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Simulation of porous medium engine using a detailed chemical kinetics model

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Abstract: The Senkin code of the Chemkin chemical kinetics package is used to simulate the combustion process of a porous medium (PM) engine fueled by n-heptane. The code is modified to incorporate the Woschni heat transfer correlation and heat transfer model within a porous medium. A detailed chemistry mechanism of NO_x formation is coupled with the detailed chemical kinetics mechanism of n-heptane. The code is applied to a zero-dimensional single-zone model of engine combustion. Influences of operating parameters on the performance of the PM engine are discussed. With the increase in the intake temperature and compression ratio, or with the decrease of the excess air ratio, the ignition timing of the PM engine obviously advances. It is found that the porous medium acting as a heat recuperator can considerably preheat the fuel-air mixture, which promotes the ignition and combustion in the cylinder. And the initial PM temperature is a critical factor controlling the compression ignition of the mixture.

Key words: porous medium (PM) engine; single-zone model; numerical simulation

A new concept of a porous medium (PM) engine, based on the combustion in a porous medium, has received attention from numerous researchers because of its potential for producing homogeneous mixtures and reducing NO_x and soot emissions[1].

Recently, development of porous burners has been encouraged by lower emission standards in recent years. As a burner of liquid fuel, the porous medium is also an efficient evaporator. Combined with the large heat capacity of the porous material, large specific surface area with excellent heat transfer in the PM volume makes the fuel droplet vaporization fast and complete[2]. The collision of the fuel droplets within the complex porous structure contributes to effective mixture formation and homogenization, which ensures homogeneous combustion in PM volume. Hanamura et al. [3] designed a reciprocating heat engine, similar to a Stirling engine, based on the technique of super-adiabatic combustion in porous media. Durst et al. [4] proposed two designs of the PM engine. In order to prove the feasibility of the PM engine, they modified a single-cylinder, air cooled diesel engine to incorporate a PM onto the cylinder head and operated it as a PM engine. The engine was operated for several hours without any damage to the PM material or showing any uncontrolled operations.

This paper develops a version of the PM engine fueled by n-heptane based on the design of Durst et al. and presents a single-zone model coupled to investigate the combustion process of the PM engine. A detailed chemical kinetics mechanism for n-heptane oxidation including 566 species and 2 669 reactions is employed, which can satisfactorily predict ignition timing for the HCCI engine[5].

1 Mathematical Model

1.1 Principle of the PM-engine

The PM-engine is here defined as an internal combustion engine with a highly porous medium (PM) chamber mounted on the cylinder head (see Fig. 1). Near the TDC of compression, fuel is injected into the PM volume. Fast fuel evaporation and mixing with air occur in the 3D-structure of the PM volume. The formation of the homogeneous mixture and the 3D-thermal self-ignition in the PM volume create a realizable condition for homogeneous combustion, which is almost independent of the engine load. Furthermore, the heat recuperation of PM may be used for heating up the compressed air and controlling the combustion temperature level.

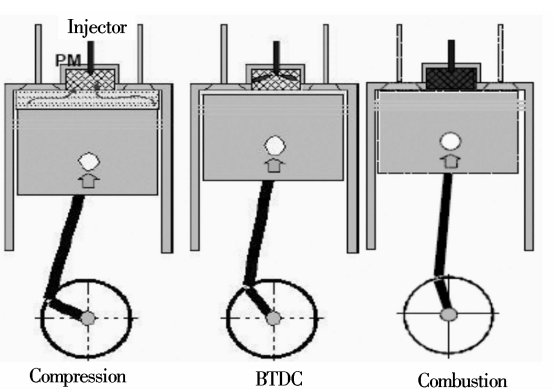

Fig. 1 Principle of the PM-engine cycle

1.2 Model assumptions

In the present model, the combustion chamber is treated as a homogeneous reactor with uniform temperature, pressure and composition. For simplicity, the assumptions concerning the porous medium used in the formulation are as follows:

1) The porous medium with high porosity is homogeneous, continuous and non-catalytic, and the pressure drop across the porous medium is negligible.

2) Fuel evaporating in the porous medium is so fast that it can be assumed that there is no time elapsing for the vaporization.

3) The effect of the porous medium is concentrated in the

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range of a 30 ° crank angle before and behind the TDC, because few mixtures stay in the PM volume when the piston is far from the TDC.

