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Modeling and analysis of heat and mass transfers of supercritical hydrocarbon fuel with pyrolysis in mini-channel

Yu Feng [a,1], Jiang Qin [b,2,*], Silong Zhang [b,3], Wen Bao [b,4], Yong Cao [a,5], Hongyan Huang [b,6]

[a] Harbin Institute of Technology, Shenzhen Graduate School, Guangdong 518055, People's Republic of China
[b] Harbin Institute of Technology, Heilongjiang 150001, People's Republic of China

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ABSTRACT

A 2D numerical model was established with unstructured mesh using Time-marching algorithms with preconditioning to investigate the heat and mass transfer of supercritical hydrocarbon fuel with pyrolysis in mini-channel. The three-parameter RK-PR EoS, which is the unified form of SRK and PR EoS, was used to describe the thermophysical properties of cracked fuel mixture including small and large hydrocarbon molecules. Then, Numerical tests indicated that the present numerical model was able to predict the variation of the supercritical reaction flow field with small velocity effectively. Then, the numerical model was employed to study the coupling relationships and interaction mechanisms of flow, heat transfer and pyrolysis in the chemical reaction flow field, and it was found that there was a chemical reaction boundary in addition to velocity and temperature boundary layers in the chemical reaction flow field. And the gradients of velocity and temperature in the flow direction increased and decreased respectively under the influence of pyrolysis. The chemical heat sink exhibited non-uniformity in the cross-section of channel. But, the non-uniformity of chemical heat sink decreased due to heat and mass transfers in the radial.

1. Introduction

Among all the advanced aeroengines used to power aircraft, rockets, and missiles, the scramjet has the largest heat load. Hydrocarbon fuel has been used as a coolant in the regenerative cooling system of a scramjet to avoid the penalty of carrying additional coolant [1,2], because the endothermic reaction of supercritical hydrocarbon fuel under high temperature can provide an extremely high chemical endothermic ability, which is also generally referred to as chemical heat sink [3,4]. Hydrocarbon fuel can produces several smaller hydrocarbon molecules in the pyrolysis reaction process to form the cracked fuel mixture with fuel and the pyrolysis distribution of hydrocarbon fuel can be called as the chemical reaction field. The pyrolysis have its effect on the flow field distribution by changing the local physical quantities such as density, C_p and so on [5]. Meanwhile, the distributions of flow and heat transfer in flow field can have its effect on the reaction rate and the residence time of hydrocarbon fuel [6]. So, there is a highly coupled relationship among flow, heat transfer and pyrolysis. Moreover, the transportation of mass and energy among hydrocarbon molecules causes a more complex heat and mass transfer problem in the flow field. It can therefore be seen from the above that a series of complex heat and mass transfers are contained in the Chemical reaction flow field of supercritical hydrocarbon fuel, which made it difficult to control the release of chemical heat sink [5,6]. So, the reasonable organization of the fuel flow and heat and mass transfers to control the release of the chemical heat sink is very important for the development of a regenerative cooling system for a scramjet.

The chemical reaction flow field of supercritical hydrocarbon fuel in a cooling channel features: (1) a real gas model is needed to describe variations of fuel physical properties under supercritical pressure [5]; (2) a highly coupled process among the flow, heat transfer and pyrolysis [5]; (3) the velocity of flow field is low, but the density is changing with the temperature and pyrolysis, and the flow field has great compressibility. So, there is a numerical stiffness problem while Time-marching algorithms was used to deal with these problems [7,8].

* Corresponding author.
E-mail addresses: yufeng@hitsz.edu.cn (Y. Feng), qinjiang@hit.edu.cn (J. Qin), zslhrb@gmail.com (S. Zhang), baowen@hit.edu.cn (W. Bao), yongc@hitsz.edu.cn (Y. Cao), huang_hy04@hit.edu.cn (H. Huang).
[1] Postdoctoral fellow, School of Mechanical Engineering and Automation.
[2] Assistant professor, College of Fundamental and Interdisciplinary Sciences.
[3] Ph.D., School of Energy Science and Engineering.
[4] Professor, School of Energy Science and Engineering.
[5] Associate professor, School of Mechanical Engineering and Automation.
[6] Professor, School of Energy Science and Engineering.

