International Journal of Heat and Mass Transfer 119 (2018) 768–776

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

Numerical study on the influence of turbulence on the pyrolysis of hydrocarbon fuel in mini-channel

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ARTICLE INFO

Article history:
Received 30 June 2017
Received in revised form 30 November 2017
Accepted 1 December 2017

Keywords:
Turbulence
Pyrolysis
Mini-channel
Hydrocarbon fuel

ABSTRACT

The turbulent heat convection with pyrolysis is very complicated and occurs in cooling system of hypersonic aircraft with hydrocarbon fuel as the coolant. Since the mixing controlled by turbulence directly affects the reaction and leads to variations in both conversion and selectivity, a 2D numerical model was established to study the influences of turbulence on the pyrolysis of hydrocarbon fuel in mini-channel. The numerical results indicated that the turbulence enhanced the heat and mass transfer in core flow. And turbulence became weak as closing to the wall, which leads to a layer distribution of reaction rate with great gradient forming near the wall. So the distribution of the reaction rate in core flow is more uniform compared with that near the wall. According to analyze the radial distribution of relative rate of that between reaction rate and mixing, the result showed that relative rate presented multi-scale in radial direction under the influence of turbulence. In addition, the increase in turbulent intensity was beneficial to the increase in uniformity of radial distribution of conversion, which was helpful to enhance the utilization level of chemical absorption capacity of fuel.

1. Introduction

In order to avoid the unacceptable weight in recirculation cooling, the regenerative cooling, using endothermic hydrocarbon fuels on board, has been considered as the most effective solution to the thermal protection of hypersonic aircraft [1–4]. A series of endothermic reactions occurs in the cooling, in which additional cooling is obtained besides the sensible convective cooling [5]. In order to increase cooling efficiency, chemical transformations have to be controlled to cool the structures exposed to high thermal stresses [6,7]. Since the chemical reaction is a non-linear transformation of mass and energy, fluid dynamics and thermodynamics greatly affect the reaction [8–10]. Therefore, it is of great significance to the basically understand the influences of flow and transfers of heat and mass on the chemical reaction for controlling the chemical transformations by an effective way.

Much work has been done on the factors of affecting reaction in chemical reactors. According to the research for such typical reactors as, fluidized bed, cracking furnace, et al., it is shown that the conversion and distribution of products are affected by heat and mass transfers [11,12]. It is pointed out in the study of combustion that turbulence is able to affect the reaction zone structure, and hence influence whole combustion characteristics [13,14]. The dissociation and recombination of nitrogen and oxygen molecules, which is exothermic reaction, occur in hypersonic flow because of aerodynamic heating. Much work shows that there is a positive feedback between turbulence and exothermic reactions, and the reaction rate is increased by the turbulent temperature fluctuations [15,16].

The regenerative cooling system with endothermic hydrocarbon fuels is actually a turbulent flow reactor [17,18]. The distribution of reaction rate is non-uniform and radial concentration gradient is high, which leads to radial mass transfer [17]. In addition, the typical wall heat flux in regenerative cooling system is high, varying from 1 to 20 MW/m^2 [19,20], and the radial temperature gradient is great. So, in regenerative cooling system, the mixing controlled by turbulence affects radial heat transfer besides

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https://doi.org/10.1016/j.ijheatmasstransfer.2017.12.002
0017-9310/

Nomenclature

A	pre-exponential factors, s^{-1}
b	coefficient of EoS
C_p	specific heat at constant pressure, J kg^{-1} K^{-1}
C_D	dissipation term
k	turbulent kinetic energy, J kg^{-1}
L	length of channel, m
P	pressure, Pa
Pr	Prandtl number
R_o	universal gas constant, 8.3145 J mol^{-1} K^{-1}
$\boldsymbol{S}$	source term, $\boldsymbol{S} = [0 \quad 0 \quad 0 \quad 0 \quad s_1 \quad \cdots \quad s_{18}]$
Sc	Schmidt number
t	time, s
$\boldsymbol{U}$	velocity vector, m/s
Y	mass fraction of species
a	coefficient of EoS, or, thermal diffusivity, m^2 s^{-1}
C	molar concentration, mol m^{-3}
D	diffusion coefficient, m^2 s^{-1}, or diameter of channel, m
E	activation energy, kJ mol^{-1}
F,G	vector of convective flux
kf	rate constant, s^{-1}
M	molecular weight, kg/mol
Pk	production term
q	heat flux, MW m^{-2}
Re	Reynolds number
s	reaction rate, kg s^{-1} m^{-3}, or, area vector, m^2
T	temperature, K
Δt	residence time, s
x,y	two coordinate directions of Cartesian coordinate system
y'	non-dimensional number distance of cooling channel, $y' = y/L$