1.3 Thermodynamics and chemical kinetics models

The single-zone model is based on the conservation of mass and energy. A modified version of the SENKIN code is used; i. e. , models for fuel direct-injection and heat transfer in porous medium are incorporated. Main changes to the code include adding a new term to the species and energy equations and, moreover, considering the heat transfer in the porous medium. The mass equation[6] for species k is expressed as

$$\frac{\mathrm{d}m_k}{\mathrm{d}t} = \dot{\omega}_k V W_k + \dot{m}_{\mathrm{f},k} \tag{1}$$

where the mass of species k in cylinder, m_k, can be written as $m_k = mY_k$, in which m is the total mass of the mixture in the cylinder and Y_k is the species mass fraction; $\dot{\omega}_k$ is the molar rate of production calculated by Chemkin[7]; W_k is the molecular weight of species k; $\dot{m}_{\mathrm{f},k}$ is the injected mass of species k per unit time; the instantaneous volume V is calculated by[5]

$$V = V_{\mathrm{PM}}\varepsilon_{\mathrm{PM}} + V_{\mathrm{c}} + \frac{\pi B^2}{4}(l + a - a\cos\varphi + \sqrt{l^2 - a^2\sin^2\varphi}) \tag{2}$$

where V_{c} is the clearance volume; V_{PM} is the total volume of the porous medium chamber; $\varepsilon_{\mathrm{PM}}$ is the porosity of the porous medium; B is the engine bore; l is the connecting rod length; and a is the ratio between l and the crank radius.

Applying the first law of thermodynamics to a closed system yields

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{1}{m\bar{c}_{\mathrm{v}}}\dot{Q}_{\mathrm{inj}} - \frac{1}{m\bar{c}_{\mathrm{v}}}\dot{Q}_{\mathrm{loss}} + \frac{1}{m\bar{c}_v}\dot{Q}_{\mathrm{PM}} - \frac{p}{\bar{c}_{\mathrm{v}}}\frac{\mathrm{d}v}{\mathrm{d}t} - \frac{v}{\bar{c}_{\mathrm{v}}}\sum_{k=1}^{K}\dot{\omega}_k W_k u_k \tag{3}$$

where T is the average temperature of mixture; t is time; p is pressure; v is specific volume; u_k is the internal energy of species k; $\dot{Q}_{\mathrm{loss}}$ is the heat transfer rate through the cylinder wall; $\dot{Q}_{\mathrm{PM}}$ is the heat transfer rate inside the porous medium; the average specific heat for constant volume, $\bar{c}_{\mathrm{v}}$, is defined as $\bar{c}_{\mathrm{v}} = \sum_{k=1}^{K} Y_k c_{\mathrm{v},k}$ and $c_{\mathrm{v},k}$ stays for the specific heat of species k.

The pressure is calculated by

$$p = \left(\sum_{k=1}^{K} X_k\right)RT = \left(\sum_{k=1}^{K}\rho\frac{Y_k}{W_k}\right)RT = \frac{\rho RT}{\overline{W}} \tag{4}$$

where ρ is the mean density of the mixture; R is a gas constant; $\overline{W}$ is the average molecular weight of all species; X_k is the molar fraction of species k.

In Eq. (3), the injection source term $\dot{Q}_{\mathrm{inj}}$[6] can be described as

$$\dot{Q}_{\mathrm{inj}} = \dot{m}_{\mathrm{f}}[u_{\mathrm{fuel}}(T_{\mathrm{inj}}) - h_{\mathrm{evap}} - u_{\mathrm{fuel}}(T)] \tag{5}$$

where $\dot{m}_{\mathrm{f}}$ is the injected mass of fuel per unit time; u_{fuel} and h_{evap} are the specific internal energy and the average heat of vaporization for fuel, respectively; T_{inj} is the temperature of the injected fuel.

Eq. (5) is derived by assuming that the injected fuel evaporates instantaneously and completely. This is a simplification of the reality, because the evaporation takes place at a finite rate and is incomplete. As fluid mechanics and evaporation are not included in the gas-phase Senkin code, the direct-injection process has to be described by the simple model. Nevertheless, the most important effects of the fuel injection are captured by the simplified approach and the modifications described above result in a simple but useful tool for studying the temperature drop in the combustion chamber caused by fuel injection.

