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Numerical Simulation of the Effect of Equivalence Ratio and Turbulence Intensity on the Combustion Characteristics and Pollutants Production in a Liquid Fuel Combustor

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Abstract

Due to the increasing development of thermal power stations with fossil fuels, optimizing the combustion process in boilers and combustion chambers are important to reduce the amount of environmental pollutants. This paper examines the equivalence ratio parameter and its effect on maximum temperature of exhaust gases from the combustor and the rate of production and emission of Nitrogen Oxides (NOx) and soot pollutants as well as the turbulence effect on these pollutants. Finite volumes method was used to solve the equations of flow field of gasoil fuel turbulent combustion.

Tesner's two-stage model and Magnussen-Hjertager's combustion model were used for modeling the process of soot formation and combustion. The amount of NOx was calculated prompt and thermal mechanisms. RNG K-E model was used for modeling the oscillating terms in the conservation equations and an eddy dissipation model was used to calculate the combustion rate. Results indicate that by increasing the equivalence rate from 0.6 to 1 due to the complete combustion, the maximum temperature of combustor and consequently, NOx increase; also, by increasing the maximum temperature of flame, the rate of soot formation in flame increases. On the other hand, high temperature of combustion chamber causes soot combustion and decreases in output. Considering the turbulence effect also increases the amount of NOx and soot due to the better combustion.

Keywords: liquid fuel combustion, turbulence, equivalence ratio, soot, NOx

Introduction

An important part of combustion pollutants results from combustion of fuel combustion is incomplete.

The main pollutants are carbon monoxide and soot. Temperature and mixing rate of fuel and air are the most important parameters affecting the rate of formation and emission of pollutants combustion. Better mixing of fuel and air reduces the carbon pollutants formation (carbon monoxide and soot) and increases the temperature and combustion efficiency. On the other hand, the flame temperature rise in hot areas significantly increases the amount of nitrogen and sulfur oxides formation. One of the other important factors in controlling the amount of nitrogen oxides and sulfur pollutants is the amount of radiation. By increasing the radiation, the maximum flame temperatures and the rate of the pollutants formation reduce significantly.

One of the factors affecting the increase of flame radiation is the formation of soot in flame and its combustion before leaving the combustion chamber. It is observed that the formation rate of nitrogen and sulfur oxides, carbon monoxide, soot and combustion efficiency were strongly linked to each other and changed by changing the rate of combustion conditions of each one.

Computer simulation is an appropriate method to study the combustion process which has found recently developed and used to calculate pollutants and many researchers have used numerical and laboratorial studies to optimize the performance conditions of boilers [1].

In this paper, the effect of equivalence ratio and turbulence on temperature, soot and NOx exhausting from combustor was analyzed by simulating the combustor internal processes.

Characteristic of Combustor

Dimensions of studied combustor are shown in table 1. All units are based on millimeters.

Table 1:Dimensions of studied combustor		
Combustor length	730	
Combustor diameter	200	
Air inlet diameter	70	
Fuel inlet diameter	30	
Outlet diameter	100	

Data used in combustor simulation are as follows:

Table 2 : Functional parameters of combustor

Described	Unit	Amount
Air mass flow rate input to the combustor	Kg/s	0.029
Input air temperature	K	300
Combustor wall temperature	K	900
Fuel particle diameter	μ	10

Equations and Numerical Solution Methods

Flow inside the combustor and combustion chambers are rotary flows and highly turbulent. Equations in these flows are partial differential equations, of which the most important equations are continuity, momentum, turbulence, energy, production rate and loss of chemical species and radiation that the profiles of combustion flow in a combustion chamber is calculated by simultaneous solution of the equation system for the geometry and certain boundary conditions. In addition to above equations for liquid fuel combustion, Lagrangian equations for trajectory of fuel particles and energy equations are also examined to calculate the fuel vaporization rate. Overall differential equation for conservation in the gas phase for variable φ is as follows [2]:

$$(\mathbf{r}\mathbf{u}_{i} + \overline{\mathbf{r}'\mathbf{u}'_{i}})\frac{\partial f_{i}}{\partial \mathbf{x}_{i}} = (1)$$
$$-\frac{\partial}{\partial \mathbf{x}_{j}} \left(\mathbf{r}\overline{\mathbf{u}'_{j}f'_{j}} + \mathbf{u}_{j}\overline{\mathbf{r}'f'} + \overline{\mathbf{r}'\mathbf{u}'_{j}f'}\right) + \frac{\partial}{\partial \mathbf{x}_{j}} \left(\Gamma_{f}\frac{\partial f}{\partial \mathbf{x}_{j}}\right) + \mathbf{S}_{f}$$

that the calculation of $\mathbf{u'_j}\mathbf{f'_j}$ oscillating terms is the task of turbulent models [3].

