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# Numerical study on the realization of compression ignition in a type of porous medium engine fueled with Isooctane

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#### ABSTRACT

The working process of a porous medium (PM) engine, characterized as periodic contact type and fueled with liquid fuel as Isooctane, is simulated by using an improved version of KIVA-3V. A modified volumeaveraged method is proposed for describing the interaction between fuel droplets and the solid phase of the PM. The improved version of KIVA-3V was validated by simulating the experiment of Zhdanok for the superadiabatic combustion of  $CH<sub>4</sub>$ -air mixtures under filtration in a packed bed. Good agreement between experimental data and computational results for the speed of combustion wave is achieved. The influences of initial PM temperature, PM structure and valve opening timing on the realization of compression ignition in the PM engine are also verified. Initial PM temperature is the crucial factor in guaranteeing the realization of the compression ignition of the PM engine. Considering influential factors, such as the properties of the PM, the compression ratio, the equivalence ratio, and the heat transfer between gas and solid phase of the PM should obtain optimized initial PM temperature. The variation in PM structure affects the convective heat transfer between the gas and solid phase and the dispersion effect of the PM. Compression ignition all can be realized in PM engines with four kinds of PM. Compression ignition is achieved at the considered four valve opening timings. Value opening timing has influence on the average temperature of the PM engine and the working of the PM engine does not allow earlier or later valve opening timing.

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#### 1. Introduction

Emission and energy saving of internal combustion engine become a major concern in both the developed and the developing world. Homogeneous mixture preparation and controllable combustion offer the most effective measure for energy saving and significant reduction of emissions of internal combustion engine. Combustion of hydrocarbon fuels within an inert porous medium (PM) provides a number of advantages, such as forming homogeneous fuel and air mixture, extending flammable limits and operating over a wide range of loads [\[1–3\].](#page--1-0) Hence, introduction of the PM combustion technique into internal combustion engine has a great potential in improving combustion efficiency and reducing NOx and CO emissions.

PM engine is a new concept for implementing homogeneous combustion in internal combustion engine. PM engine concept, firstly proposed by Durst and Weclas based on PM combustion technique, promises well in attaining the homogeneous combustion and meets the requirements of energy saving and emission reduction [\[4\].](#page--1-0) They proposed two type of PM engine, one is permanent contact type and another is periodic contact type. In PM engine with permanent contact type of PM chamber, the working process is similar to that of conventional engine. The main difference in the working process between PM engine with periodic contact type of PM chamber and conventional engine results from the existence of a valve in PM engine, which realize the periodic contact of the PM chamber and engine cylinder.

The PM contacts periodically with the working gas in the engine cylinder of the PM engine as periodic contact type. [Fig. 1](#page-1-0) shows a schematic working process diagram of the periodic type PM engine. The valve between the PM chamber and engine cylinder closes and fuel is injected in the PM chamber at the end of the expansion stroke, as shown in [Fig. 1](#page-1-0)d. Low pressure and high temperature in the PM provide conditions for the rapid evaporation of fuel droplets. Because the amount of oxygen in the PM chamber is very few, the mixture of evaporated fuel vapor and gas cannot be ignited in the closed PM. During the exhaust, intake and compression stoke, the value remain closed. Near the TDC (Top Dead Center) the valve opens and the compressed air flows from the cylinder to the hot PM. Homogenous combustion then will be accomplished in the PM chamber.

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Fig. 1. Schematic drawing of the working process of periodic contact type PM engine.

Until now, PM engine has not received much attention in engine research communities. Durst and Weclas performed experiments on a test PM engine with permanent contact type of PM chamber, which was modified by inserting a SiC PM into the engine head between the intake and exhaust valves [\[4\].](#page--1-0) Their results demonstrated many attracting characteristics of the PM engine in comparison with that of the original engine, such as a very low emission level, higher cycle efficiency, and low combustion noise. Based on a multi-zone combustion model, Jan Macek modeled the working process of a PM engine fueled with methane and hydrogen respectively, and discussed some important issues concerning its practical applications [\[5\].](#page--1-0)

In this study, the working process and some influential factors for the realization of compression ignition of a PM engine fueled with Isooctane, in the case of periodic contact between the engine cylinder and the PM, are investigated by using an improved version of CFD code KIVA-3V [\[6\]](#page--1-0).

#### 2. Numerical models

The KIVA-3V code is incorporated with the chemical kinetics software Chemkin-3.0 [\[7\]](#page--1-0). The solving of one more energy conservation equation for describing the change in the temperature of solid phase of the PM is realized. An interaction model describing the impingement and heat transfer between fuel droplets and the solid phase of the PM is also included in the version of KIVA-3V. The simplified Rossland model is used to compute the heat radiation in the PM and the Ergun equation for the flow resistance caused by the PM. The dispersion effects of the PM on energy and species diffusion are considered. We use a reduced chemical kinetic mechanism that consists of 38 species participating 69 elementary reactions [\[8\]](#page--1-0) for modeling the oxidation of Isooctane in the PM engine. Numerical computation is carried out under the experimental conditions conducted by Zhdanok et al. [\[9\]](#page--1-0) to validate the reasonability of the modified version of KIVA-3V code [\[10\]](#page--1-0).

