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Different Oxygen Levels of Dimethyl Ether Combustion Influence Numerical Simulation

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Abstract

Aiming at the dimethyl ether itself with oxygen, this paper simulate that how much less oxygen quantity Dimethyl ether combustion required than liquefied petroleum gas in the same fuel quantity, and obtain optimum normoxia of dimethyl ether desired. This paper simulated dimethyl ether, liquefied petroleum gas (LPG) combustion with the air for 10%, 20%, 30%, 40%, 50%, 90% Oxygen levels. Under the different oxygen levels ,the study found that the best oxygen levels dimethyl ether combustion needed is around 30%, and the best oxygen levels liquefied petroleum gas (LPG) combustion needed is around 50%, so that Oxygen levels dimethyl ether needed is less than liquefied petroleum gas (LPG) needed in the same amount of fuel.

Key words: Dimethyl ether combustion; Energy conservation and emission reduction; air normoxia; Numerical Simulation.

1. Introduction

Dimethyl ether gradually replace Liquefied petroleum gas (LPG) in most of the ceramic kiln plant at present, and more and more be replaced , the main reason is the dimethyl ether own oxygen, good combustion performance, high thermal efficiency, no residue, no black smoke in the process of burning , low carbon monoxide and nitric oxide emissions, it is a kind of clean fuel [1-4]. Under the same heat condition, dimethyl ether combustion efficiency is increased 5% with natural gas, liquefied petroleum gas, and other gas phase comparison, such as shown in table 1. With liquefied petroleum gas (LPG) compared, dimethyl ether need less air, and this can avoid polluting air into influence the quality of ceramic fire, so product has good gloss with the dimethyl ether burning. Therefore, dimethyl ether instead of other fuel will become a mature technology in the near future.CH_3-O-CH_3

Table 1 the contrast of chemical and physical properties of Dimethyl ether and other alternative fuel contrast [5-7]

Material	DME	Methanol	Ethanol	CNG	LPG
Chemical formula	CH3-O-CH3	CH3-OH	CH3- CH2OH	CH4	C3H8

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Low calorific value（MJ/kg）	28.43	19.5	26.8	50.0	46.5
Liquid density（g/ml）	0.668	0.79	0.784	0.43	0.51
Boiling point（℃）	-25	65	78	-162	-42
Ignition temperature（℃）	235	450	420	650	507
Theory air-fuel ratio（kg/kg）	9.0	6.5	9.0	17.2	15.7
Gasification latent heat	410	1110	904	-	426
Carbon content（%）	52.2	37.5	52.2	75.0	81.8
Hydrogen content（%）	13.0	12.5	13.0	25.0	18.1
Oxygen content（%）	34.8	50.0	34.8	0	0

2. Turbulent combustion model

1. Control equation:

Continuity equation:

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u_x)}{\partial x}+\frac{\partial\left(\rho u_y\right)}{\partial y}+\frac{\partial\left(\rho u_z\right)}{\partial z}=0 \tag{1}$$

Momentum equations:

$$\frac{\partial\left(\rho u_x\right)}{\partial t}+\nabla\cdot\left(\rho u_x \vec{u}\right)=-\frac{\partial p}{\partial x}+\nabla\cdot\left(\mu grad u_x\right)+S_{u_x} \tag{2}$$

$$\frac{\partial\left(\rho u_y\right)}{\partial t}+\nabla\cdot\left(\rho u_y \vec{u}\right)=-\frac{\partial p}{\partial y}+\nabla\cdot\left(\mu grad u_y\right)+S_{u_y} \tag{3}$$

$$\frac{\partial\left(\rho u_z\right)}{\partial t}+\nabla\cdot\left(\rho u_z \vec{u}\right)=-\frac{\partial p}{\partial z}+\nabla\cdot\left(\mu grad u_z\right)+S_{u_z} \tag{4}$$

Where S_{u_x} 、 S_{u_y} 、 S_{u_z} is generalized source term, and $S_{u_x}=\rho f_x+S_x$， $S_{u_y}=\rho f_y+S_y$，$S_{u_z}=\rho f_z+S_z$

