Computational fluid dynamics simulation to predict the effect of the equivalence ratio on the temperature distribution in a pyrolysis furnace

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Abstract. This research investigated numerically the effect of the equivalence ratio on the temperature distribution in an industrial non-premixed flat flame burner with methane as the fuel. The burner configuration is a wall-fired one to produce a flat flame with a large cross-sectional area to effectively radiate heat to tubes contained in a pyrolysis furnace. The temperature distribution was predicted by using a phenomenological model consisting of mass balance, energy balance and momentum balance with computational fluid dynamics approach. Fluid flow was explained by the $k-\varepsilon$ turbulent momentum balance, and the reaction rate was approached to eddy dissipation model. Simulation results show that the change in the equivalence ratios affects the temperature distribution so that this variable needs to be adjusted with certain considerations for pyrolysis process.

1. Introduction
Some equipment in process industries need to be heated, and most heat sources come from burners. In the early 1800s, furnaces were simply equipped with input air and gas, and then the two streams were mixed and burned in furnaces. This process worked well to obtain the desired temperature of furnaces, but this approach was not suitable for many applications. The resulting flame was often too large, the mixing was slow, and in gases with low heating values flame often was not produced, unless the furnace temperature is high or the input air/gas was preheated. The necessity to obtain a combustion process with better gas/air mixing, intensity and flame stability is one of the trigger factors to develop burners so far. One of the factors influencing combustion processes is equivalence ratio, which is the ratio between fuel and air.

Pyrolysis is a process utilizing heat from burners to produce olefins from hydrocarbon molecules. The process involves gas phase reactions take place inside tubes made of special alloys located in a furnace. Pyrolysis reactions is very endothermic. Therefore, non-premixed burners were used to generate high-temperature flame transferring heat to tubes by radiation. The general situation of a combustion process in a pyrolysis furnace with a burner can be seen in figure 1. Burners are arranged in parallel with generated flame facing pyrolysis tubes (black colour in the figure 1) arranged side by side.
In order to engineer a combustion process generating flat flame many aspects need to be considered, among others are process parameters and geometry parameters. Engineering works will be easier and cheaper if simulation methods are used. Researches on simulation related to flat flame have been carried out by several researchers. Schoegl simulated radiation effects on automatic stabilization on burners [1]. They used a one-dimensional energy balance with radiation heat being modelled by a radiative diffusion approximation. Moghaddam et al. investigated geometric parameter effect on thermal efficiency and pollution emission in a multi-hole flat flame burner [2]. They used a two-dimensional model consisting of continuity equation, momentum transfer equations and mass transfer equations. Francisco Jr et al. were curve-fitted measurement results of laminar flame velocity using a flat flame burner to a flame asymptotic model assuming one-step reaction. Their work estimated adiabatic flame velocity and its corresponding overall activation energy [3]. Lazic et al. investigated numerically the effect of the change in a furnace chamber height on heat transfer rate in a furnace enclosure [4]. The formulation of mathematical model of heat exchange in the furnace was based on a well-stirred zone model consisting of a system of simultaneous energy balance equations for the volume and surface zones. Mayr et al. used computational fluid dynamics (CFD) to investigates a semi-industrial furnace fired by a natural gas flat flame burner, which operates under different O/N ratios in an oxidizer [5]. The simulations were confronted with temperature measurements inside the furnace and with measurements of the surface temperature of a quarl.

There are many correlations between fluid dynamics and chemical reactions in a burner [6]. In order to generate flames with large surface area suitable for pyrolysis processes in an industrial furnace fired by a methane flat flame burner, the present research coupled fluid dynamics, mass and heat transfers as well as chemical reactions in a three-dimensional furnace system into a set of transport equations and then solved numerically. The effect of the equivalence ratio on the flame form was investigated. COMSOL Multiphysics modelling software was used to simulate the model.

2. Modelling

In order to ease convergent calculations, the following assumptions were considered:

- The burner was an industrial non-premixed one with 100% methane as the fuel.
- The system operated in steady state.
- The flame form was identified by observing the temperature distribution in the furnace.
- A global combustion reaction was used.
- Eddy-dissipation model was considered, rather than chemical kinetic model.
- Fluid mixing was dominated by convection.
- The energy balance taken into account only heat conduction and convection.
- The model geometry was half burner with one side of symmetry.
The geometry of the flat flame burner in this study refers to Baukal [7]. The basic geometry of the flat flame burner is in accordance with figure 2. The arrangement of the burners and the pyrolysis tubes in the pyrolysis furnace can be seen in figure 3, which is the top view of figure 2. The red line in figure 3 is the system boundary to be modelled in this study.