#### 2.1. Governing equations

Gas phase radiation in PM is negligible and the PM is assumed inert and does no influence on the chemical reactions. Heat transfer between gas and solid matrix is considered. The conservation equations for gas phase energy, solid phase energy, gas species and momentum in PM domain are given as follows. Other relevant conservation equations can be found in the related Ref. [\[11\].](#page--1-0)

The gas phase energy conservation equation is

$$
\frac{\partial}{\partial t} \left( \varepsilon \rho_g c_p T_g \right) + \nabla \bullet \left( \rho_g c_p \vec{u} T_g \right) + \varepsilon \sum_i \omega_i h_i W
$$
\n
$$
= \nabla \bullet \left( \varepsilon \lambda_g' \nabla T_g \right) + h_p (T_s - T_g) \tag{1}
$$

where  $\varepsilon$  is the porosity of the PM,  $T_g$  is the temperature of the gas phase of the PM,  $T_s$  is the temperature of solid phase of the PM.  $\lambda'_g$ is the corrected thermal conductivity of gas in the PM [\[12\],](#page--1-0)  $\lambda_{\rm g}^\prime = \Big(\epsilon + {\rm 0.1} \Big[{\rm Pr} \Big(\frac{\rho_{\rm g} u d_{\rm p}}{\mu}$  $\left(\varepsilon + 0.1 \left[ \Pr\left(\frac{\rho_g u d_p}{u}\right) \right] \right) \lambda_g$ , where  $\lambda_g$  is the thermal conductivity of the gas phase in the PM and  $d_p =$  $\frac{\sqrt{4\varepsilon/\pi}}{PPC}$  (cm) [\[13\]](#page--1-0).

The solid phase energy conservation equation is

$$
\frac{\partial}{\partial t}[(1-\varepsilon)\rho_s c_s T_s] = \nabla \bullet [(1-\varepsilon)\lambda_s \nabla T_s] - h_p (T_s - T_g) - \text{div} q_r \tag{2}
$$

where  $h_n$  is the volume heat transfer coefficient [\[14\]](#page--1-0) between the gas and solid phase of the PM, which is derived from  $\frac{h_p d_p^2}{\lambda_g} = \left[0.0426 + \frac{1.236}{L/d_p}\right]$ Re<sub>dp</sub>, where Re<sub>dp</sub> =  $\rho ud_p/\mu$ .  $\lambda_s$  is the thermal conductivity of the solid phase in the PM. The radiant heat flux in the solid phase of the PM is modeled with the simplified Rossland model in which the radiant heat flux is expressed as  $q_r(x) = -\frac{16}{3} \frac{\sigma T_s^3}{\beta} \frac{dT_s}{dx}$ ,  $\beta = \frac{3}{d_p(1-\epsilon)}$  [\[15\]](#page--1-0). The radiation characteristics of the PM are described by the parameters of porosity  $\varepsilon$  and pore diameter  $d_p$ . So, Eq. (2) can be rewritten as the following.

$$
\frac{\partial}{\partial t}[(1-\varepsilon)\rho_s c_s T_s] = \nabla \bullet (\lambda_{\text{eff}} \nabla T_s) - h_p (T_s - T_g)
$$
\n(3)

 $\lambda_{\text{eff}}$  is the effective thermal conductivity of the PM and is solved by the following equation:  $\lambda_{eff} = \lambda_e + \lambda_r$ , where  $\lambda_e = \lambda_s(1 - \varepsilon)$  and  $\lambda_r = 16\sigma T_s^3 d_p (1-\varepsilon)/9.$ 

The species conservation equation is

$$
\frac{\partial}{\partial t}(\varepsilon \rho_g Y_i) + \nabla \bullet (\rho_g \vec{u} Y_i) + \nabla \bullet (\rho_g \varepsilon Y_i V_i) - \varepsilon \omega_i W_i = 0 \tag{4}
$$

where  $V_i = -(D + D_{\parallel m}^d) \frac{1}{Y_i} \nabla Y_i$ ,  $D_{\parallel m}^d/D = 0.5Pe$  [\[14\]](#page--1-0),  $Pe = \rho_g C_p u d_p / \lambda_g$ . The momentum equation is

$$
\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_j u_i) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] + S_i
$$
(5)

The Ergun model modified by Macdonald et al. [\[16\]](#page--1-0) is used to calculate the last term on the right-hand side of Eq. (4).  $S_i = -(\frac{\mu}{\alpha}u_i + C_2\frac{1}{2}\rho u_{mag}u_i), \text{ where } \alpha = \frac{D_p^2}{150}\frac{\varepsilon^3}{(1-\varepsilon)^2}, C_2 = \frac{3.5}{D_p}\frac{(1-\varepsilon)}{\varepsilon^3}, D_p \text{ is}$ the equivalent particle diameter of the PM. Gas densities are computed from the ideal gas equation of state for a multi-component mixture,  $P = \rho_g RT_g / \overline{W}$ .

#### 2.2. Interaction model between fuel droplets and solid phase of the PM

Experimental research about interaction between fuel spray and porous medium was ever reported [\[17\].](#page--1-0) For simulating the interaction between fuel liquid jet and the solid phase of the PM, an implemented volume-averaged method is proposed. In the method, the solid phase of the PM in one control volume is regard as an assumed ball located at the center of the control volume. The diameter of the ball is derived according to the porosity and the volume of the control volume. The ball occupies some space but has no impact on the fluid flow in the control volume. When fuel droplet impinges on the surface of the assumed ball, the variation in the velocity of the droplet and the heat transfer between the fuel droplet and the solid phase of the PM are determined by the interaction model, which was developed in Ref. [\[18\]](#page--1-0).

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