Energy equation:

$$\frac{\partial(\rho E)}{\partial t}+\nabla\cdot\left[\vec{u}(\rho E+p)\right]=\nabla\cdot\left[k_{eff}\nabla T-\sum_j h_j J_j+\left(\tau_{eff}\cdot\vec{u}\right)\right]+S_h \tag{5}$$

Where E is total energy of micro group and contains the internal energy, energy and potential energy, namely $\frac{\partial\left(\rho u_x\right)}{\partial t}+\nabla\cdot\left(\rho u_x \vec{u}\right)=-\frac{\partial p}{\partial x}+\nabla\cdot\left(\mu grad u_x\right)+S_{u_x}$, h is effective heat enthalpy(J/kg), h_j is enthalpy of components j, namely $h_j=\int_{T_{ref}}^{T} C_{p,j}dT$, them $T_{ref}=298.15K$; k_{eff} is effective heat conduction coefficient (W / (m K)), namely $k_{eff}=k+k_t$, k_t is the turbulence heat conduction coefficient ,according to the turbulence model used to determine; J_j is the diffusion fluxes of components j; S_h contains chemical reaction heat and other volumetric heat source user defined [8].

2. Turbulence model:

Standard k-model transport equations:

$$\frac{\partial(\rho k)}{\partial t}+\frac{\partial\left(\rho k u_i\right)}{\partial x_i}=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]+G_k+G_b-\rho\varepsilon-Y_M+S_k \tag{6}$$

$$\frac{\partial(\rho\varepsilon)}{\partial t}+\frac{\partial\left(\rho\varepsilon u_i\right)}{\partial x_i}=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial\varepsilon}{\partial x_j}\right]+C_{1\varepsilon}\frac{\varepsilon}{k}\left(G_k+C_{3\varepsilon}G_b\right)-C_{2\varepsilon}\rho\frac{\varepsilon^2}{k}+S_\varepsilon \tag{7}$$

Where G_k is the turbulence because average speed gradient produce; G_b is the turbulence because the influence of buoyancy produce; Y_M is the influence of total dissipation rate because of compressed turbulent pulse inflation; And $C_{1\varepsilon}$、 $C_{2\varepsilon}$、 $C_{3\varepsilon}$ is experienced constant and a default value in FLUENT ,namely $C_{1\varepsilon}=1.44$、 $C_{2\varepsilon}=1.92$、 $C_{3\varepsilon}=0.09$; σ_k、 σ_ε is perlong number corresponding turbulent kinetic energy and dissipation rate and a default value in FLUENT, namely $\sigma_k=1.0$、 $\sigma_\varepsilon=1.3$; Pr_t is turbulent kinetic perlong number, namely the default value is $\mathrm{Pr}_t=0.85$; g_i is gravity acceleration component in the i direction; β is thermal expansion coefficient; M_t is Mach number of turbulent kinetic; a is sound velocity [9-11].

3. The simplification of geometric model and the decision of boundary condition

This paper simulation spindle ceramic kiln, as shown in figure 1 , this simplified model is Shown below : ① Geometric structure construction under the foundation of the actual shuttle type furnace; ②There are no gap among the spake、kiln wall and kiln car (kiln bottom), namely without any cold air into the furnace influencing combustion in the firing process; ③ Burner is the round entry with air and fuel concentric jet ;④ Uniform layered materials is simplified to the uniform distribution cylinder in furnace [12-13], as in figure 2 shown.