Assuming that the fuel is injected by a sinusoidal law, $\dot{m}_{\mathrm{f}}$ is then given by

$$\dot{m}_{\mathrm{f}} = \frac{\pi q_{\mathrm{m}}}{2(t_{\mathrm{E}} - t_{\mathrm{B}})}\sin\frac{\pi(t - t_{\mathrm{B}})}{(t_{\mathrm{E}} - t_{\mathrm{B}})} \tag{6}$$

where q_{m} is the total mass of fuel injected per cycle; t_{E} and t_{B} are the time of fuel injection start and end, respectively.

The overall wall heat loss $\dot{Q}_{\mathrm{loss}}$ is described by the model of Woschni. The heat transfer inside the porous medium $\dot{Q}_{\mathrm{PM}}$ is calculated by a submodel developed in this paper as described below. The variation in the mean temperature $\mathrm{d}T/\mathrm{d}t$ can be calculated by Eq. (3). Combined with Eq. (1) for the mass variation, an ordinary differential equation set of $(K + 1)$ order is built. Under the given initial conditions, the variations in the temperature and species mass fraction are obtained by solving the equation set with the Dvode package of Chemkin which is a variable-coefficient ordinary differential equation solver, with fixed-leading coefficient implementation.

1.4 Heat transfer model for the cylinder wall

The overall wall heat loss is defined as

$$\dot{Q}_{\mathrm{loss}} = -hA(T - T_{\mathrm{w}}) \tag{7}$$

where h is the heat transfer rate coefficient; A is the total area of the combustion chamber including the wall area of the porous medium chamber; and T_{w} is the wall temperature.

The approximation of Woschni is used to calculate the heat rate coefficient:

$$h = 129.8B^{-0.2}P^{0.8}T^{-0.53}\omega^{0.8} \tag{8}$$

where T and P denote the average gas temperature and pressure; B is the cylinder bore; ω is the mean gas velocity.

1.5 Model of heat transfer in porous medium

Studies on porous medium burners[2] show that the evaporation of liquid fuel in a hot porous medium is fast. Considering the assumption of Lucien[6] for HCCI that the injected fuel evaporates instantaneously, we assume that the injected fuel evaporates instantaneously and completely in the porous medium; i. e. , no liquid appears in the porous medium at any time. Thus, the heat transfer in the porous medium occurs only between gas and the solid matrix.

A model for the heat transfer in the porous medium has

been developed, in which the energy equation of the solid matrix is incorporated and the heat transfer rate between gas and the solid matrix is calculated.

The heat transfer rate in porous medium $\dot{Q}_{PM}$ can be described as

$$\dot{Q}_{PM} = h_v V_{PM}(T_s - T_g) = C_{PM} m_{PM} \frac{dT_{PM}}{dt} \quad (9)$$

$$m_{PM} = \rho_{PM} V_{PM}(1 - \varepsilon_{PM}) \quad (10)$$

where T_g and T_s are the temperature of the gas mixture in porous spacing and that of the solid porous media, respectively; h_v is the volumetric heat transfer coefficient between solid and gas. C_{PM}, ρ_{PM} and ε_{PM} are the specific heat, density and the porosity of the porous medium, respectively.

The energy equation for the solid phase[8] is

$$\rho_s c_s \frac{dT_s}{dt} = h_v(T_g - T_s) \quad (11)$$

During the intake stroke and the early compression stroke, only a small amount of air is in contact with the hot porous medium, and the PM-heat capacity has little influence on the in-cylinder air thermodynamic conditions. The heat exchange process intensifies with continual compression. Near the TDC, most of the combustion air is contained inside the PM volume and contacts directly with the solid framework of the PM. Thus, the heat exchange process in the porous medium happens mainly near the TDC. Accordingly, the range over which the porous medium has substantial effects is assumed to be a 330° crank angle up to a 390° crank angle.

1.6 Model of chemical kinetics

In this study, a detailed mechanism for n-heptane oxidation is introduced into the Chemkin code based on the mechanism of Lawrence Livermore National Laboratory (LLNL) with 544 species and 2 446 reactions[9]. The LLNL mechanism has been validated by comparisons with a wide variety of experimental data for HCCI[10]. In these experiments, engine operating conditions are as follows: inlet temperature is 323 K up to 450 K; the equivalence ratio is 0.2 up to 1.5; inlet pressure is 0.1 MPa up to 0.25 MPa; engine speed is 1 000 r/min up to 3 000 r/min.

