NUMERICAL COMBUSTION MODELLING OF A GAS-BURNER

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ABSTRACT

In this paper numerical simulation of combustion over a sample of a prevalent gas-burner, and effects of parameters such as environment geometry, main parameters of chimney, effect of free and forced convection on the environment, in radiation modelling situation and without radiation has been studied. Since offering proposals to improve the efficiency of a system is required for completing identification of the system, gas-burner is set in different cases in the environment to have better recognition of the manner of gas-burner heat transfer to the environment. For study of radiation effects, a geometric model considering radiative heat transfer and without radiation is simulated and the results compared together. Furthermore, the distribution of environmental temperature in normal conditions, and advert to mass fraction of combustion products are the other cases which have been studied.

Keywords: Combustion, Radiation, Furnace, Gas-burner, Chimney

NOMENCLATURE

\( a \) Absorption coefficient
\( E \) Internal energy
\( H \) Enthalpy
\( I \) Radiation intensity
\( m \) Mass
\( n \) Refractive index
\( P \) Pressure
\( \dot{Q} \) Heat capacity of the gas-burner
\( \mathbf{r} \) Location vector
\( S \) Path length
\( \mathbf{S} \) Radiation direction vector
\( \mathbf{S}' \) Propagation direction vector
\( T, T_i \) Temperature
\( T_o \) Atmosphere temperature
\( T_{\text{max}} \) Maximum temperature of gas-burner surface
\( T^* \) Nondimensional temperature
\( \tau_{ij} \) Tension tensor
\( \sigma \) Stephan-Boltzman constant
\( \sigma_s \) Propagation constant
\( u \) Velocity
\( \Delta P_{\text{bouyancy}} \) Buoyancy temperature difference
\( \Delta P_f \) Friction pressure difference of the chimney
\( \Phi \) Phase function
\( \Omega' \) Body surface angle
\( \delta_{ij} \) Kronecker delta
\( \varphi \) Ratio of stochiometric air to actual air
\( \gamma \) Oxygen percent
\( \mu \) Viscosity
\( \rho \) Density

1. INTRODUCTION

Significant of fossil fuel combustion for producing energy in industry, automotive transportations and home consumption is clear to everyone. More than 90 percent of the world consumption of energy is produced from fossil fuels. Ever-increasing need of human to energy, danger of finishing fossil fuels and biological destructive effects arising from combustion of fossil fuels, caused researchers to design cleaner combustion devices with higher efficiencies. Simulation of combustion process with the purpose of studying the amount of pollutants produced by combustion needs perfect identification of this phenomenon from chemical point of view (hydrocarbon oxidization, quick reaction parameters, etc.), thermodynamic point of view (hypothesis of chemical reaction with infinity speed and computing the released heat), and fluid mechanics point of view (turbulent flow with change of density and have potential to produce turbulence in the case of releasing heat). According to the following formula, the best case for inflammation complex of natural gas is to observe fuel-air ratio 1 to 10 (Dryer and Glassman, 1973).

\[
\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}
\]
According to the above formula, one volume of methane needs to have 2 volumes of oxygen for complete combustion, and because oxygen is one fifth of the air, one volume of methane needs to have 10 volumes of air. Of course for complete combustion we need to have 25 percent of excess air. The above reaction is one stage reaction between methane gas and air, because the main product of combustion of methane is carbon monoxide (CO); which is made by initial process between methane and air, and in high temperature of the flame composes with the oxygen in the air and generates carbon dioxide (CO$_2$). But if there is not enough air available, or the flame is not complete and uniform, there is not enough time for carbon monoxide to oxidize and convert to carbon dioxide and will be released.