Figure 1 furnace and **material form** of ceramic kiln

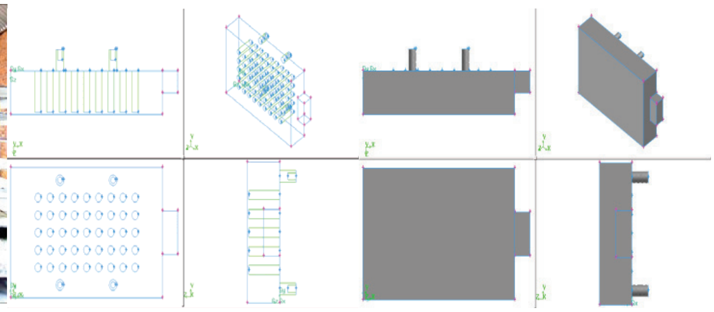


Figure 2 geometric model of spindle ceramic kiln

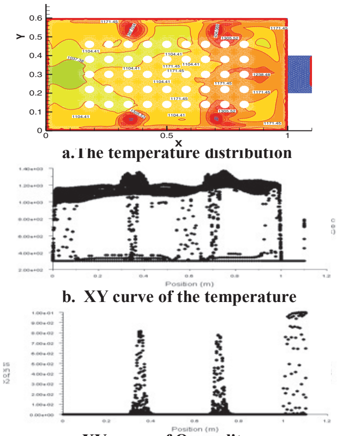
In the simulation process, fuel and the air turbulence intensity is significant at the entrance, so fuel by discrete phase is injected into the chamber in a fixed position, and the air by continuous phase is injected into the chamber in the burner entrance .Determine the fuel and air entry conditions, create PDF form, set the burning chemical components and fuel and air temperature, use velocity entrance boundary conditions for the entry boundary conditions [14-15].Kiln wall, kiln crown, the kiln and materials form were used the different two types of wall; The discrete areas of grid are fluid. According to the actual calculation and field measurement, we concluded that the inlet velocity of fuel is 47.73 m/s, hydraulic diameter is 0.03 m/s; The inlet velocity of flame retardant air is100 m/s, hydraulic diameter is 0.02 m/s; The environmental temperature is 300 K, the outlet pressure is 5 Pa, the outlet hydraulic equivalent diameter is0.16 m/s; And it suppose that the material of the Kiln bottom (the kiln car), kiln wall and spake is fireclay brick, the whole simulation process ignore absorption and heat release effect from porcelain body and glaze materials of physical chemical reaction, only includes the heat transfer process of the burning of fossil fuels, kiln wall, porcelain body itself and smoke [16], so its whole combustion process is assumed to the adiabatic combustion process.

4. Dimethyl ether、 liquefied petroleum gas and the different oxygen levels air Combustion

Because of the dimethyl ether itself with oxygen, through the comparison and analysis of the situation of the same volume of dimethyl ether and liquefied petroleum gas (LPG) combustion in the different oxygen levels air condition, mainly from combustion temperature, oxygen quantity and other combustion performance, it is realize the technical improvement of the dimethyl ether alternative liquefied petroleum gas (LPG).

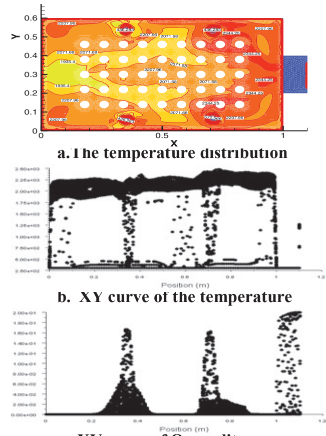
4.1 Dimethyl ether Combustion in the different oxygen levels air

It simulated the change rule of dimethyl ether combustion with the different oxygen levels air for 10%, 20%, 30%, 40%, 90%by using fluent software, the simulation results as in figure 3 to figure 7 shown. we can see when oxygen levels is 10% and 20% the average temperature of the insulation combustion is very low respectively for 1150 K and 2100 K, but it is in growth trend ; And when oxygen level is 30%, the average temperature of the insulation combustion continues to increase to 2750 K; When oxygen levels increases to 40%, the average temperature of the insulation combustion is about 2750 K as the same as oxygen levels is 30%; It is find that the average combustion temperature in whole chamber is no increase trend when we continue to increase the oxygen levels to 90%, but it drops a little, and uniformity degree of combustion temperature distribution in the whole furnace is increases, this is because the rest of the oxygen molecules in the furnace influence to the combustion. From the oxygen levels of the furnace to see, when oxygen levels is 10% and 20%, in addition to vents and exit, other parts of the furnace are no oxygen; When oxygen levels increases to 30%, 40%, 90%, the average Oxygen quality score of the furnace is 5%, 15%, 60% respectively after the completion of the combustion, so the rest of the oxygen is more and more.