Momentum equations of fluid particles are derived by using the external forces' balance on the droplet [4] that in the assumption direction of x is as follows:

$$\frac{du_{p}}{dt} = F_{D}(u - u_{p}) + \frac{g_{x}(r_{p} - r)}{r_{p}} + F_{x}$$
(2)

in which, *u* is axial velocity of gas, ρ_p is density of droplet, and, ρ is fluid density around the droplet, and u_p is axial velocity of fuel droplet. F_D is also determined from the following equation:

$$F_D = \frac{18\,\boldsymbol{m}_g \boldsymbol{C}_D \,\mathrm{Re}}{24\,\boldsymbol{r}_p \boldsymbol{d}_p^2} \tag{3}$$

In this equation, μ_g is viscosity of gas, ρ_p is density of droplet, and d_p is diameter of droplet. C_D and Re are drag coefficient and local Reynolds number, respectively.

Energy conservation equation on liquid fuel droplet, assuming an monotonous temperature inside the droplet regardless of superficial evaporation, is expressed as follows:

$$m_l C_{p,l} \frac{dT_l}{dt} = \dot{Q}_l - \dot{Q}_v \tag{4}$$

in which the total heat transferred to the droplet, Q_{ν} is the energies spent to evaporate the fuel droplet and T_l is temperature of drop. $C_{p,l}$ and m_l are specific heat and mass, respectively [4].Combustion model used in this study is Magnussen-Hjertager's model. [5], [2].

Chemical formula of heavy liquid fuel (gasoline) is presented as $C_{16}H_{29}$. Combustion of heavy fuel vapor is often done with excess air.

Equation of conservation mass fraction of each species is written as follows:

$$\frac{\partial}{\partial x_i} \left(r u_i m_j \right) = \frac{\partial}{\partial x_i} \left(\Gamma_{mj} \frac{\partial m_j}{\partial x_i} \right) - \frac{\partial}{\partial x_i} \left(r \overline{u_i m_i} \right) + S_{mi} \quad (5)$$

That the term containing fluctuation rate of velocity is modeled as follows:

$$- \overline{ru_i m_j} = C_m \frac{rk^2}{e} \frac{\partial m_j}{\partial x_i}$$
(6)

The term $S_{m,i}$ is considered as the appropriate source term for production or consumption of chemical species which is determined from the following equation due to the used combustion model:

$$S_{m,i} = n'_{i}M_{w,i}Ar\frac{e}{k} \times$$

$$min(\frac{Y_{Fuel}}{n'_{Fuel}M_{w,Fuel}}, \frac{Y_{Oxygen}}{n'_{Oxygen}M_{w,Oxygen}})$$
(7)

Pollutants Formation Models

In this study, Tesner's two-stage model [6] was used for modeling the nucleation rate and soot formation. Three mechanisms are mainly discussed for the production of NOx in combustion [2 & 7], which include heating mechanism [2], the fuel mechanism [2] and prompt mechanism [2].

Boundary Conditions and Numerical Solution

Produced computing grid and boundary conditions are shown in figure 2. Finite volumes method and fluent6.3 numerical code were used for numerical solution of equations. RNG k- ε model was used to calculate the turbulences of flow and Discrete Ordinate model is used for modeling the radiation.



Figure 1 : Computing grid and boundary conditions

Results

Distribution of mass fraction, NOx and soot for the initial conditions of combustor (equivalence ratio 1) are shown in figures 2 and 3, as is observed, NOx has maximum amount in areas with maximum temperature. About soot, by increasing the maximum temperature of flame, formation of soot rate in the flame increases. On the other hand, high temperature of combustion chamber results in soot combustion and reduces soot in output.





Figure 3 : Distribution of soot mass fraction

Effect of equivalence ratio parameter on the maximum temperature of combustor exhausting gases and the amount of NOx and soot are shown in figures 4 to 6. By increasing the flow rate of intake air (decreasing the equivalence ratio to one), maximum temperature of combustion chamber increases due to the complete combustion. Due to further intake air, the maximum temperature of flame is reduced because the mixture is cooling. As figure 5 shows, NOx pollutant increases at first in the output of the combustor by increasing the maximum temperature and then decreases.



Figure 4 - Effect of equivalence ratio on maximum temperature of combustor exhaust gases



Figure 5: Effect of equivalence ratio on exhaust NOx mass fraction

But increasing the flow rate of air has a complex effect on soot formation. The amount of soot formation in flame increases by increasing the flow rate and consequently by increasing the maximum flame temperature (and resolution of input fuel). On the other hand, high temperature of combustion chamber results in soot combustion and decreasing in output. Also, excess air causes the better mixing of fuel and air and decreasing the amount of soot (figure 6).



Figure 6:Effect of equivalence ratio on output soot mass fraction

As figure 7 and 8 show, regarding the turbulence effect, the amount of NOx pollutant and soot (at equivalence ratio 0.6) increases due to combustion improvement.



Figure 7 : Turbulence effect on NOx mass fraction



Figure 8 :Turbulence effect on soot mass fraction

Conclusion

By reducing the equivalence ratio to 1 (increasing the flow rate of input air) maximum temperature of combustion chamber increases because of complete combustion, but further amount of intake air, the maximum flame temperature is reduced due to cooling the mixture.

NOx pollutant also increases at first by increasing the maximum temperature and then decreases. Better mixing of fuel and air, decreases the carbon pollutants and increases temperature and combustion efficiency. Also, regarding the turbulence effect, NOx pollutant and soot increases due to combustion improvement.

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