Effects of mesh type on a non-premixed model in a flameless combustion simulation

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Abstract. Flameless combustion is a recently developed combustion system, which provides zero emission product. This phenomenon requires auto-ignition by supplying high-temperature air with low oxygen concentration. The flame is vanished and colorless. Temperature of the flameless combustion is less than that of a conventional case, where NOx reactions can be well suppressed. To design a flameless combustor, the computational fluid dynamics (CFD) is employed. The designed air-and-fuel injection method can be applied with the turbulent and non-premixed models. Due to the fact that nature of turbulent non-premixed combustion is based on molecular randomness, inappropriate mesh type can lead to significant numerical errors. Therefore, this research aims to numerically investigate the effects of mesh type on flameless combustion characteristics, which is a primary step of design process. Different meshes, i.e. tetrahedral, hexagonal are selected. Boundary conditions are 5\% of oxygen and 900 K of air-inlet temperature for the flameless combustion, and 21\% of oxygen and 300 K of air-inlet temperature for the conventional case. The results are finally presented and discussed in terms of velocity streamlines, and contours of turbulent kinetic energy and viscosity, temperature, and combustion products.

1. Introduction
Flameless combustion is a recently developed combustion system, which provides zero emission product. According to work done by Gupta and Arghode [1], flameless combustion is developed from a high temperature air combustion (HiTAC) in an industrial furnace. This technology is investigated to apply with a high thermal intensity gas turbine in a term of flameless oxidation or colorless distributed combustion (CDC). This phenomenon provides ultra-low NOx of about 1 ppm and reduces carbon-monoxide (CO) emission at the operation point. Flameless combustion is promoted by controlling hot product gas recirculation to provide fast fuel/oxidizer mixing at high temperature, which results in a distributed combustion condition, and avoid hot spot region formed in gas turbine combustor.

Flameless combustion is commonly designed in non-premixed combustion regime in order to discretely and directly inject oxidizer and fuel in a confined volume to avoid the direct mixing and reaction of fuel and combustion air prior to the operation point. Fast diluted of oxidizer and internal recirculation are turbulent flow phenomena which induced reactants to form a turbulent-combustion couple relation.

Abuelnuor et al. [2] mention that flameless oxidation reactions are combustion with oxidizer dilution inlet, and the oxygen concentration must be reduced to below 7\% to suppress the peak temperature along
with internal recirculation inside a combustion chamber to maintain stable combustion. At low oxygen concentration environment, it is difficult for the combustion to occur. To overcome this problem, the inlet air must be preheated until it is reached a fuel auto-ignition temperature in order to sustain the oxidation reaction. When these two conditions meet, the flame is suddenly vanished and the peak temperature is decreased to around 1,000-1,300 K, the reaction is distributed entirely over the combustion region and the emission is suppressed to zero emission.

Duwig et al. [3] used planar laser-induced fluorescence (PLIF) and Rayleigh scattering measurements to study turbulent combustion interactions in distributed reaction regimes of flameless combustion in a laboratory-scale jet burner. Oxygen depletion reactions are varied from equivalent ratio 0.8 to a very lean case at 0.4. All cases are observed by detecting CH$_2$O/OH signal. The results indicated a complex and intermittent interplay between turbulent flow and chemical reaction involving a coherent structure arising in a jet shear layer. They concluded that a stronger intermittent and the high dilution drive the invisible reaction in a particular case.

Hossieni et al. [4] investigate biogas flameless combustion by applying numerical simulation. They used standard k-ε model with the two-step combustion model developed by Westbrook and Dryer (WD model). This model consists of combustion reaction in equation (1) and oxidation of carbon-monoxide (CO) and carbon-dioxide (CO$_2$) reaction in equation (2) including with gas phase kinetic file from Arrhenius equation in equation (3) where $A_i$ is pre-exponential factor $\beta_i$ is temperature coefficient and $E_i$ is activation energy.