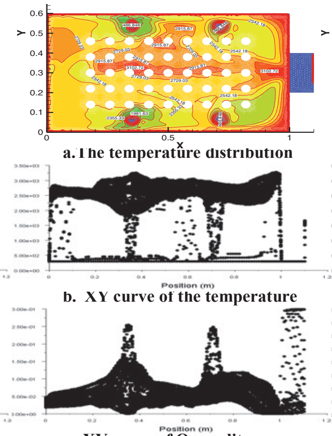
a. The temperature distribution; b. XY curve of the temperature; c. XY curve of O_2 quality score

Figure 3 combustion rule when oxygen levels is 10% in Z = 0.1



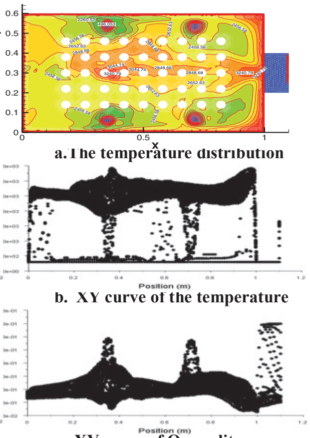
a. The temperature distribution; b. XY curve of the temperature; c. XY curve of O_2 quality score

Figure 4 combustion rule when oxygen levels is 20% in Z = 0.1



a. The temperature distribution; b. XY curve of the temperature; c. XY curve of O_2 quality score

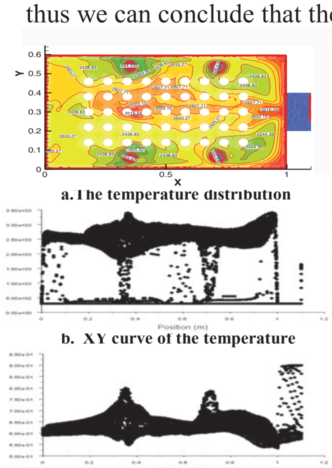
Figure 5 combustion rule when oxygen levels is 30% in Z = 0.1



a. The temperature distribution; b. XY curve of the temperature; c. XY curve of O_2 quality score

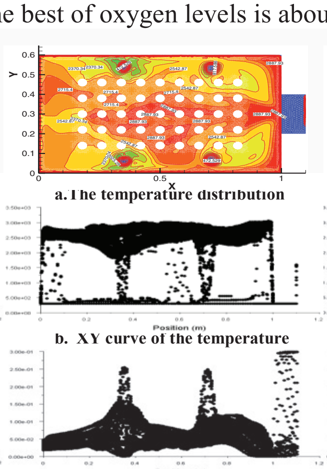
Figure 6 combustion rule when oxygen levels is 40% in Z = 0.1

From the above we can conclude that when the oxygen levels is 10% and 20%, combustion temperature is low in the whole furnace, this is because oxygen quantity is insufficient and others haven't enough time to burn in the furnace and is expelled, if Only the oxygen levels increase constantly, combustion temperature will increase; When oxygen levels increase to more than 30%, the combustion temperature will no longer increase, but will decrease, thus we can conclude that the best of oxygen levels is about 30% what dimethyl ether combustion need.



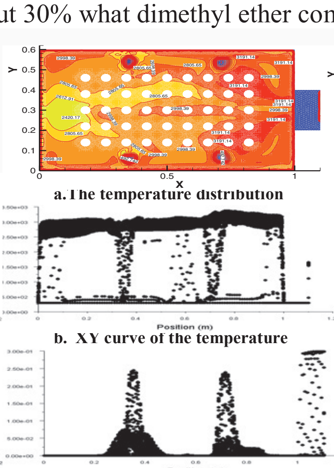
a. The temperature distribution; b. XY curve of the temperature; c. XY curve of O_2 quality score

Figure 7 combustion rule when oxygen levels is 90% in Z = 0.1



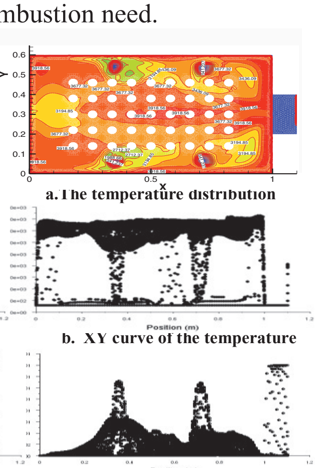
a. The temperature distribution; b. XY curve of the temperature; c. XY curve of O_2 quality score