Greek

ρ	density, kg m^{-3}
$\alpha,\delta_1,\ \delta_2$	coefficients of EoS
ω	reaction rate of reactant, mol s^{-1} m^{-3}
λ	thermal conductivity, W m^{-1} K^{-1}
$\boldsymbol{\Gamma}$	Preconditioning matrix, $\boldsymbol{\Gamma} = [P \quad u \quad v \quad T \quad Y_1 \quad \cdots \quad Y_{18}]$
μ	viscosity, Pa s
τ	characteristic time, s
$\beta^*,\beta,\alpha,\delta$	constants of k-ω turbulent model

Subscripts

R	reactant (Hydrocarbon fuel)
v	viscosity
t	turbulence flow
in	inlet
h	heat transfer
eff	effective (the total influence cased by molecular motion and turbulence)
k	turbulent kinetic energy
c	core flow
r	reaction
l	laminar flow
i,j	species
out	outlet
m	mass transfer
ω	specific dissipation rate
w	wall

the radial mass transfer, which is different from turbulent flow reactor in previous study. Moreover, the heavy hydrocarbon fuel pyrolyse to light hydrocarbon molecules with smaller molecular mass, so thermo-physical properties of fluid in cooling undergo a change with pyrolysis in a large temperature range, which causes the enhancement of turbulence. And, the typical hydraulic diameter of cooling channel is small, in the range of 0.5–2 mm [2]. Since the distribution of boundary layer in mini-channel is different from that in the channel with larger hydraulic diameter, turbulence has a more significant influence on the pyrolysis in mini-channel [21–24]. In order to controlling pyrolysis in cooling, much work has been done on the factors of affecting pyrolysis in recent years. The factors in these works could be grouped as physical and chemical factors. The physical factors include residence time, wall heat flux, pressure, geometry of cooling channels, etc [25–29]. And the chemical factors include reaction mechanism, products distribution, catalytic crack, coke, etc [30–35]. However, less previous work focused on the influence of turbulence on the pyrolysis of hydrocarbon fuel in cooling mini-channel.

Therefore, a 2D numerical model was established using coupled method based on Time-marching algorithm with preconditioning for studying the influence of turbulence on the pyrolysis of hydrocarbon fuel in cooling mini-channel. The influence of heat and mass transfer, which is caused by turbulence, on the pyrolysis was analyzed. And the distribution of relative rate between pyrolysis and mixing in mini-channel was discussed. In addition, the influence of turbulence intensity on the distribution of reaction rate was studied as well.

2. Numerical model and methodology

2.1. Computational methods

The conservation equations of mass, momentum, energy and species, which were used to describe the heat convection with pyrolysis of hydrocarbon fuel in cooling mini-channel, can be written as,

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

Eq. (1) is a preconditioned governing equation, in which the preconditioning scheme was employed to circumvent the stiff problem of convective terms when Time-marching algorithms is used to solve the compressible flow with low Mach number [36]. The standard enthalpy of formation in flow field was used to calculate the energy transformation between internal and chemical energies. Mass fractions of products, including 18 species, were calculated by solving 18 species equations, and mass fraction of hydrocarbon fuel was determined as 1 minus the sum of products. The source term caused by pyrolysis and reflecting mass transformation relationship between hydrocarbon fuel and products can be written as

$$s_i = \omega_i \cdot M_i \tag{2}$$

Since the flow field in boundary layer was focused on in this paper, the k-ω two equations turbulent model was used in present study because of its good accuracy and high numerical stability to the boundary layer [37].