The system was simplified and drawn in COMSOL as a three-dimensional furnace box containing half burner with its symmetry plane being at the \( x = 0 \) plane, as can be seen in figure 4. Figure 4(a) is the three-dimensional drawing of the system bounded by the red line in figure 3, and figure 4(b) is the half burner drawing. The size of the system is \( 10 \times 15 \times 50 \) cm.

Fuel enters the burner through five inlets: the left main fuel inlet, the middle main fuel inlet, the right main fuel inlet and two wing fuel inlets. In the system being modelled, the left main fuel inlet and the right main fuel inlet are mirrors of each other so that only one of them, i.e. the left main fuel inlet was drawn. The main fuel inlet was divided into two equal halves. Two wing fuel inlets were represented by one of them. Air enters from the centre of the burner.

![Figure 2](image2.png)  
**Figure 2.** The basic geometry of the flat flame burner [7].

![Figure 3](image3.png)  
**Figure 3.** The top view of the system boundary [7].

![Figure 4](image4.png)  
**Figure 4.** The geometry of (a) the part of the furnace and (b) the half burner.
2.1. \( k-\varepsilon \) turbulent momentum balance

Model describing the turbulent flow phenomenon in the furnace is as follows [8, 9]:

\[
\rho (u \cdot \nabla) u = \nabla \left[ -p I + (\mu + \mu_T)(\nabla u + (\nabla u)^T) - \frac{2}{3} \rho k I \right] + F
\]

(1)

\[
\rho (u \cdot \nabla) k = \nabla \left[ (\mu + \frac{\mu_T}{\sigma_k}) \nabla k \right] + P_k - \rho \varepsilon
\]

(2)

\[
\rho (u \cdot \nabla) \varepsilon = \nabla \left[ (\mu + \frac{\mu_T}{\sigma_\varepsilon}) \nabla \varepsilon \right] + C_{\varepsilon_1} \frac{\varepsilon}{k} P_k - C_{\varepsilon_2} \rho \frac{\varepsilon^2}{k}
\]

(3)

where \( \rho \) is the fluid density, \( u \) is the velocity, \( p \) is the pressure, \( \mu \) is the fluid viscosity, \( g \) is the gravitational force, \( F \) is the other additional force, \( k \) is the turbulence kinetic energy and \( \varepsilon \) is the turbulence dissipation.

The turbulent/eddy viscosity is described by

\[
\mu_T = \rho C_\mu \frac{k^2}{\varepsilon}
\]

(4)

2.2. Mass balance

Mass balance involving five components of the combustion, \( \text{CH}_4, \text{O}_2, \text{N}_2, \text{CO}_2 \), and \( \text{H}_2\text{O} \), is as follows:

\[
(u \cdot \nabla c_j) = \nabla \cdot (D_j \nabla c_j) + R_j
\]

(5)

where \( c_j \) is the \( i \)-species concentration, \( D_j \) is the \( i \)-species diffusion coefficient and \( R_j \) is the \( i \)-species reaction rate.

The following global combustion reaction of methane with air was used:

\[
\text{CH}_4 + \frac{2}{\phi} \left( \text{O}_2 + 0.79 \text{N}_2 \right) \rightarrow \text{CO}_2 + 2\text{H}_2\text{O} + a\text{O}_2 + \frac{2}{\phi} 0.21\text{N}_2
\]

(6)

where \( \phi \) is the equivalence ratio and \( a \) is stoichiometric coefficient of excess oxygen. The combustion reaction was approached by Eddy dissipation model involving the following equation:

\[
R_A = AB \frac{\varepsilon}{k} \min \left( C_{\text{CH}_4} \frac{C_{\text{O}_2}}{2}, 0.5 \times \frac{C_{\text{CO}_2} + C_{\text{H}_2\text{O}}}{3} \right)
\]

(7)

2.3. Energy balance

Energy balance in the furnace involves heat convection and conduction, which is expressed as follows:

\[
\rho \dot{c}_p \mathbf{u} \cdot \nabla T = \nabla \cdot (k \nabla T) + Q
\]

(8)

where \( T \) is the temperature, \( \dot{c}_p \) is the fluid heat capacity, \( k \) is the heat conductivity and \( Q \) is the reaction heat.