Figure 8 combustion rule when oxygen levels is 27% in Z = 0.1



a. The temperature distribution; b. XY curve of the temperature; c. XY curve of O_2 quality score

Figure 9 combustion rule when oxygen levels is 30% in Z = 0.1



a. The temperature distribution; b. XY curve of the temperature; c. XY curve of O_2 quality score

Figure 10 combustion rule when oxygen levels is 40% in Z = 0.1

From figure 3 to figure 7, we can conclude that the combustion temperature is highest when oxygen levels is 30%, and residual oxygen is the least, this is the best oxygen levels dimethyl ether combustion needed. However through detailed calculation, the best oxygen level is 27%the fuel needed. SO it simulated the change rule of dimethyl ether combustion with air of the oxygen levels for 27%, by using fluent software, as in figure 8 shown. From the figure 9, we can see that this compared with oxygen levels for 30%, its average combustion temperature is in 2750 K, and its temperature distribution is more uniform than oxygen levels for 30% in the furnace, remaining oxygen quantity is almost the same as oxygen content for 30%.Therefore we find that oxygen level what the dimethyl ether combustion need is less than 30% slightly.

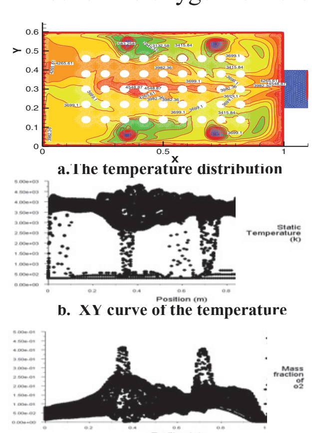
4.2 Liquefied petroleum gas (LPG) Combustion in the different oxygen levels air

Most of the ceramic kiln plant still use liquefied natural gas (LPG) as fuel at present, mainly due to its high calorific value, no smoke, no carbon residue, convenient operation, etc. we can see its main composition is C_3H_8 whose volume fraction is 90.7% from table 2, and it itself no own oxygen elements. The combustion process of liquefied petroleum gas (LPG) compared with dimethyl ether, dimethyl ether need the amount of oxygen more than liquefied petroleum gas when combustion effect is the best.

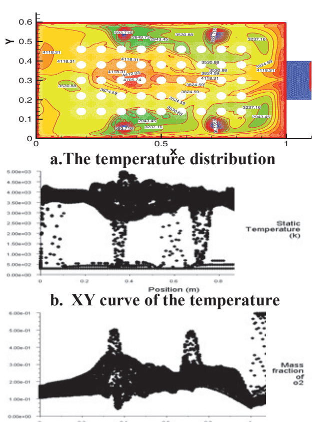
Table 2 liquefied gas components

C_3H_8	C_3H_6	C_4H_{10}	C_4H_8	C_5H_{12}	Other
90.7	3.5	3.8	0.1	0.5	1.4

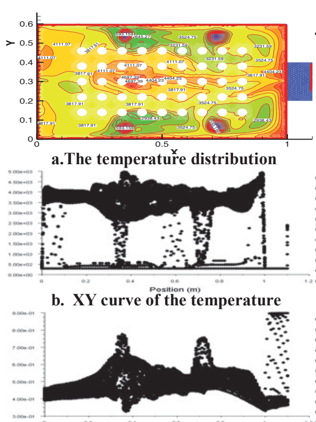
It simulated the change rule of liquefied petroleum gas (LPG) combustion with the different oxygen levels air for 30%, 40%, 50%, 60%, 90% by using fluent software, the simulation results as in figure 9 to figure 13 shown. we can see when oxygen levels is 30% and 40% the average temperature of the insulation combustion is very low respectively for 2750 K and 3600 K, but it is in growth trend; And when oxygen level is 50%, the average temperature of the insulation combustion continues to increase to 3800 K; When oxygen levels increases to 60%, the average temperature of the insulation combustion is about 3800 K as the same as oxygen levels is 50%; It is find that the average combustion temperature in whole chamber is no increase trend when we continue to increase the oxygen levels to 90%, but it drops a little, and uniformity degree of combustion temperature distribution in the whole furnace is increases, this is because the rest of the oxygen molecules in the furnace influence to the combustion. From the oxygen levels of the furnace to see, when oxygen levels is 30% and 40%, in addition to vents and exit, other parts of the furnace are no oxygen; When oxygen levels increases to 50%, 60%, 90%, the average Oxygen quality score of the furnace is 5%, 10%, 60% respectively after the completion of the combustion, so the rest of the oxygen is more and more.