2. MODELS AND GOVERNING EQUATIONS

The flow regime in the combustion chamber under studied is turbulent with change in density of the chemical species, which is aroused from the combustion. The governing equations on this phenomenon are conservation of mass, momentum, transmission of species and energy in the cylinder coordinate system with the assumption of steady with respect to time. For modelling the terms aroused from turbulent assumption k-ε method, and for modelling the combustion flow and calculating transmission of species Eddy-Dissipation method has been used (Subramaniam and Howarth, 2000). Equations of transmission of species (N-1 equations which N is the number of species) can be expressed as (Pope, 1990).

\[
\frac{\partial}{\partial x_i} (\rho u_i m_{\phi}) = - \frac{\partial}{\partial x_j} J_{i,j} + R_i
\]

(2)

Where

\[
J_{i,j} = \left( \rho D_{i,j} + \mu \frac{\partial m_{\phi}}{\partial x_j} \right)
\]

(3)

And diffusion factor of species is calculated as follows:

\[
D_{i,j} = (1 - \rho X_{i}) / \sum \rho_{j \neq i} X_{j} / D_{i,j}
\]

(4)

Also the momentum equation can be written as below:

\[
\frac{\partial}{\partial x_j} (\rho u_i u_j) = - \frac{\partial P}{\partial x_j} + \frac{\partial}{\partial x_j} (\rho \tau_{ij})
\]

(5)

Where tensor stress is

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

(6)

Conservation of energy equation in this process with chemical reaction (combustion) is

\[
\frac{\partial}{\partial x_j} [u_j (\rho E + P)] = \frac{\partial}{\partial x_j} (\lambda_{\phi} \rho T - \sum \sigma_{i,j} J_{i,j}) + S_h
\]

(7)

Where $S_h$ is the source term aroused from the heat released from the chemical reaction, also

\[
E = h - \frac{P}{\rho} + \frac{u^2}{2}
\]

(8)

Where, h is calculated from the ideal gas definition. Effective heat conduction factor, which is heat conduction factor of fluid and turbulence effects on it, with using the RNG k-ε method calculated as below:

\[
\lambda_{\phi} = \alpha C_{\phi} \mu_{\phi} \epsilon
\]

(9)

For calculating the turbulence effects on the properties of flow and calculating the effective heat conduction factor and effective viscosity two assistance equations (k-ε) has been utilized (Muradoglu et al., 2001). Also $\mu_\varepsilon$ is the turbulent viscosity determined from the following equation (Muradoglu et al., 2001):

\[
C_\mu = 1.92, \quad \sigma_\varepsilon = 1.3, \quad \sigma_k = 1.0, \quad C_{2\varepsilon} = 1.92, \quad C_{I\varepsilon} = 1.44
\]

2.1 Combustion of Methane-Air

In this study combustion of methane-air assumed with two stage combustion mechanism as mentioned below (Dryer and Glassman, 1973):

\[
\text{CH}_4 + 1.5\text{O}_2 \Rightarrow \text{CO} + 2\text{H}_2\text{O} \quad \text{(step 1), (reaction 1)},
\]

\[
\text{CO} + 0.5\text{O}_2 \Rightarrow \text{CO}_2 \quad \text{(step 2), (reaction 2)}.
\]

On the basis of this mechanism, the products of methane oxidization are carbon monoxide and water vapour. In the next stage carbon dioxide formed from carbon monoxide oxidization. Because of complete oxidization of methane in dilute complexes, in combustion with excess air the equation of combustion is expressed as (Dryer and Glassman, 1973):

\[
\text{CH}_4 + 2\left( \frac{\phi + 100 - \gamma N_1}{\phi} \right) \Rightarrow \text{CO}_2 + 2\text{H}_2\text{O} + \left( \frac{1 - \phi}{\phi} \right) \text{O}_2 + \frac{2(100 - \gamma N_1)}{\phi}
\]

(11)

In this equation $\phi$ is the ratio of the amount of stoichiometric air to the amount of actual air and $\gamma$ is the oxygen percentage exists in the air, which is 22% in normal conditions. This equation in bound of $0 \leq \phi \leq 1.0$ is the governing equation for the complete combustion with excess air. Mass of entrance fuel ($m_f$) is calculated in
terms of fuel heat capacity (LCV), molecular mass ($M_f$) and gas-burner heat capacity ($Q$)

$$m_f = \dot{Q} \cdot M_f / LCV$$  \hspace{1cm} (12)

Which LCV is calculated in terms of enthalpy of combustion products ($H_p$) and enthalpy of reactants ($H_r$).