Combustion reaction:

$$CH_4 + \frac{3}{2}O_2 \rightarrow CO + 2H_2O$$

(1)

Carbon-dioxide oxidation reaction:

$$CO + 1/2O_2 \leftrightarrow CO_2$$

(2)

Arrhenius equation:

$$k_{fi} = A_iT^{\beta_i}exp(-\frac{E_i}{RT})$$

(3)

Arrhenius equation describes a reaction rate in energy form. The fluctuation combustion can be solved from a standard k-ε model and energy equation. Arrhenius equation is weakly implied turbulent combustion phenomena present in a real flameless combustion. Mancini et al. [5] investigates a flameless burner with a strong oxidizer jet and two weak natural gas jets by simulation method. The Reynolds-Averaged Navier-Stokes equation (RANS) and the eddy break up sub-model with two step reaction scheme are applied to predict turbulent non-premixed behavior. They found that the error in predictions of the entrainment was caused by a combustion reaction that slightly occurs within the natural gas jets. The temperature rises within the fuel jets resulting from the entrainment of the hot combustion products. These results present the failure of RANS equation with the two-step reaction scheme.

Pope [6] introduced a PDF method for a turbulent reactive flow where turbulent and combustion are distributed over a probability density function (PDF) which developed from the Heaviside and Dirac delta function adaptation (4)-(6). Pope [6] also proposed that a mean and variance of any parameters such as velocity, temperature and mixture fraction can be described as in equation (7)-(11), respectively. Mean and variance can then be distributed in PDFs as defined in equations (12) and (13) called a joint-PDF equation. This PDF can be coupled solving with other parameters such as pressure, enthalpy and radical mixture which is more approached to a real turbulent combustion regime.
Heaviside function (Unit step function) is
\[ H(y) = \begin{cases} 
0, & y \leq 0, \\
1, & y > 0, 
\end{cases} \]  
(4)

Dirac delta function (Impulse function) is a derivative of Heaviside function as
\[ \delta(y) = \frac{dH(y)}{dy} \]  
(5)

The distribution of Dirac delta function is
\[ \int_{-a}^{a} \delta(y) dy = H(a) - H(-a) = 1 \]  
(6)

Distribution function of velocity as a probability density function (PDF) generating from the distribution of Dirac delta function is
\[ F_{u}(V) \equiv P(U < V) \]  
(7)

Derivative of the distribution function of velocity is
\[ f_{u}(V) \equiv \frac{dF_{u}(V)}{dV} \]  
(8)

Mean velocity distribution \((U)\) is given by
\[ < U > = \int_{-\infty}^{\infty} V f_{u}(V) dV \]  
(9)

Variance of \(U\) can be written as
\[ D(U) = < u^{2} > = \int_{-\infty}^{\infty} (V - < U >)^{2} f_{u}(V) dV \]  
(10)

where \(u\) is a velocity fluctuation as
\[ u \equiv U - < U > \]  
(11)

PDF distribution function \(Q\) of mean velocity \(U\) and mean temperature \(\phi\) (joint PDF equation) is
\[ < Q(U, \phi) > = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} Q(V, \phi) f_{u\phi}(V, \phi) dV d\phi \]  
(12)

where \(f_{u\phi}(V, \phi)\) is a derivative of probability density function (PDF) \(F_{u\phi}(V, \phi)\) represent in
\[ f_{u\phi}(V, \phi) = \frac{\partial^{2} F_{u\phi}(V, \phi)}{\partial V \partial \phi} \]  
(13)

Ren et al. [7] applied the PDF method for solving turbulent non-premixed flame problem by comparing the method between an eddy dissipation concept (EDC) and PDF. The results demonstrate that EDC predicted a thinner flame with higher flame temperature than the PDF method. Compared with experiment data, EDC provides over-prediction for flame temperature and OH concentration while PDF model yields more accurate prediction.

The literature review above shows the relation between combustion and turbulence. Both are random base phenomena which required a proper type of mesh. Selecting an improper mesh can lead to numerical error caused by fluctuating parameters. Therefore, this research aims to identify suitable meshing in terms of mesh types, namely tetrahedral and hexagonal, with turbulent non-premixed combustion model (PDF model) for a flameless combustion simulation then compares and discusses results from each case.

2. Methodology
This study is a part of a flameless combustion design for industrial application. Flameless combustion is a new type of combustion with high efficiency with zero emission. This combustor could play a major role in a future technology for gas turbine or drying process heat source. The design uses computational fluid dynamics (CFD) to simulate phenomena inside a combustor. Mesh selection is the first major step
before varying other parameters in a further calculation process to prevent inaccurate results. The study of mesh effects started by selecting a geometrical model (refer to Hossieni et al. [3]) as demonstrated in figure 1. The model has full length of 600 mm and a 5-mm single fuel inlet hole at the center surrounding by 8 holes of air inlet with the same diameter. The outlet diameter is 50 mm.