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Nomenclature

A_f	pre-exponential factors, s^{-1}
C_p	specific heat capacity at constant pressure, J kg^{-1} K^{-1}
D	diffusion coefficient, m^2 s^{-1}; diagonal matrix
F, G	vector of convective flux
L	length of channel, m/s; upper triangular matrix
k_f	reaction rate constant
$M^{\pm}_{(4)}$	split Mach numbers
n	component number
$P^{\pm}_{(5)}$	split pressure
R_o	universal gas constant, 8.3145 J mol^{-1} K^{-1}
s	area, m^2
T	temperature, K
V	volume, m^3
Y	species mass fraction
u^+	dimensionless friction velocity
y^+	dimensionless friction distance

Greek

ρ	density, kg m^{-3}
λ	eigenvalue of Jacobian matrix; thermal conductivity, W m^{-1} K^{-1}
τ	viscous stress, N m^{-2}
ω	chemical reaction rate, kg s^{-1} m^{-3}

Subscripts

in	inlet
i	species
a	speed of sound, m/s; thermal diffusivity, m^2/s;
C_v	specific heat capacity at constant volume, J kg^{-1} K^{-1}
E	activation energy, kJ/mol
H	specific total enthalpy, J kg^{-1}
k	karman constant
M	molecular weight, kg/mol
m	mass flux
P	pressure, Pa
Q	conservation variable
S	source term
t	time, s
U	velocity vector, m/s; lower triangular matrix
X	species mole fraction
u,*v*	*x*-component and *y*-component of velocity, m/s
Z_c	critical compressibility factor
Θ	scaling factor
ε	preconditioning factor
μ	dynamic viscosity, Pa s
γ	ratio of specific heat
out	outlet
v	viscosity

Much work has been done on chemical reaction flow field. For example, Hu et al. [9], Lan et al. [10], built a multi-dimensional calculation model for the convection heat transfer in ethylene cracking furnace. Sheu et al. [11] built supercritical reacting flow numerical models for Norpar-13 and analyzed the influence of thermal pyrolysis on the convective heat transfer of Norpar-13. Ward et al. [12] built Proportional Product Distribution Chemical Model (PPD) based on experimentally measured proportional distributions of n-decane. Meanwhile, they developed a two-dimensional reacting flow numerical model and analyzed the influence of pressure on thermal pyrolysis from the view point of reaction mechanism. Ruan et al. [1] and Bao et al. [5] developed a supercritical hydrocarbon reacting flow numerical model using commercial CFD package base on pressure-based numerical algorithm and analyzed the supercritical hydrocarbon fuel reaction flow field in detail. However, all these models mentioned above have their own limitations, it is of great necessity to develop a numeric calculation model, in which physical property method of stronger universality and coupling solution method for flow controlling and composition equations are used.

Therefore, a 2D numerical model was established using Time-marching algorithms with preconditioning, and the flow controlling and composition equations were solved in a coupled way. The RK-PR EoS demonstrated over a wide range of thermodynamics and hydrocarbons was used to describe the *P*–*V*–*T* behaviors [13,14]. The present scheme was validated by two benchmarks and experimental effectively. Then, the velocity, temperature and pyrolysis contours in supercritical hydrocarbon chemical reaction flow field were analyzed using the numerical model verified. And the factors having their effects on the release of chemical heat sink were proposed.

2. Numerical model and methodology

In order to avoid phase change and to improve the heat transfer in the cooling process, the operational pressure of hydrocarbon fuel in the cooling panel is kept above the supercritical pressure in the regenerative cooled scramjet. As shown in Fig. 1, the scramjet engine consists of a series of ramps which experiences the highest heat flux. The typical ramp heat flux of a scramjet ranges from 2 to 20 MW/m^2 and can go up to 700–800 K. Thermal pyrolysis of fuel occurs at a temperature above 800 K in cooling channel [15], of which hydraulic diameter is 0.5–2 mm. Hydrocarbon fuel cools the combustion chamber flowing through the cooling channel. In the heat convection of hydrocarbon fuel with wall, hydrocarbon molecules crack into several smaller molecules, such as CH_4, C_2H_4, C_2H_6 and so on, with the release of chemical heat sink.

The numerical study on the supercritical chemical reacting flow field is based on conservation equations of component, momentum and energy, equation of state and accurate evaluations of transport properties. Because of the coupling characteristics among flow, heat transfer and pyrolysis in the chemical reaction flow field of supercritical hydrocarbon fuel, a numerical model of coupling solution was established using Time-marching algorithms.

2.1. Time-derivative preconditioning

Coupling solution method for flow controlling and composition equations was used to solve supercritical hydrocarbon reaction flow field on the base of Time-marching algorithms. However, in the low subsonic Mach number regime, the convective terms of governing equations become stiff, because of large condition number, Time-marching algorithms converges very slowly [16]. In order to circumvent this numerical difficulty, preconditioning scheme for real-fluid was employed in this paper. Because ideal gas is a special case of real-fluid, preconditioning scheme for real-fluid is suitable to ideal gas [16]. The 2D, preconditioned N–S system can be written in Cartesian coordinates as shown below:

$$\Gamma\frac{\partial Q}{\partial t}+\frac{\partial(F-F_v)}{\partial x}+\frac{\partial(G-G_v)}{\partial y}=S \tag{1}$$

Vector of primitive variables Q are chosen as: