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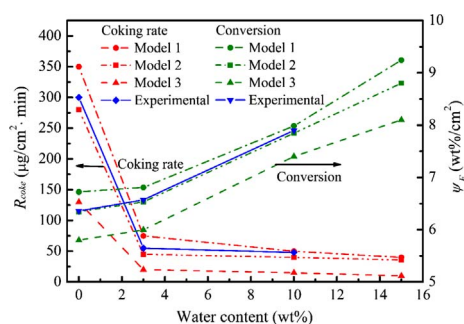
Numerical study of catalytic steam reforming of aviation kerosene at supercritical pressures



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GRAPHICAL ABSTRACT



Conversion and coking rate of RP-3 under different water contents.

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ABSTRACT

A new two-dimensional numerical model is proposed for supercritical catalytic steam reforming of Chinese aviation kerosene No. 3 (RP-3) in order to suppress the coke formation during regenerative cooling of scramjet engines. A well-established wall catalytic steam reforming mechanism is used together with the newly proposed coke formation models to account for the coke formation during wall catalytic steam reforming reaction of RP-3. This wall catalytic steam reforming and coking model is coupled with computational fluid dynamics (CFD) codes to provide information of the flow field variables in the mini-channel reactor. The model is validated against experimental results. The effects of water content, pressure and inlet flow velocity on the wall catalytic reforming of RP-3, particularly on the coke formation, are then studied and analyzed. The simulation results show that higher water content and higher pressure can effectively suppress coke formation and increase the conversion of RP-3. The increase of inlet flow velocity, however, can reduce coke deposits but results in low conversion of RP-3.

1. Introduction

The high heat load on the combustor chamber of scramjet engines at high flight Mach numbers ($Ma > 5$) necessitates the regenerative cooling using endothermic hydrocarbons [1,2]. The strong endothermic thermal cracking (e.g. pyrolysis) of hydrocarbons takes place when heated above certain temperatures. Thus, additional cooling capacity

besides the physical heat absorption can be obtained by endothermic reactions occurring simultaneously with traditional sensible convective heat transfer [3–6]. Meanwhile, the thermal cracking of hydrocarbons also produce smaller combustible molecules (e.g. hydrogen, carbon monoxide and methane) which can promote combustion performance of fuels in the combustor chamber [5]. Different thermal cracking models of hydrocarbons coupled with computational fluid dynamics

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Nomenclature			
a	model parameter	\tilde{Y}_i	species mass fraction
A	model parameter, Pa	y^+	the dimensionless width
A_{cell}	area of the cell surface at wall, m^2	<i>Greeks</i>	
b	model parameter	β	model parameter, $\text{m}^2 \cdot \text{MPa} \cdot \text{s} / \text{kg}$
D	diffusion coefficient, m^2 / s	λ	thermal conductivity, $\text{W} / (\text{m} \cdot \text{K})$
e_t	total energy, J / kg	ρ	density, kg / m^3
h	model parameter	τR	accumulated reaction time, min
Δh_s	specific heat of chemical reaction, W / m^2	ψ	conversion of fuel
ΔH_s	heat of reaction, MW	<i>Subscripts</i>	
K_1	model parameter, $\text{kg} / (\text{m}^2 \cdot \text{MPa} \cdot \text{s})$	c	catalytic reaction
K_2	model parameter, $\text{kg} / (\text{m}^2 \cdot \text{s})$	<i>coke</i>	coke deposits
K_3	model parameter, 1	<i>coke, pre</i>	coke precursor
K_M	model parameter, $\text{kg} / (\text{m}^2 \cdot (\text{MPa})^2 \cdot \text{s})$	d	diffusion
K_W	model parameter, 1	F	fuel
m_{coke}	the total mass of coke deposits	H	hydrogen
n_i	the moles of species i , mole	i	species
MW_i	molecule weight, kg / kmol	m	the m th species
P	pressure, Pa	M	methane
Q_r	reaction heat, $\text{J} / (\text{mol})$	n	normal direction
R	chemical reaction rate, $\text{mol} / (\text{m}^3 \cdot \text{s})$	r	the r th reaction
\tilde{S}_i	chemical reaction source term, $\text{kg} / (\text{m}^3 \cdot \text{s})$	R	residence
S_{in}	total interior surface of the reactor, cm^2	s	specific area
T	temperature, K	w	wall
\tilde{u}	Favre-averaged velocity vector, m / s	W	water
U_0	inlet flow velocity, m / s	<i>wall cell</i>	cells at the surface of the reactor
\dot{w}	chemical reaction rate, $\text{mol} / (\text{m}^3 \cdot \text{s})$		
X	axial coordinate along the reactor, m		
Y	radial coordinate, m		