### 2.2 Eddy-Dissipation Combustion Model

In turbulent flows with chemical reactions Aranius rate of reaction (for laminar flows) or Eddy-Dissipation rate of reaction (for turbulent flows) or both calculated according to the definition of the problem for using in the source term of the transmission of the species equation. In this study rate of reaction is used from Eddy-Dissipation model on the basis of Magnesen & Hertager, 1976. The source term of $i$ specie in the reaction calculated according to the number of reaction stages as below

$$R_i = M_i \cdot \sum_{k=1}^{N_g} R_{i,k}$$ \hspace{1cm} (13)

The effect of turbulence on the rate of reaction is calculated on the basis of Magnesen-Hertager model.

### 2.3 Radiative Transfer Equation

In high temperatures call off from radiation effects can intensely affect the results. Due to flame high temperature in the reaction zone, radiation effects could be noticeable in the combustion process. The radiative transfer equation (RTE) for an absorbing, emitting, and scattering medium at position $\vec{r}$ in the direction $\vec{\Omega}$ is

$$\frac{dI(\vec{r},\vec{\Omega})}{ds} + (a + \sigma_s)I(\vec{r},\vec{\Omega}) = \sigma T^4 \frac{a}{4\pi} \int I(\vec{r},\vec{\Omega}) \Phi(\vec{r} \cdot \vec{\Omega}) d\Omega$$  \hspace{1cm} (14)

$(a + \sigma_s)s$ is the optical thickness or opacity of the medium. The refractive index $n$ is important when considering radiation in semi-transparent media (Fluent User’s Guide, 2001). In the DTRM and the DO (which is considered in this study) models the radiative transfer equation (RTE) is considered in the direction $\vec{\Omega}$ as a field equation and is written as

$$\nabla \cdot (I(\vec{r},\vec{\Omega}) + (a + \sigma_s)I(\vec{r},\vec{\Omega})) = \sigma T^4 \frac{a}{4\pi} \int I(\vec{r},\vec{\Omega}) \Phi(\vec{r} \cdot \vec{\Omega}) d\Omega$$ \hspace{1cm} (15)

### 3. NUMERICAL MODELLING OF COMBUSTION IN GAS-BURNER

One of the most important parts in numerical solving is producing proper geometry of the under studied system which has the least errors in meshing (Tannehill et al., 1997]. General structure of stove with chimney as below:

1- Furnace and crossing chamber of hot gases produced by combustion to the chimney.
2- Outer casing of the gas-burner.

The computational model used is shown in Figures 1 and 2 with its geometric dimensions. It should be pointed out that modelling sensitivity is on furnace and crossing chamber of hot gases. One of the other important steps in numerical solving is producing proper grid with needed precision in different parts.

1. **Figure 1** Side view of the furnace of the gas-burner
2. **Figure 2** Front view of the furnace of the gas-burner
quadrilateral forms are tested at entrance surface of fluid in which the best results come from the rectangular grid. Since radiation plays the main rule in heat transfer of bodies with atmosphere, effect of radiation phenomenon of gas-burner to the atmosphere is studied (Adams, 1993).

![Figure 3 Grids and overall view of the gas-burner and its environment](image)

Schematic of meshing is shown in Figure 3. In this case the gas-burner is placed in atmosphere with determined dimensions meters and the heat sensed with the walls calculated with or without considering radiation. To calculate mean heat transfer coefficient on the casing of gas-burner contacted with the atmosphere, the gas-burner is placed in cubic atmosphere with 3 meter length of each side which this atmosphere is contacted to 300K air from four sides. In Figure 2 meshing model and whole view of the gas-burner and its atmosphere are shown. For modelling radiation the Discrete Ordinate model is chosen (Fluent User’s Guide, 2001).

4. BOUNDARY CONDITIONS

In this modelling, entrance surface of fuel and air is considered to be a part of a cylindrical tube with a determined cross section. On the other hand, with determining the amount of fuel and air and mass fraction of each of them in entrance (with the assumption of combustion with excess air), velocity of entrance flow is calculated, and is given as entrance values. In this paper gas-burner is studied in two different ways:

1- Modelling of gas-burner and its surrounding in order to study atmosphere effects on efficiency of the gas-burner (e.g. room dimensions, distance between walls, and quota of radiation heat transfer to free convection)

2- Modelling of gas-burner and imposing atmosphere effects on gas-burner walls with imposing convection heat transfer boundary conditions (for studying distribution of different variables, manner of function and recognition of combustion phenomenon gas-burner, study the effect of chimney, etc.)