In the mechanism, the reactions of nitrogen are not included. Thus, a mechanism including 22 species and 123 elementary reactions is distilled from the GRI 3.0 chemical kinetics mechanism, which has been used for combustion in porous medium by Ellzey[8]. As a result, the new mechanisms consist of 566 species and 2 669 reactions. Compared with the LLNL mechanism, approximately the same ignition times for compression combustion processes are predicted[5].

1.7 Engine specifications and operating conditions

Based on the design of Durst et al.[4], a PM engine model derived from a D6114ZG diesel engine is simulated in this paper. It is a typical medium-duty diesel engine and fueled with n-heptane. The basic parameters of the PM engine are listed in Tab. 1. The intake pressure is maintained at 0.1 MPa throughout the study, simulating naturally aspirated operation; the intake temperature of air is 300 K, much lower than that in HCCI(400 K)[11]; the excess air ratio is 2.0; the injection of fuel starts at a BTDC 25° crank angle and ends at a BTDC 10° crank angle.

Tab. 1 Specifications of PM engine

Parameters	Value
Fuel	n-heptane
Bore/mm	114
Stroke/mm	135
Connecting rod length/mm	216
Compression ratio	13
Engine speed/(r · min^{-1})	2 000
Intake temperature/K	300
Intake pressure/MPa	0.1

Note: 0° crank angle is taken to be TDC intake, so TDC is 360° crank angle.

Parameters relevant to the porous medium chamber are as follows. The initial temperature of the PM is 1 050 K. The dimension of the porous medium body mounted on the cylinder head is 40 mm in diameter and 50 mm high. The material of porous ceramic foams is silicon carbide with the porosity $\varepsilon_{PM} = 0.87$, density $\rho_{PM} = 510$ kg/m^3 and specific heat $C_{PM} = 824.7$ J/(kg · K). For convenience of comparison, the operating parameters can be changed separately. The computations are conducted from the beginning of a compression stroke 180° crank angle to the end of a expansion stroke 540° crank angle.

For the PM engine, the existence of the porous medium chamber enlarges the total space volume of the combustion chamber. Sequentially, the actual compression ratio of the PM engine is smaller than that of the original engine. Fresh air has been assumed as the initial mixture composition in the PM engine.

2 Results and Discussion

It is well known that the auto-ignition temperature of hydrocarbon fuels used in engines has often been determined according to the sudden jump in the in-cylinder gas pressure or temperature[11]. Hence, as key parameters for controlling the auto-ignition process, the changes in the in-cylinder gas pressure or temperature are mainly investigated in this paper.

2.1 Influence of the initial temperature

The effect of the intake temperature on the in-cylinder temperature and pressure is shown in Fig. 2. The injection of fuel starts at a BTDC 25° crank angle and ends at a BTDC 15° crank angle. It can be seen that the crank angle position of the auto-ignition varies within a 5° crank angle, as the intake

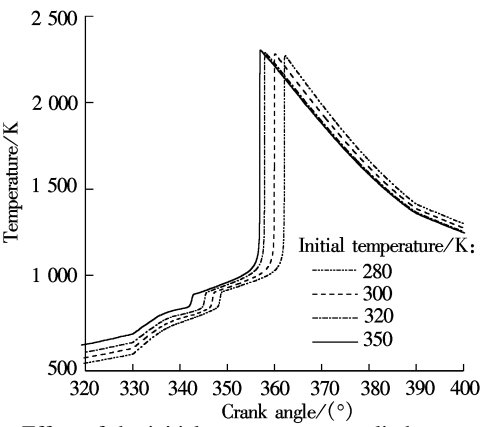

Fig. 2 Effect of the initial temperature on cylinder temperature

temperature changes from 280 to 350 K. Even at a low intake temperature (280 K), the ignition can still take place. It means that the intake temperature is not a decisive factor for ignition, which is different from that of the HCCI engine and indicates a characteristic of the PM engine. Because at the end of compression stroke, the porous medium with high heat capacity and large specific surface area influences the thermodynamic properties of the charge in the cylinder significantly. Thus, to realize compression ignition in the porous medium engine, it is not necessary to preheat the intake gas, and the ambient temperature for the intake gas is high enough.

