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Numerical investigation of distribution of reaction rate during convective heat transfer with endothermic chemical reaction

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ABSTRACT

The reaction rate for thermal chemical reaction is an intensive quantity characteristic of process, and reflects the general influence of such factors as heat transfer and mass transfer on the chemical reaction. The distribution of reaction rate during convective heat transfer with endothermic chemical reaction in channel was numerically investigated using a 2D model. Simulation results indicated that there was a layer distribution of reaction rate in the flow field, which was similar to a thermal boundary layer. The reaction rate near wall was much higher than that in the core flow region, and there was a dramatic increase in reaction rate in the very thin layer near the wall. Moreover, the distribution of reaction rate was affected by the negative feedback effect of transformations of mass and energy. The distribution of reaction rate, which was contrary to the thermal boundary layer, could be eventually obtained because the distribution of reaction rate could change over a short distance once the heat absorbed by reactant was less than the internal energy transformed into chemical energy.

1. Introduction

The convective heat transfer with endothermic chemical reaction plays an important role in such engineering applications as regeneratively cooled scramjet, the real gas effects in hypersonic flight, etc. [1–6]. In order to accurately control the heat transfer process in the optimization design for engineering applications [6,7], it is therefore of great importance to better understand the endothermic chemical reaction in flow field. However, endothermic chemical reaction in the convective heat transfer is very complicated, because the chemical reaction is a non-linear transform process of mass and energy in addition to the complicated reaction mechanism [7–9], and there is a strongly coupled relationship between heat and mass transfers and chemical reaction [9–12].

The convective heat transfer with pyrolysis of hydrocarbon fuel has drawn much attention from the research community in recent years because of its effect on the thermal protection of scramjet [13–15], which is the best choice for the propulsion of aerospace plan, hypersonic missile, and fully reusable launch vehicle. Much work has been done in recent years on the influence of residence time, chemical reaction mechanism [16,17], pressure [18,19], heat and mass transfers [9,12], additive [20], etc., on endothermic chemical reaction. For example, Zhou et al. [18] and Ward et al. [19] studied through experiments the influence of pressure on pyrolysis of n-decane. Meng et al. [21], Hou et al. [22] and Fan et al. [23] studied the flow and heat-transfer behavior of thermal pyrolysis of n-decane. Jiang et al. [16] and Vandewiele et al. [17] studied the pyrolysis characteristic of hydrocarbon fuel. Qin et al. [9,12] performed numerical investigations on the influence of heat and mass transfer on the endothermic chemical reaction in the cooling mini-channel. Such factors as, heat and mass transfers, were separately considered in their studies. However, since the heat transfer and mass transfer are coupled together in flow field, when one of them is changed, another one is changed as well. Meanwhile, it could be seen from reaction rate function that the heat and mass transfers could affect the chemical reaction. So, the heat and mass transfers could affect the chemical reaction together, and the effect cased by them could not be split. The reaction rate for a given endothermic chemical reaction is the measure of the changes in concentrations of the reactants or products and energy, and reflects the general influence of heat and mass transfers on the chemical reaction. So, the general influence of these factors on chemical reaction can be better understood through the distribution of reaction rate. However, the detailed distribution of reaction rate has not been well understood yet so far.

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Nomenclature

A	pre-exponential factors, s^{-1}
D	diameter, m
E	activation energy, kJ/mol
k_f	rate constant, 1/s
m	mass flux
$\boldsymbol{Q}$	conservation variable
r	radius, m
t	time, s
U	velocity vector, m/s
Y	mass fraction of composition
x,y	the two coordinate directions of Cartesian coordinate system
a,b	coefficients of EoS
C	mole fraction of species
F,$\boldsymbol{G}$	vector of convective flux
L	length of channel, m
P	pressure, Pa
R_o	universal gas constant, 8.3145 J mol^{-1} K^{-1}
S	source term
T	temperature, K
v	specific volume, m^3/kg
u, υ	x-component and y-component of velocity, m/s

Greek

ρ	density, kg m^{-3}
ω	reaction rate, kg s^{-1} m^{-3}
$\boldsymbol{\Gamma}$	preconditioning matrix
δ_1, δ_2	coefficients of EoS

Subscripts

in	inlet
R	reactant
out	outlet
v	viscosity

Therefore, a numerical model was established using Time-marching algorithms with preconditioning and validated by benchmarks and experiment. And, the distribution of reaction rate during the convective heat transfer with endothermic chemical reaction in channel was then numerically investigated using the numerical model established.