![Fluid domain and its dimensions](image1.png)

**Figure 1.** Fluid domain and its dimensions

Next mesh types are selected as tetrahedral and hexagonal in figures 2 and 3, respectively. Both mesh types are generated by ANSYS 16.2 meshing and note that hexagonal mesh is constructed by multi-zone meshing method. Then mesh quality is adjusted by advanced sizing function: proximity and curvature. The number of elements is 270,312 elements which is comparable to Hossieni et al. [3]. The mesh edge sizing effect is also included. The boundary condition at inlet for flameless mode and conventional mode are shown in table 1. Biogas is applied as fuel for both cases.

![Tetrahedral mesh generated by ANSYS meshing](image2.png)

**Figure 2.** Tetrahedral mesh generated by ANSYS meshing
Figure 3. Hexagonal mesh generated by ANSYS meshing

Table 1. Boundary condition

| Boundary Conditions                  | Value                          |
|--------------------------------------|--------------------------------|
| Biogas Composition                   | CH\(_4\) 60\%, \text{CO}_2 40\%|
| Oxidizer Composition (Flameless mode)| N\(_2\) 95\%, \text{O}_2 5\%    |
| Oxidizer Composition (Conventional mode)| N\(_2\) 79\%, \text{O}_2 21\%  |
| Inlet Air Temperature (Flameless mode)| 900K (627\(^\circ\)C)          |
| Inlet Air Temperature (Conventional mode)| 300K (27\(^\circ\)C)          |
| Inlet Fuel Temperature               | 300K (27\(^\circ\)C)          |
| Equivalent ratio \(\phi\)            | 1                              |
| Pressure                             | 1 atm                          |
| Inlet air speed                      | 30 m/s                         |

For turbulent model, the RNG k-\(\varepsilon\) model is chosen along with energy equation, as shown in equations (14)-(21), and a PDF non-premixed combustion. This PDF method of ANSYS FLUENT 16.2 is developed by Pope [6]. In each iteration, PDF method is solved by calculating mean mixture fraction and mixture fraction variance in equations (19) and (20), respectively. Then, it uses both parameters to create a beta function as in equations (22)-(24) (see figure 4), instead of Dirac delta function as in Pope [6]. PDF function is mapped into other parameters such as enthalpy, pressure, velocity by equation (12) which prior solving from turbulent model and energy equation. This represents the randomness and interconnection between turbulent and combustion phenomena. The results are compared with species transport methane-air 2 step in equations (1)-(3). Second-order upwind numerical scheme is applied in all cases. Finally, all results are compared and discussed.

Continuity equation:

\[
\frac{\partial \rho}{\partial t} + \nabla (\rho \vec{v}) = 0
\]  

(14)

RNG k-\(\varepsilon\) turbulent model – k equation:

\[
\frac{\partial}{\partial \tau} (\rho k) + \frac{\partial}{\partial x_i} (\rho k u_i) = \frac{\partial}{\partial x_j} \left( \alpha_k \mu_{eff} \frac{\partial k}{\partial x_j} \right) + G_b + G_k - \rho \varepsilon - Y_M
\]  

(15)

RNG k-\(\varepsilon\) turbulent model – \(\varepsilon\) equation:

\[
\frac{\partial}{\partial \tau} (\rho \varepsilon) + \frac{\partial}{\partial x_i} (\rho \varepsilon u_i) = \frac{\partial}{\partial x_j} \left( \alpha_k \mu_{eff} \frac{\partial \varepsilon}{\partial x_j} \right) + c_1 \varepsilon \frac{\varepsilon}{k} (G_k + C_3 \varepsilon G_b) - C_2 \varepsilon \rho \frac{\varepsilon^2}{k} - R_e
\]  

(16)

Ideal gas equation:

\[ P = \rho RT \]  

(17)
Energy equation in term of enthalpy (H) of all species:
\[
\frac{\partial}{\partial t} (\rho H) + \nabla \cdot (\rho \mathbf{v} H) = \nabla \cdot \left( \frac{k_t}{\sigma_t} \nabla H \right)
\] (18)

Mean mixture fraction in term of atomic mass fraction:
\[
f = \frac{Z_i - Z_{i,\text{LOX}}}{Z_{i,\text{fuel}} - Z_{i,\text{LOX}}}
\] (19)