have been proposed to shed light on the mechanistic study of regenerative cooling using endothermic hydrocarbons [6–8].

However, coke deposits produced during thermal cracking of hydrocarbons can adversely affect the efficiencies of regenerative cooling and subsequent combustion. In some cases, severe coke deposition can block the regenerative cooling channel and even cause the shutting down of engines [5]. Three types of coke deposits are reported in the literature including the filamentous coke, condensation coke and deposited coke [9]. The investigation of coke formation derived from the thermal cracking of hydrocarbons demonstrate that coke are primarily formed via metal-catalyzed mechanism and free-radical mechanism [10]. Coke deposits can also be formed via Diels-Alder reaction between dienes [11]. In addition, the precursors of coke deposits are found to be polyolefins and polycyclic aromatic hydrocarbons (PAH). In the present study, the wall catalytic steam reforming and coking reactions of RP-3 are investigated. All coke deposits are assumed to be generated only at the heated wall surface of the mini-channel reactor according to the coke formation models in the present study. This is because the mini-channel is heated from outside and the high temperature at the metal wall surface is conducive to coke formation.

Various attempts including the addition of passivating coatings (e.g. alumina coating), the addition of sulfide to the alloy wall surface are carried out to inhibit the coke formation during thermal cracking of hydrocarbons [12–14,15]. It is found that the hydrogenation reaction is conducive to inhibiting coke formation in the thermal cracking process of hydrocarbons [16]. Catalytic steam reforming of hydrocarbons, which can produce high levels of hydrogen and effectively reduce coke formation, has been studied by many researchers [5,17–21]. The coke formation is suppressed because the hydrogen generated by catalytic steam reforming of hydrocarbons can significantly inhibit the formation of coke precursors i.e. polyolefins and PAH [5].

Compared with the study of thermal cracking of hydrocarbons, however, there is little report on the study of catalytic steam reforming

of hydrocarbons, particularly the RP-3 (Chinese aviation kerosene No.3). Although experimental studies of wall catalytic steam reforming of RP-3 have been reported [5,20,21], the amount of coke deposits are mainly obtained by indirectly calculating the pressure differences between two ends of the channels and no distribution information of coke formation is obtained in these studies. Considering the complexity of the reaction mechanism as well as the difficulty in obtaining accurate information of coke formation and distribution under wall catalytic steam reforming of RP-3, it is therefore necessary to develop a kinetic model with proper assumptions to describe catalytic steam reforming reactions of RP-3 for regenerative cooling, in which chemical reactions are coupled with heat transfer and fluid flow. In the present study, a novel two-dimensional numerical model is established for supercritical wall catalytic steam reforming of aviation kerosene (RP-3) which consists of well-established chemical mechanisms of wall catalytic steam reforming reactions and newly proposed coke formation models. The above chemical reaction models are coupled with CFD codes to study the key operating parameters influencing the wall catalytic steam reforming of RP-3 and the coke formation including water content, pressure and inlet flow velocity in the present study. It is aimed to provide a simple and accurate numerical model for catalytic steam reforming of hydrocarbons with consideration of coke formation, thus providing better insight into the operation and design of regenerative cooling systems of scramjet engines for hypersonic propulsion.

2. Methodology

2.1. Governing equations

The governing equations in the present study including the mass, momentum and energy conservation equations as well as species mass fractions conservation equation take the following steady state Favre-averaged form [22]:

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