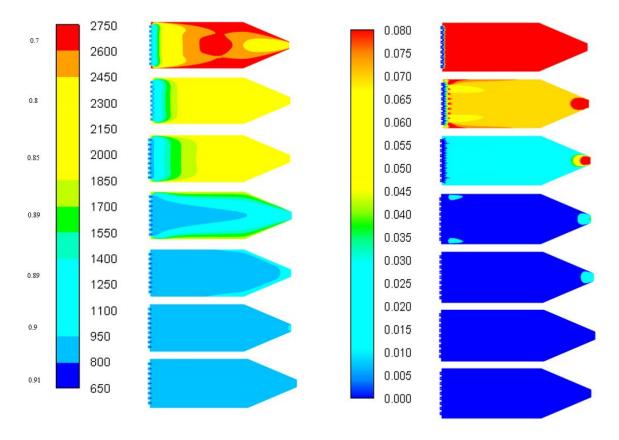
In order to summaries results it can be seen that with increasing in number of inlets both the emission levels and unburned hydrocarbons is significantly decreasing. Based on above

results 61 inlets is being choose to perform all the simulation and analysis because 61 inlets have the minimum value of CO emission and unburned hydrocarbons.

### **3.3.** Contours with different oxidizer concentration ( $\gamma$ )

It can be seen in **Figure 12** that by increasing the concentration of CO2 temperature is decreasing, which could allow burner to be design with low and cost-effective materials. It can also be notice that flame is diffusing at 0.895 due to the insufficient ratio of oxygen in oxidizer at  $\gamma$  0.895 about 89.5% is CO2 and 11.5% of O2.

Through this it could be easier to choose a range of concentration with required temperature and flame speed. it is also studied that during the numerical result between 0.8-0.85 range fuel and oxidizer is well mixed. At 0.91 there is there is no combustion as can be seen the turbulent flame speed is zero and inlet temperature is equal to burner temperature. At 0.9 there is a temperature but without any flame.



a) Temperature (K) with different  $\gamma$ 

b) Turbulent flame speed (m/s) with different  $\gamma$ 

**Figure12.** Representing contours with different values of  $\gamma$ .

### Results with different $\gamma$ .

γ	Unburned Hydrocarbons at outlet
0,7	5.82x10 <sup>-9</sup>
0,8	4x10 <sup>-12</sup>
0,85	5.56x10 <sup>-9</sup>
0,89	8.28x10 <sup>-3</sup>
0,895	6,91
0,9	70,45
0,91	479,18

Table 3. Unburned hydro carbons with different concentration of oxidizer.

Table 4: CO emission	with different	concentration	of oxidizer
		concentration	OI UNIGIZOI

γ	CO emission at outlet ppm	
0,7	10539,64	
0,8	1315,67	
0,85	301,04	
0,89	0,34	
0,895	263,44	
0,9	743,99	
0,91	1662,768	

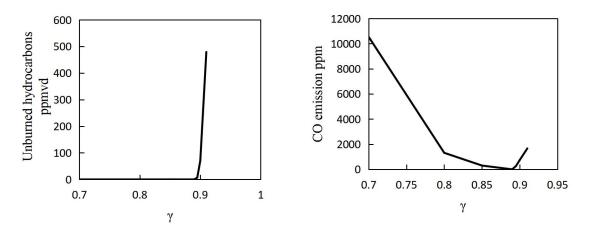


Figure 13. Unburned hydrocarbons at outlet with different value of  $\gamma$  (concentration).

Figure 14. CO emission at outlet with different value of  $\gamma$  (concentration).

If summaries, it can be seen that between 0.8-0.85 the flame speed temperature is in normal range along with minimum CO emission and minimum unburned hydrocarbon in outlet.

# 4. Conclusion

- Choosing maximum number of inlet because it provides minimum emission and unburned hydrocarbons at outlet
- It is been notice during simulation that the most effective value where we have minimum unburned hydrocarbons and CO emission is in between the range of 0.8-0.85.
- It is observed that between 0.8-0.85 flame and temperature is stable.
- It is also seen that by increasing concentration of CO2 temperature decreases also flame speed.
- It is confirming that at 0,915 there is no reaction and flames speed is also 0 which is also confirms from energico reactions.

### **Author Contributions**

Conceptualization, SO and IK; methodology, SO; software, MMS; validation, MMS, PG; formal analysis, SO; investigation, MMS, ANR; resources, SO; IK, writing—original draft preparation, MMS; writing—review and editing, SO; visualization, PG; supervision, IK; project administration, SO; funding acquisition, SO. All authors have read and agreed to the published version of the manuscript.

# **Conflict of interest**

The authors declare no conflict of interest.

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