Fig. 2 also shows that the gas temperature obviously increases since the preheating effect of the porous medium comes into operation at a condition of $\lambda = 2.0$, CR = 13. When the fuel injection starts (BTDC 25° crank angle), the temperature curves become smooth. Next to this, an obvious two-stage ignition process including low and high temperature kinetic reactions is displayed. With the increase in the initial temperature, both the low and high temperature reactions advance. The ignition process of the PM engine in the cylinder zone is approximated with an HCCI engine and completely identical to the chemical kinetics mechanism of high carbon fuel.

It is noted that for an HCCI engine, the initial temperature must be high enough to enable an auto-ignition. However, the PM engine can be ignited with lower initial temperature(280 K), so the auto-ignition in the PM engine is not restricted by the initial gas temperature.

2.2 Influence of the compression ratio

Fig. 3 shows the effect of the compression ratio on the in-cylinder temperature of the PM engine. It can be seen that the auto-ignition cannot occur at the compression ratio of 8. With increasing compression ratios, the ignition timing obviously advances and the maximum temperature in the cylinder greatly increases. For the PM engine, the compression ratio is an important factor influencing the auto-ignition timing; however, it is not similar to that of the HCCI engine. The hot porous medium greatly influences the temperature of the mixture before ignition, which promotes the occurrence of the low temperature reaction. Therefore, the ignition and combustion in the cylinder occur more easily. In order to pursue a balance between heat efficiency and emissions of NO_x and HC, it is still important to choose a proper compression ratio to maintain the ignition near the TDC.

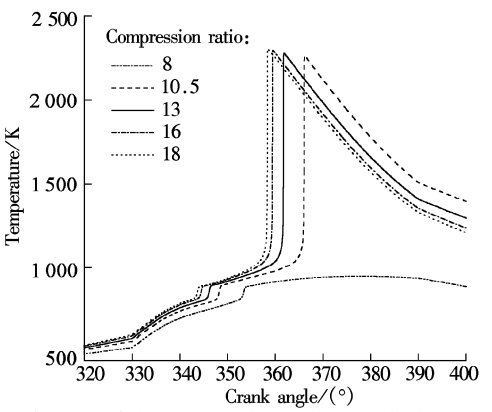

Fig. 3 Influence of the compression ratio on cylinder temperature

2.3 Influence of the excess air ratio

Fig. 4 shows the effect of the excess air ratio λ on the temperature in the PM engine at a condition of CR = 13, T_0 = 300 K, p_0 = 0.1 MPa. At $\lambda = 1.0$, the maximum temperature is extremely high and the ignition delay reaches the shortest. With increasing excess air ratios, the maximum temperature evidently drops and the time of the auto-ignition in the cylinder occurs late, until it cannot ignite for $\lambda = 4.5$. That is because a high excess air ratio means less injected fuel for the same air intake, and an excess lean mixture retards the ignition and heat release. Moreover, the calculation indicates that the combustion efficiency increases with the increase in excess air ratios, because sufficient oxygen ensures more complete combustion. Furthermore, it is easy to understand that the exhaust concentrations of NO, CO_2 and CO, as a function of the excess air ratio, will also decrease. It can be concluded that the excess air ratio must be properly determined to ensure the ignition and low emissions for the PM engine.