Those transfer equations were solved numerically step by step to achieve convergent results. First, the turbulent flow equations were solved to estimate the velocity. The calculated velocity was then used as the input to the mass transfer equations, then solved to predict the species concentrations. The calculated species concentrations were inputted to the heat transfer equation to assess the temperature. With the step by step calculations, the density and viscosity in the mass and momentum transfer equations were set constant by taking the properties of the combustion products in the stoichiometric state.
3. Results and discussion

In order to find out the effect of the equivalence ratio on the temperature distribution in the furnace, the equivalence ratio was varied. Equivalence ratio is the actual fuel-to-air ratio relative to the stoichiometry ratio. As shown in the figure 4, the middle and left main fuel inlets are located in the area of the air inlet. The inlet tips are tilted towards the fired wall with the 57° angle to the horizontal plane. The wing fuel inlet is also tilted with the 68° angle to the horizontal plane.

The inlet air velocity is 42.6 m/s, and the inlet fuel velocity is 21.3 m/s. The simulation results are shown in figure 5.

![Figure 5. The temperature profiles at the equivalence ratios of (a) 0.6, (b) 1.0, (c) 1.4 and (d) 3.0.](image)

The temperature in the vertical direction for the equivalence ratio of 0.6 is more unevenly distributed than that at 1.0. This happens because the excess air for the equivalence ratio of 0.6 gives a quenching effect on the flue gas. The heat released by the combustion reaction is partly used to increase the temperatures of the combustion products and the unconverted fuel. Since more excess air exists for the equivalence ratio of 0.6, more molecules absorb heat, leading to lower adiabatic flame temperature. As a result, the temperature distribution in the vertical direction is rather unevenly distributed. The temperature decreases relative to the furnace height.

The decrease in the temperature to z-direction (vertical) was evaluated along three red vertical lines, i.e. at \( x = 0 \) m, \( x = 2.7 \) m and \( x = 5.4 \) m the symmetry plane as can be seen in figure 6. The temperature profile in various equivalence ratios can be seen in figure 7.

For the equivalence ratios of 0.6, 1.0 and 1.4, the highest temperature occurs at the line \( x = 0 \). This line is located at the symmetry plane of the model system. The temperature decreases along the \( x \) direction. This happens because the less fuel molecules are burned at locations farther from the symmetry plane in \( x \) direction. From the burner upwards, the temperature increases. The temperature reaches its peak at different heights, depending on \( x \) positions. At \( x = 0 \), the peak temperature is at the height of 3 m - 4 m. The highest peak temperature exists for the equivalence ratio of 1.0, i.e. 2500 K, indicating that the combustion at this ratio is the most efficient. The peak temperature in the lean mixture is slightly below the stoichiometric mixture, indicating that the almost complete combustion reaction occurs. After reaching the peak, the temperature decreases. The cause of the decrease depends on the equivalent ratio. In the fuel lean mixture, the decrease in the temperature due to the quenching is more dominant than the heat transport in the \( y \) direction. In the stoichiometric mixture and the fuel rich mixture, the decrease in the temperature is caused by the heat transportation in the \( y \) direction. This is also as the basis of the steepest decline of the temperature curve at the fuel lean mixture.
Figure 6. The location of the red lines for temperature analysis at (a) $x = 0$ m, (b) $x = 2.7$ m and (c) $x = 5.2$ m from the symmetry plane.

Figure 7. The temperature profiles along the red lines described in figure 6 for the equivalence ratios of (a) 0.6, (b) 1.0, (c) 1.4 and (d) 3.0.
For the equivalence ratio of 3 the temperature curve at \( x = 0 \) is flat, indicating that the rate of the heat formation is comparable to the rate of the heat transportation to the \( y \) direction.

In general, it can be observed from the simulation results that the flat flame occurs for all equivalence ratios. This can be seen from the small temperature difference at \( x = 0, x = 2.7 \) and \( x = 5.4 \). The difference in the temperature in \( x \) direction is high at the low part of the furnace, and then decreases, and then is almost constant after the height of about 16 m, which is around 500 K.

Of the four equivalence ratios studied in this research, the equivalence ratio of 3.0 give the most uniform temperature distribution in term of the small temperature difference along the vertical direction, and the most stable flame in term of the nearly constant temperature along the vertical direction.

4. Conclusions
The simulation of the flat flame burner in the furnace for pyrolysis has been carried out. In general, the flat flame occurs for all equivalence ratios under the study. The equivalence ratio of 3.0 is the best since it gives the most uniform temperature distribution and the nearly constant temperature along the vertical direction. Therefore, the reacting mixture of 3.0 in the equivalence ratio is suitable for use in pyrolysis furnaces.

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