Mean mixture fraction transport equation:
\[
\frac{\partial}{\partial t} (\rho f \tilde{f}) + \nabla \cdot (\rho \mathbf{v} f \tilde{f}) = \nabla \cdot \left( \frac{\mu_t}{\sigma_t} \nabla f \tilde{f} \right)
\] (20)

Mixture fraction variance transport equation:
\[
\frac{\partial}{\partial t} (\rho f'^2 \tilde{f}^2) + \nabla \cdot (\rho \mathbf{v} f'^2 \tilde{f}^2) = \nabla \cdot \left( \frac{\mu_t}{\sigma_t} \nabla f' \tilde{f} \right) + C_g \mu_t (\nabla \tilde{f})^2 - C_d \rho \frac{\tilde{f}^2}{k} f'^2
\] (21)

Beta function PDF:
\[
P(f) = \frac{f^{\alpha-1}(1-f)^{\beta-1}}{I_0^{\alpha-1}(1-f)^{\beta-1} df}
\] (22)

where \(\alpha\) and \(\beta\) are:
\[
\alpha = \tilde{f} \left[ \frac{f(1-f)}{f'\tilde{f}^2} - 1 \right]
\] (23)
\[
\beta = (1 - \tilde{f}) \left[ \frac{f(1-f)}{f'\tilde{f}^2} - 1 \right]
\] (24)

**Figure 4.** Beta function probability density function

The difference in each case is observed by contour and streamline plots of the following parameters: velocity, temperature and turbulent parameters. They are also compared with theoretical values from literature review mentioned above. The conclusion is expected to provide a guidance for further flameless simulation in term of mesh types and turbulent combustion model selection.

3. Results discussion
3.1 Mesh types comparison
The simulation results indicate that tetrahedral mesh is sensitive to the randomness of turbulent fluctuation than hexagonal mesh as seen in both the temperature distribution in figure 5 and streamlines.
in figure 6. Figure 5 demonstrates a rough result of flameless and conventional modes. In flameless mode, the peak temperature is suppressed by the effect of dilution oxidizer and temperature is rapidly dropped, but in conventional mode the peak temperature arises by a concentrated oxidizer and fuel. PDF method demonstrated the strongly turbulent interplay between streamlines and temperature distribution. The randomness jumping between tetrahedral mesh causes streamline and internal recirculation distort in both cases with severely induced temperature distribution that represent an unstable combustion zone. Flameless combustion is the most stable combustion phenomena, so the tetrahedral mesh prediction is substantially unacceptable, the turbulent randomness has extremely effected on this mesh type.

The hexagonal mesh shows more stable results. In figure 7, the temperature distributions show the distinction between flameless and conventional modes. In flameless mode, temperature is distributed symmetrically across the entire combustor and temperature is drastically dropped compared to a conventional one which characterizes the flameless phenomena. The peak temperature in conventional mode is confined only in a small range of combustion regions. In figure 8, the streamlines is fully aligned along the combustion length. It is concluded that the randomness in turbulent scheme has less effect on this mesh type. The internal recirculation is not severely distorted as in a tetrahedral mesh. The turbulent
combustion still has a major interplay by inducing the temperature distribution as a streamline-contour mapping in figure 8. The results show a successful prediction of flameless combustion in agreement with literature review mentioned earlier.

![Temperature Contour](image)

**Figure 7.** Temperature distribution contour comparison of Hexagonal mesh case for flameless mode and conventional mode.

![Velocity Streamline](image)

**Figure 8.** Streamline comparison of Hexagonal mesh case for flameless mode and conventional mode.

### 3.2 The effect of edge sizing

In the last subsection, the results show that hexagonal mesh has a more reliable result than the tetrahedral type due to the less sensitivity to turbulent randomness. In this section, the hexagonal mesh is further improved by using edge-sizing functions to vary the details of edge sizing as demonstrated in figure 9. Edge sizing 1 sets the number of division around combustor circumference to 30. Edge sizing 2 is a biased division along combustion chamber length with a bias type shown in figure 9 with a bias factor 30. Finally, edge sizing 3 sets around all of inlet holes circumference with number of division 10. The boundary condition is similar to the latest cases with biogas fuel. The number of elements is 260,805 elements which is comparable to 270,312 elements in Hossieni et al. [3]. The PDF model and RNG turbulend3 scheme are also applied.
When applying an edge-sizing function, the temperature results represented more smoothly distribution in both flameless and conventional mode. Streamlines arrangement is more symmetrical than the case without edge sizing function. Now the turbulent kinetic energy is included in the results. In conventional mode, turbulent kinetic energy has a strong influence on flow pattern than flameless mode. In flameless mode, fuel stream flow is weaker causing the internal recirculation to form more symmetric flow patterns. In contrast, stronger fuel stream in conventional mode causes streamlines collision within reaction zone which increases turbulent kinetic energy.

