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Review

Numerical simulation of catalysis combustion inside micro free-piston engine

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ABSTRACT

In order to investigate the catalytic combustion characteristics concerning homogeneous charge compression ignition (HCCI) in micro power device, numerical simulations with a 3D computation model that coupled motion of free piston and fluid dynamics of methane–air mixture flow were carried out and detailed gas-phase and surface catalytic reaction mechanisms of methane–air mixture were applied to the catalytic reactions model, a series of mathematical formula are established to predict the characteristics of compression ignition condition, impacts of catalysis on temperature, pressure, work capacity and other factors were analyzed respectively. Simulation results reveal that catalytic combustion facilitates the improvement of energy conversion efficiency and extends the ignition limit of methane–air mixture obviously, the ignition timing is brought forward as well, while compression ratio decreases and ignition delay period shrinks significantly. Numerical results demonstrate that the existence of catalytic wall helped to restrain the peak combustion pressure and maximum rate of pressure rise contributing to the steadily and reliability of operation inside micro free-piston power device.

Contents

1. Introduction . . . 243
2. Numerical simulation models . . . 245
 2.1. Physical model. . . . 245
 2.2. Mathematical model . . . 245
 2.3. Chemical kinetics model . . . 245
 2.4. Model validation . . . 246
3. Dynamic grid implementation and numerical computation method . . . 247
4. Results and discussion . . . 247
 4.1. Influence of the catalysis on the compression ignition timing and compression ratio. . . . 247
 4.2. Influence of catalysis on combustion limits . . . 249
 4.3. Influence of the catalysis on temperature, pressure in the micro combustion chamber . . . 249
 4.4. Influence of the catalysis on work capacity of the micro free-piston engine . . . 250
5. Conclusion . . . 250
 Acknowledgments . . . 251
 References . . . 251

1. Introduction

With the development of micro-electro mechanical system (MEMS) [1] and micro machining technology, considerable progress has been made at miniaturization of electro-mechanical equipment in recent years [2,3], yet their primary power source,

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Nomenclature

A	cross-sectional area of the piston
A_L	the clearance area
At	the area in contact with the high temperature gas
D_n	diameter of free piston
e	unit mass with fluid internal energy
$F_{S,j}$	diffusion flow
h_h	the convective heat-transfer coefficient
u_i	absolute velocity in the x_i direction
k_r	reaction rate constant of the R_{th} reaction
L_n	length of combustor u_{rs}
m	mass of free piston
P_0	the external atmospheric pressure
$P_t\,(x, y, z)$	pressure
P_∞, T_∞	ambient pressure and temperature
K_S	number of elementary reactions on surface
M_S	molar mass of components R_S
$N_g + N_S$	number of ingredients
q_i	energy flux of x_i direction
R_S	reaction rate of mass of the component
R_m	the mixed gas constant
s_h	energy generation source
s_i	momentum generated source phase
s_m	quality generation source
t	time
$T_t\,(x, y, z)$	temperature
T_w	the wall temperature
u_n	velocity component of Stenfan flow
ε_{rs}	override parameters
V	the compressed volume of the piston
$\overline{v}$	the average velocity of the piston
v_{rs}, v'_{jr}	chemistry equivalent coefficient
V_t	chamber volume
x_i	cartesian coordinate
x_j	concentration of j component
$y(P, P_o, \gamma)$	indicates the stream function
$Y_{nt}\,(x, y, z)$	concentration of each component

Greek variables

ρ	denotes fluid density
τ_{ij}	stress tensor
Θ_S	surface coverage of the component S

i.e., batteries, remain essentially unchanged, but their intrinsically lower energy densities and short lifetimes impose a fundament limitation [4]. The batteries have quite low specific energy (0.6 kJ/g for alkaline battery and 1.2 kJ/g for lithium battery) compared to hydrogen (140 kJ/g) and hydrocarbon fuels, miniature power plants based on kinetic energy are prominently potential and promising [5]. However, there are two major challenges in maintaining stable combustion inside a micro reactor, fame quenching due to heat loss and insufficient fuel reaction time on the micro scale [6,7]. The catalytic combustion with HCCI is one of the critical approaches to solve problems proposed above in micro power device [8–11] and there are a few exclusively superiority reflected in a few aspects: catalytic reactions often have lower activation energies than homogeneous reactions. Using the catalyst wall can ensure intensive reactions and reduce heat loss through the reactor and radical depletion on the wall.

In order to improve the thermal efficiency and combustion stability of micro combustors, various efforts have been made regarding optimization of thermal management and the use of catalysts [12–14,8]. Aichlmayr [15–18] at Departments of Mechanical Engineering and Chemistry of the Minnesota University made great efforts and conducted a series of single shot combustion experiments on the rapid compression expansion machine to investigate micro HCCI combustion. Mikalsen and Roskilly [19] use a computational fluid dynamics engine model as well as a zero dimensional single-zone model to investigate the in-cylinder gas motion, combustion process and nitrogen oxide formation in a free-piston diesel engine and compare the results to those of conventional engine. Ju and Xu [20] theoretically and experimentally studied mesoscale flame propagation and extinction of premixed flames in channels. Their results showed that channel width, flow velocity, and wall thermal properties have dramatic effects on the flame propagation and lead to multiple flame regimes and extinction limits. Yang et al. [11] performed comparative experiments of methane, methanol and ethanol combustion in micro channel bed combustors. They evaluated the performances of combustors with the ZSM-5 zeolite supported nanometer-sized Pt as the catalyst, but the efficiencies in the packed bed combustor were not analyzed in detail. Smyth et al. [21], and Evans and Kyritsis [22] investigated catalytic micro-combustion flows over small-scale flat plates for methane and propane fuel. Their numerical simulation and experimental results indicated that the catalytic reaction of hydrogen (methane) can be self-sustained in a platinum tube with a 0.1-mm (0.4-mm) inner diameter. Being limited by the size, it is difficult to obtain information inside a micro-reactor by systematic experimental studies and, in fact, most previous works acquired only outlet information. Besides effects of the piston initial velocity, piston mass, micro-combustor geometric parameter, equivalence ratio and leakage on critical initial kinetic energy were analyzed by Wang et al. [23], the mathematical formula was obtained for predicting the critical compression ignition condition.

The studies mentioned above show that the research on the micro free piston is nearly in the fundamental stage, but dynamic model of catalytic combustion inside micro power device is still not fully understood or well documented. The aim of this study is to conduct catalytic combustion process and investigate the impact factors on catalytic combustion inside micro free-piston device, a 3D computation model that coupled motion of free piston and fluid dynamics of methane–air mixture flow is built through computational fluid dynamics (CFD) software, CFD software coupled with CHEMKIN [24] is used to perform these calculations. By compiling a user-defined function (UDF) file, the motion law of free piston is defined. The catalyst was coated at the bottom of the micro chamber of 20 mm length; the influences of catalytic combustion on ignition timing, compression ratio, temperature, pressure, combustion limits, and work capacity were investigated. The research of this paper could enrich the theory of combustion in the micro chamber, which has reference value for the analysis on steadily and reliability of operation inside micro free-piston power device.

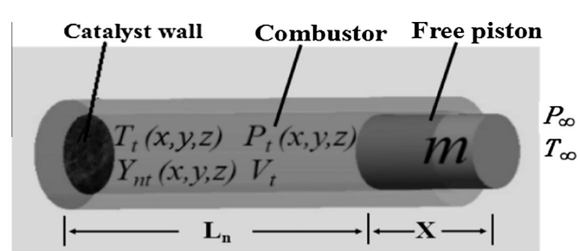

Fig. 1. Physical model.