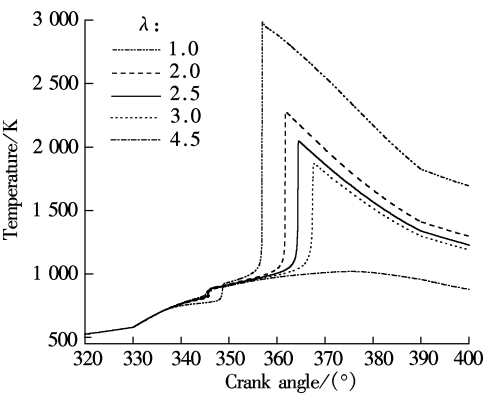

Fig. 4 Effect of the excess air ratio on cylinder temperature

2.4 Influence of the initial temperature of porous medium

Fig. 5 shows the effects of the initial temperature of the porous medium on the temperatures of the in-cylinder gas and the porous medium at a condition of $N = 2\,000$ r/min, $\lambda = 2.0$, CR = 13, $p_0 = 0.1$ MPa, $T_0 = 300$ K. It can be seen that the combustion cannot occur with an initial temperature of the porous medium as low as 900 K. With the increase in the initial temperature of the porous medium, ignition evidently advances and the maximum gas temperature also increases. The initial PM temperature is one of the crucial factors determining the auto-ignition timing. To guarantee the ignition in the PM engine at a given compression ratio, the initial PM temperature should be maintained at a high level. However, excessive high initial PM temperatures will result in an increase in the combustion temperature; consequently, the emission of NO_x will increase. There should be an optimal initial PM temperature, which can, on the one hand, realize the compression ignition of the PM engine and guarantee the next working cycle, and, on the other hand, avoid the rise of NO_x emissions.

As shown in Fig. 5, the temperature of the porous medium stays at a relatively steady level during a working cycle and its changes are limited to within 50 K. The initial temperature of the PM is mainly determined by the properties of the porous medium and heat transfer with the porous medium.

3 Conclusions

A single-zone combustion model using the Senkin code of

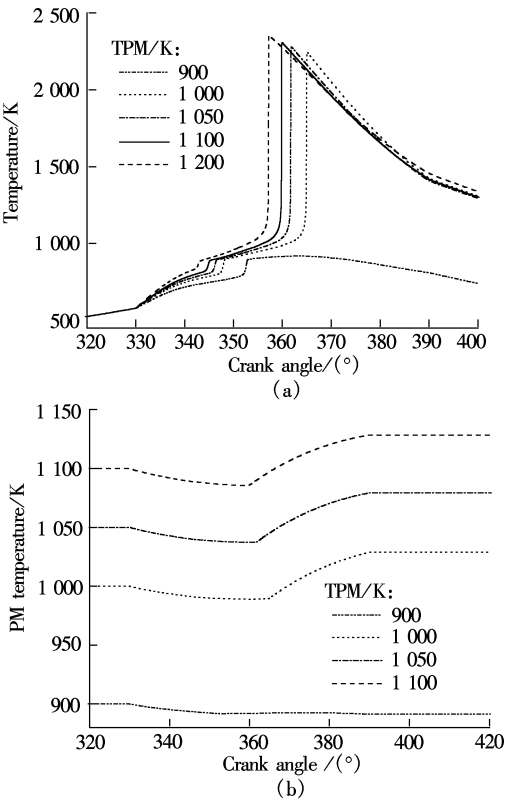

Fig. 5 Effect of the initial temperature of the porous medium on in-cylinder and PM temperature. (a) In-cylinder temperature; (b) PM temperature

the Chemkin kinetic solver, which has been modified to incorporate models for heat transfer in the porous medium and for the fuel injection, etc., is developed to simulate the combustion process of a PM engine. From the numerical investigation, the following conclusions can be made:

1) The PM engine is modified by a direct injection engine. A homogenous mixture formation and high initial temperature for the fuel are not needed as in the HCCI engine.

2) For the PM engine, the effect of the compression ratio on the ignition is not so important as in an HCCI engine because the heat recovered by the PM enhances the ignition in the cylinder. This means that the operating range of the PM engine can be expanded more readily to large loads than in the case of the HCCI engine.

3) At a given compression ratio, the initial temperature of the porous medium is a crucial factor for determining the ignition timing in the PM engine. During a working cycle, the PM temperature has only a slight change (within 50 K).

4) There should be an optimal match among the compression ratio, the initial temperature of the porous medium and other operation parameters, which can guarantee the compression ignition in the PM engine and also reduce the emission of NO_x.

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多孔介质发动机详细反应动力学模型

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摘要: 应用 Chemkin 化学动力学软件包中的 Senkin 模块模拟了正庚烷在多孔介质发动机中的燃烧过程. 通过修改 Senkin 程序,结合了 Woschni 传热模型和多孔介质换热模型,并在正庚烷详细氧化机理中加入氮氧化物的生成机理,将此程序纳入发动机燃烧的零维单区模型. 对多种工况参数进行计算,讨论了运行参数对发动机性能的影响. 当进气温度、压缩比增大,或过量空气系数降低时,多孔介质发动机着火时刻会明显提前. 结果表明:多孔介质对混合气具有预热作用可强化发动机的点火燃烧,多孔介质的初始温度是决定压燃点火的决定性因素.

关键词: 多孔介质(PM)发动机;单区模型;数值模型
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