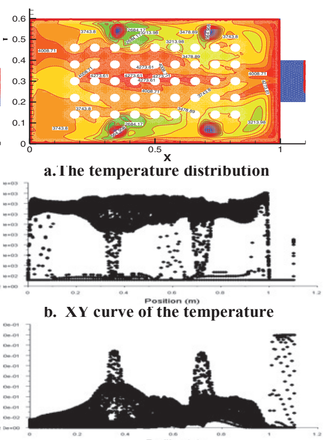
a. The temperature distribution
b. XY curve of the temperature
c. XY curve of O_2 quality score
Figure 11 combustion rule when oxygen levels is 50% in Z = 0.1



a.The temperature distribution
b. XY curve of the temperature
c. XY curve of O_2 quality score
Figure 12 combustion rule when oxygen levels is 60% in Z = 0.1



a.The temperature distribution
b. XY curve of the temperature
c. XY curve of O_2 quality score
Figure 13 combustion rule when oxygen levels is90% in Z = 0.1



a. The temperature distribution
b. XY curve of the temperature
c. XY curve of O_2 quality score
Figure 14 combustion rule when oxygen levels is45% in Z = 0.1

From the above we can conclude that when the oxygen levels is 30% and 40%, combustion temperature is low in the whole furnace, this is because oxygen quantity is insufficient and others haven't enough time to burn in the furnace and is expelled, if Only the oxygen levels increase constantly, combustion temperature will increase; When oxygen levels increase to more than 50%, the combustion temperature will no longer increase, but will decrease, thus we can conclude that the best of oxygen levels is about 50% what liquefied petroleum gas combustion need.

From figure 9 to figure 13, we can conclude that the combustion temperature is highest when oxygen levels is 50%, and residual oxygen is the least, this is the best oxygen levels liquefied petroleum gas combustion needed. However through detailed calculation, the best oxygen level is 45%the fuel needed. SO it simulated the change rule of liquefied petroleum gas combustion with air of the oxygen levels for 45%, by using fluent software, as in figure 14 shown. From the figure 14, we can see that this compared with oxygen levels for 50%, its average combustion temperature is in 3750 K, and its temperature distribution is more uniform than oxygen levels for 50% in the furnace, remaining oxygen quantity is almost the same as oxygen content for 30%.Therefore we find that oxygen level what the liquefied petroleum gas r combustion need is less than 50% slightly.

5. Conclusion

1. In the same oxygen levels, the burning temperature of dimethyl ether is less than the liquefied petroleum gas, as in table 3 shown. And compare the situation of the dimethyl ether and the best oxygen levels air combustion with liquefied petroleum gas, the liquefied petroleum gas (LPG) combustion temperature is higher than dimethyl ether, this is because calorific value of dimethyl ether is lower than natural gas, liquefied petroleum gas, and other gas , so the theory combustion temperature is lower than other gas. But from the economic point to see, the prices of dimethyl ether is lower than other fuel gas and can reduced by 5% when the combustion efficiency of dimethyl ether is the same as liquefied petroleum gas. It is a kind of clean fuel, no residual, no black smoke, low carbon monoxide and nitric oxide emissions, and porcelain products which use it have better gloss and higher quality.

Table 3 the adiabatic combustion temperature of Dimethyl ether, liquefied petroleum gas (LPG) with different oxygen levels

Project	Highest temperature			Average temperature		
	30%	40%	50%	30%	40%	50%
DME	3102.72	3240.79	3229.96	2729.03	2652.63	2643.97
LPG	3191.14	3918.56	4265.61	2805.65	3750.32	3699.1

2. Compare with liquefied petroleum gas (LPG), we find that oxygen level what the dimethyl ether combustion need is less than 30% slightly, but the liquefied petroleum gas combustion need is less than 50% slightly, so amount of oxygen levels dimethyl ether needed is less than liquefied petroleum gas, and the entrance of the air can be done a bit small

Acknowledgments

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