**Figure 9.** Position of edge sizing

**Figure 10.** Temperature, Turbulent kinetic energy contour and streamline after using edge sizing functions.
3.3 The effect of turbulent combustion model

The combustion model is compared between two-step species transport model and PDF model for non-premixed combustion. Hexagonal mesh type and edge sizing function mentioned in subsection 3.2 are applied to each case. In figure 11, the results show that both models can be used to superficially estimate flameless combustion characteristics. The difference of these two models can be detected when observed deeply in a turbulent scheme. In flameless case, the two-step model has less influence to turbulent than PDF model. Two-step model represents the less large scale fluctuation when observed from streamlines which causes less disturbance to a temperature distribution. In contrast, the non-premixed model results in less turbulent kinetic energy but more disturbed in streamlines and excessively interplay with combustion reaction.

Two-step species transport with RNG k-ε  
PDF non-premixed model with RNG k-ε  

Figure 11. Comparison of two-step species transport and PDF non-premixed combustion for flameless combustion in term of temperature contour and velocity streamlines.

In figure 12, several parameters along the longitudinal axis are collected and analysed including temperature, velocity, O₂, CO₂, CO mass fraction and turbulent kinetic energy. The results from conventional and flameless cases are compared in both two-step species transport and PDF non-premixed combustion models which show similar trend of velocity and temperature along an axis. Two-step species transport indicate a slightly over-predicted turbulent kinetic energy but still maintain a similar trend to the PDF model in both cases. Mass fraction of conventional cases has major effects from altering turbulent combustion model than flameless cases, especially on CO₂ – CO reaction in peak temperature zone. Two-step species transport predict more CO₂ and less CO in combustion region. In contrast, PDF model shown less CO₂ production at peak temperature but more CO which indicate an incomplete combustion. In fact, CO₂ – CO reaction is the slowest chemical reaction of all combustion mechanism which require more reaction time. Two-step model predicted reaction faster than expect, this could be a noticeable results for further calculation.
Figure 12. Comparison of two-step species transport and PDF non-premixed combustion in terms of temperature, velocity, CH₄, CO₂, CO, O₂ mass fraction, turbulent kinetic energy and enthalpy of both flameless and conventional cases. CC = Conventional Case and FC = Flameless Case.
4. Conclusion
This research studies the effect of mesh types for simulations of flameless turbulent non-premixed combustion. Mesh effect study is important to investigate prior to a further design process. An inappropriate mesh selection can lead to significantly inaccurate results. The study chooses two types of mesh which are tetrahedral and hexagonal to simulate with boundary condition of 5% of oxygen and 900 K of air-inlet temperature for the flameless combustion, and 21% of oxygen and 300 K of air-inlet temperature for the conventional case. Applying Probability Density Function (PDF) method for non-premixed turbulent combustion in both mesh types and boundary conditions. PDF method is a simulated randomness from beta function that distribute on others parameters such as velocity, temperature and mass fraction to represent turbulent flow behaviour.

The results concluded that tetrahedral mesh is an inappropriate mesh type for turbulent combustion due to its high sensitivity to turbulent randomness. Hexagonal represents more stable solution in streamlines with less disturbed from turbulence. However, turbulent randomness affected conventional combustion than flameless combustion due to collision of a high velocity fuel and oxidation stream in a combustion regime. Hexagonal mesh is chosen to study edge sizing by applying edge sizing function around combustor and inlet holes circumference with edge bias along combustor centreline. The results from edge sizing function give more stable combustion for both flameless and conventional cases.

Finally, the turbulent combustion models are compared. Two-step species transport and PDF turbulent non-premixed model are applied to both flameless and conventional combustions. The results demonstrated the similarity of two model on predicting large scale phenomena. The results are slightly different due to turbulent interplay. Flameless cases again admit less effect from altering turbulent combustion model than the conventional one. Note that CO₂ – CO reaction has different prediction in both turbulent combustion model in conventional mode. Two-step species transport predict the formation of CO₂ significantly higher than PDF model in combustion zone around peak temperature region, indicating the difference in residence time prediction of reaction that could be noticeable in a further work.

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