2. Numerical model and methodology

In our prior numerical studies, based on finite volume method, a compressible reacting flow numerical model was established using coupled method based on Time-marching algorithm with preconditioning [12].

2.1. Simulation method

A complete set of conservation equations of mass, momentum, energy and species were numerically solved to properly handle the convective heat transfer with chemical reaction [12]. Because of the coupling characteristic among heat and mass transfer and chemical reaction, coupling solution method for flow controlling and species equations was used to solve conservation equations on the base of Time-marching algorithms. A preconditioning scheme was used to circumvent the stiff problem caused by a large condition number when the Time-marching algorithms were used to solve the compressible flow field with low

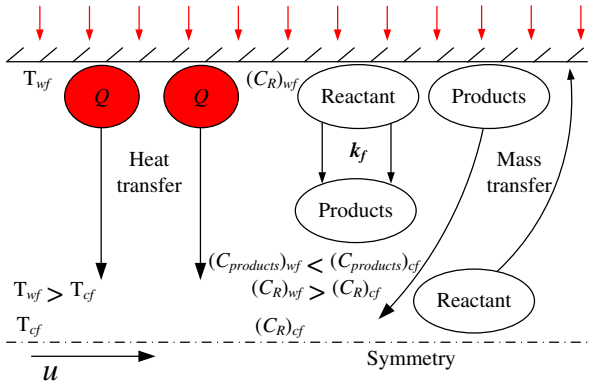

Fig. 1. Schematic diagram of energy and mass transfers.

velocity [24]. The 2D preconditioned N-S system could be written in Cartesian coordinates as shown below:

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

where $\boldsymbol{Q}=[P,u,v,T,Y_1\cdots Y_{n-1}]$. The energy transformed to chemical energy was obtained by calculating the enthalpy difference between the species before and after the chemical reaction.

The governing equations were discretized using finite volume scheme. The convection term and diffusive term were discretized by AUSM+ and central difference scheme respectively [12]. LU-SGS implicit method was employed to solve the discretized equations [12].

2.2. Chemical kinetics model

N-decane is the main composition of hydrocarbon fuel, and the thermo-physical properties of n-decane are similar to those of hydrocarbon fuel used as the coolant in the regenerative cooling process [25]. So, n-decane has been used as the working fluid for many current studies. The proportional product distribution (PPD) model of n-decane proposed by Ward et al. [25] for mild conversion, was adopted for the study:

$$\begin{aligned} C_{10}H_{22}\Rightarrow & 0.151H_2+0.143CH_4+0.256C_2H_4+0.126C_2H_6 \\ & +0.230C_3H_6+0.180C_3H_8+0.196C_4H_8+0.102C_4H_{10} \\ & +0.171C_5H_{10}+0.124C_5H_{12}+0.195C_6H_{12}+0.089C_6H_{14} \\ & +0.169C_7H_{14}+0.072C_7H_{16}+0.152C_8H_{16}+0.012C_8H_{18} \\ & +0.053C_9H_{18}+0.003C_9H_{20} \end{aligned} \tag{2}$$

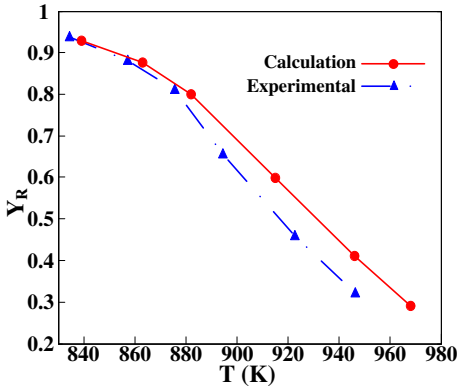

Fig. 2. Comparison of experimental results with calculations of outlet reactant conversion with channel diameter of 1 mm.