Since modelling of atmosphere around gas-burner cause the calculation time to threefold increase, essential space for computer (RAM) to increase 50%, and also decrease the rate of convergence. It is observed that with correctly imposing atmospheric effects on heat transfer from gas-burner surface, we can save a lot of time and memory for calculations. This boundary condition is used for study of combustion in internal chamber of gas-burner.

With the assumption of pre-mixed combustion with excess air and governing equations of combustion, entrance velocity is considered to be $0.24 \text{ m/sec}$ and temperature to be $300K$, with mass fraction of 0.044 for methane and 0.2222 for oxygen. Entrance velocity is calculated on the basis of gas-burner capacity and entrance mass fraction of fuel and air. In this research, the amount of excess air is considered to be 22%, and it can be increased be up to 40%. On the basis of mentioned values, consumption of this gas-burner is about $0.5 \text{ m}^3/\text{hour}$.

Calculations of the produced model for determined values of fuel and air is performed, and the results show that the mean heat transfer coefficient of about $20\text{w/m}^2\text{.K}$ is a proper value for imposing the free convection heat transfer effect of the atmosphere.

5. ANALYSIS OF EFFECTIVE VARIABLES ON THE GAS-BURNER EFFICIENCY

5.1 Furnace

After combining together, fuel and air enter the furnace chamber and ignited. Because of this ignition, temperature of combustion products increased and their density decreased, and this lightness cause them to move upward. As mass fraction of species shows in Figures 3 and 4, oxidization process of CO to CO$_2$ still continues among the movement of hot gases until the entire produced CO from the first reaction is consumed in the furnace. It is also observed that up to specific height of flame, the process is concomitant with producing CO, but above that height, produced CO is consumed and CO$_2$ & H$_2$O is produced. Afterwards, final combustion products (CO$_2$ & H$_2$O) and residual excess air enter the second reservoir of the gas-burner. Variations of mass ratio of oxygen along the path of combustion gases movement in the furnace and along the reaction with 22% excess air is observed from Figure 5. One of the most important purposes of placing the second reservoir is to decrease the exit velocity of produced gases of combustion, and increase the amount of heat transfer from hot gases to the atmosphere.
Excessive decrease in diameter of connection pipe between the furnace and the reservoir prevents the combustion products from egression, and cause flame asphyxia (producing noxious CO gas), and distribute it to the atmosphere. On the other hand, with increasing the diameter of these pipes, velocity of exiting combustion products from the furnace to the reservoir increased, and the amount of heat transfer from the furnace to the atmosphere decreased, and the efficiency of the gas-burner decreased.

5.2 Effect of Gas-Burner Dimensions on Efficiency and Flame Maximum Temperature

Dimensions of combustion chamber are an important design parameter because of:

1- Direct correlation between heat transfer surface and gas-burner dimensions

2- Effect of combustion chamber dimensions on cooling and extinguishing the flame or imperfect combustion in diffusion flames.

In diffusion flames, on the contrary to pre-mixed flames, the necessary air for combustion is obtained from atmosphere around the flame. In these torches, with decrease in combustion chamber dimensions, the flame cannot obtain its essential air for complete combustion from the atmosphere; so with decrease in combustion chamber dimensions, the amount of CO pollutants (from incomplete combustion) increased until the flame quenched. Also the other effect of decrease in combustion chamber dimensions is that the rigid wall comes closer to the flame which accounts for cooling the flame and quenching it (Dryer and Glassman, 1973). But in household gaslight devices, a section of combustion air, which exists before ignition, is mixed with the fuel and only a small quota of it is secured from the atmosphere. We can consider the gas-burner as almost complete pre-mixed torches. Since decrease in combustion chamber dimensions has no effect on density of species unless this decrease is enormous that there is not enough space and time for combustion reaction completion (Kempf et al., 2005).

The results show that with 20 percent increase in gas-burner length, the amount of heat transfer will increase 18.5 percent. Also 20 percent increase in gas-burner width (from 250mm to 300mm) leads to 6 percent increase in the amount of heat transfer. In both situations, the reason of increase in heat transfer is raise in the exchange surface of heat transfer. Also surface increase in YZ plane direction (Figure 2) has much larger effect comparing with XZ direction. In addition, gas-burner dimensions in X&Z directions has been increased 10 percent of their initial value, and the results shows 12 percent increase in the amount of heat transfer with the atmosphere

5.3 Effect of Radiation Heat Transfer for the Sake of Increase in Gas-Burner Efficiency

Temperature distribution considering radiation heat transfer with respect to height of room centre and without it is shown in Figure 6. In this case, the gas-burner is situated in an open environment, but it is under a roof of 3 meters height. The temperature of atmosphere is considered to be 27°C (300K). As shown in Figure 7, in the case of without radiation, temperature region of more than 310K (those heated more than 5 degrees) is situated near the roof, and there is not considerable change in the temperature of beneath surfaces, which is the place for people presence. We can note increase in radiation heat transfer contribution in heating equipments as one of the useful methods in reduction of energy consumption. In this method of heating, in equipments such as gas-burner, due to rather high temperature of its wall with respect to atmosphere, has some contribution in warming the atmosphere. As it is observed in Figure 8 (in comparison with Figure 7), with absorbing radiation energy from the gas-burner surface via ground, about 5°C temperature difference is created in height of 20 centimeters, which is increased with approaching the surface.
Figure 6 Variations of oxygen mass fraction with respect to furnace height

It should be noted that the ground and the roof of the atmosphere is considered to be adiabatic in this paper and its heat dissipation is not taken into consideration.

5.4 Effect of Chimney in Gas-Burner Efficiency

The chimney has no role in securing the air for combustion in a gas-burner, assuming complete mixing of fuel and air before the combustion, but the created suction in the chimney makes up for the pressure loss in the exiting path of combustion products, and this helps the designer to increase the amount of heat transfer between the gas-burner and atmosphere with designing more complicated paths (but with higher pressure loss), and the gas-burner efficiency will be increased consequently.

High pressure loss in the exiting path of gases leads to leak the combustion products from the seams and even return of these products to the atmosphere around the gas-burner which is jeopardous and mortal for inhabitants. Effective parameters in increasing the produced suction in the chimney are increase in chimney length (because of buoyancy increase), and increase in chimney diameter for reducing dissipations in the chimney. The following equation shows the balance between the pressure loss due to buoyancy $\Delta p_{\text{bouncy}}$, and the pressure loss due to friction of chimney wall $\Delta p_f$, and the flow pressure loss in passing the furnace and the expansion reservoir behind the gas-burner $\Delta p_s$ (Kempf et al., 2005):

$$\Delta p_{\text{bouncy}} = \Delta p_f + \Delta p_s$$  \hspace{1cm} (16)

$$\Delta p_f = \mu \left| \frac{\partial V}{\partial y} \right|_{\text{wall}}$$  \hspace{1cm} (17)

In this equation, $V$ is the fluid velocity inside the chimney, and the wall index represents the velocity variations on the chimney wall. Increase in chimney diameter leads to faster exiting of combustion products and reduce the gas-burner efficiency. On the other hand, intense decrease in diameter causes high pressure drop and flame quenching.

6. BOUNDARY CONDITIONS AND VARIOUS GEOMETRIES ON THE GAS-BURNER EFFICIENCY

6.1 Heating Effects in a Confined Environment with 3 Lateral Walls and 1 Open Surface

For studying the heating dissipation of gas-burner in small environments with open doors and windows, the gas-burner is situated in a cubic place with three lateral walls, and one side is modelled open to the outside environment. The goal is to study the volume of entering air from cold environment (and the amount of exiting warm air to the outside
environment) from the room. For the study of heating dissipation of the gas-burner in small environments with open doors and windows, the results show that the temperature distribution is formed stratifiedly from near the roof to the ground of the room. Also the maximum temperature difference with respect to 30°C environment is in the region of ascension of warm air from over the gas-burner to the roof and in the space beneath the roof. This temperature difference decreases to 5°C with approaching the ground. In adjacent to the outside environment, because of entering cold air, the reservoir shows lower temperature than other regions. The cold air enters the environment from wide area (between roof and ground), and after heating with the gas-burner, transmitted to the outside. The volume of loosing warm air due to this transmission, is calculated about 3.5 kilogram per minute (about 3.5 cubic meter per minute), that we can say that the air of the room is substituted about 17 times.

For studying the manner of temperature distribution in above conditions, the temperature is non-dimensionalized in the environment with this equation:

$$ T^* = \frac{T_i - T_{\text{max}}}{T_{\text{max}} - T_0} $$

(18)

Where $T^*$ is the non-dimensional temperature, $T_i$ is the temperature of the regarding point, $T_0$ is the environment temperature (which is assumed 300K in this paper), and $T_{\text{max}}$ is the maximum temperature of the gas-burner surface.

Also for comparing the results with the gas-burner model in an environment surrounded with four lateral walls, temperature distribution in four different heights between two parallel walls of the room which has more symmetric temperature distribution between them is studied with a horizontal line passing through the centre of the room, and Figure 9 shows this distribution. Figure 10 also shows a graphic display of the path of the air particles due to the motion created by temperature difference in a room with 3 walls.

Figure 9 Temperature distribution around the gas-burner with radiation effects

Figure 10 Non-dimensional temperature distribution with respect to height in the centre of the room, in two cases of three and four walls

6.2 Heating Effects in an Environment Surrounded with 4 Lateral Walls

The heating dissipation effects in walls are studied with modelling of a gas-burner in an environment surrounded with walls which are open to air with 300K temperature and convection heat transfer coefficient of 20W/m².K. In Figure 11, non-dimensional temperature distribution is shown like Figure 9 in four different heights.
temperature distribution, the increasing region with height which is occurred near the walls is smaller. Instead, the region of decreasing temperature with height becomes larger, that is more effective on warming of inhabitants of the room.

Non-dimensional temperature distribution versus height of the room centre in two cases of room modelling with 3&4 walls are compared to each other in Figure 10. In both figures, there is a temperature increase with height up to the roof proximity, and this is because of warm air agglomeration and reduction of air flow velocity in upper direction in the roof proximity because of heat transfer with the roof and 90 degree change in movement direction in this region. It is evident that this is the reason of temperature decrease in the roof proximity. Naught of direct exiting of air flow from the room surrounded with 4 walls leads to higher average temperature distribution in Figure 12, that there is about 15 percent temperature increase in all points with respect to the case of room with three walls.

3. CONCLUSIONS

The results show that with 20 percent increase in gas-burner length, the amount of heat transfer will increase 18.5 percent. Also 20 percent increase in gas-burner width (from 250mm to 300mm) leads to 6 percent increase in the amount of heat transfer. In both situations, the reason of increase in heat transfer is raise in the exchange surface of heat transfer. Increasing lateral surface can significantly increase the gas-burner efficiency, but we can't change the gas-burner dimensions excessively because it has an elegant appearance and size and this is an important factor in residential areas. But we can create this surface increase with setting some fins on the gas-burner surface.

Another appropriate use of this heating is in small and close rooms without exiting of air flow from the environment. In this case we can achieve 15 percent efficiency increase. On the other hand, in small regions and with considering the convection phenomenon, radiation contribution in correct temperature and heat distribution is very high. Approximate 15 percent temperature increase in the room model with radiation is a proof of this claim.

Modelling of the heating device in two geometric environments, room with four walls, room with three walls and one open surface that are widely used gas-burner, discloses advantages and disadvantages, temperature distribution and heat transfer trend in each of these environments. Non-dimensional temperature distribution is useful indicator to compare the gas-burner efficiency in these two environments.

3. RECOMMENDATIONS FOR FURTHER WORK

- The computational findings were not validated using experimental results.
- Work is currently under way to conduct experimental measurements using reduced scale models of heating device using various geometric configurations.

REFERENCES


