



Numerical study of fluid flows and heat transfer of aviation kerosene with consideration of fuel pyrolysis and surface coking at supercritical pressures



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ABSTRACT

A computational fluid dynamics (CFD) model has been developed and applied for numerical studies of fluid flows and heat transfer of the aviation kerosene RP-3 with consideration of both fuel pyrolysis and surface coking in a circular cooling tube at a supercritical pressure of 5 MPa. A detailed pyrolytic chemical reaction mechanism, which contains 18 species and 24 elementary reactions, and a modified kinetic model for considering the surface coking reactions are incorporated in the CFD model. The effects of the surface heat flux and inlet flow velocity on the complex physicochemical process of supercritical-pressure turbulent heat transfer of RP-3 are examined. Results reveal that the endothermic fuel pyrolysis improves the convective heat transfer by two means: providing extra heat absorption through the endothermic chemical reactions and thus decreasing the bulk fluid temperature, and increasing the flow velocity and consequently increasing the convective heat transfer coefficient. The equivalent surface heat flux from the endothermic chemical reactions can contribute to around 70% of the total surface heat flux at the high fluid temperature region. As the aviation kerosene RP-3 is thermally decomposed, the main surface coking precursors, propene and aromatics, are produced. As a result, carbon deposition accumulates on the interior surface of the cooling tube, particularly at a low inlet flow velocity and/or a high surface heat flux.

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1. Introduction

Regenerative cooling has been considered as an effective approach for the thermal protection of many propulsion and power-generation systems, including the rocket, supersonic combustion ramjet (scramjet), and advanced gas turbine engines [1,2]. The engine fuel, prior to its injection and burning in a combustor, is forced to flow through micro cooling channels surrounding the combustion chamber and/or other high-temperature components to cool and protect the propulsion system. The process is defined as regenerative cooling since a large amount of waste heat is absorbed by the engine fuel and redelivered into the combustor. The operating pressure in the cooling process is generally higher than the critical pressure of the fuel, which is around 2–3 MPa for a typical hydrocarbon material. This leads to fluid flows and heat transfer at supercritical pressures. Many experimental and numerical studies have been conducted to obtain fundamental understanding of the supercritical-pressure cooling process [3–10].

It was found that strong variations of the thermophysical properties, such as fluid density, heat capacity, and viscosity etc., exert significant impacts on the fluid dynamics and heat transfer characteristics.

As the speed of the advanced air-breathing flight systems moves into the hypersonic regime ($Ma > 5$), the demand on the cooling capacity of the engine fuel significantly increases. An endothermic hydrocarbon fuel is thus needed for the regenerative cooling process. When the temperature of the endothermic hydrocarbon fuel rises above a certain value, e.g., 750 K, the fuel is thermally decomposed into many low-molecular-weight chemical species and in the process, absorbs an extra amount of heat. Therefore, in addition to the physical cooling capacity with increasing fluid temperature, an endothermic fuel significantly increases its heat-absorbing capacity by means of the pyrolytic chemical reactions [11–14]. During fuel pyrolysis, the formation of olefins and aromatics, however, can lead to carbon deposition or coking on the cooling channel surface [15–18]. This is an undesirable phenomenon in the supercritical-pressure cooling process, since surface coking blocks the flow passage of a cooling channel and can eventually terminate fluid flows and heat transfer.

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Nomenclature

A	surface area, m^2	Y_i	species mass fraction
C	constants in turbulent model or molar concentration, mol m^{-3}	<i>Greeks</i>	
e_t	total energy, J kg^{-1}	ε	turbulent dissipation rate, $\text{m}^2 \text{s}^{-3}$
E_a	activation energy, J kmol^{-1}	λ	thermal conductivity, $\text{W m}^{-1} \text{K}^{-1}$
G_k	turbulence generation term	ρ	density, kg m^{-3}
h	convective heat transfer coefficient, $\text{W m}^{-2} \text{K}^{-1}$	σ	turbulent Prandtl number
h_i	enthalpy of species i , J kg^{-1}	τ	viscous stress tensor, Nm^{-2}
k	turbulent kinetic energy, J kg^{-1}	μ	viscosity, $\text{kg m}^{-1} \text{s}^{-1}$
p	pressure, Pa	<i>Subscripts</i>	
\dot{q}''	surface heat flux, W m^{-2}	b	bulk parameter
\dot{Q}'''	volumetric heat absorption rate, W m^{-3}	d	diffusion
r	radial coordinate, mm	<i>endo</i>	endothermic value
R	universal gas constant, $8.314 \text{ kJ kmol}^{-1} \text{K}^{-1}$	i	species
S_i	chemical source term of species i , $\text{kg m}^{-3} \text{s}^{-1}$	k	parameter related to turbulent kinetic energy
SC	surface coking	w	wall
t	time, s	ε	parameter related to turbulent dissipation rate
T	temperature, K		
\mathbf{u}	velocity vector, m s^{-1}		
x	axial coordinate along the flow direction, mm		

Much effort has been expended to study fuel pyrolysis and surface coking phenomena at supercritical pressures. The pyrolytic chemical reaction mechanisms of a variety of hydrocarbon fuels, including n-tetradecane, C10–C14 normal alkanes and their mixtures, decalin, tetralin, n-decane, JP-7, and RP-3, have been experimentally investigated under near-critical and supercritical conditions [19–23]. The polycyclic aromatics from supercritical fuel pyrolysis have been identified as the key coking precursors [15,16]. The effect of fuel type on the pyrolytic reactivity and deposition propensity under supercritical conditions was also analyzed [17].

Numerical modeling and simulation of fluid flows and heat transfer with fuel pyrolysis at supercritical pressures have been carried out to obtain a comprehensive understanding of the physicochemical process. Ward et al. [24,25] developed a one-step proportional product distribution (PPD) model for consideration of the mild thermal decomposition (fuel conversion less than 25%) of n-decane and n-dodecane at supercritical pressures and conducted numerical studies of fluid flows and heat transfer with fuel pyrolysis. Ruan et al. [13] further simplified the PPD model of n-decane and applied it to investigate the effect of fuel pyrolysis on flow dynamics and heat transfer characteristics. Zhu et al. [26] also derived a global reaction model for the mild thermal cracking of n-decane at supercritical pressures and carried out numerical simulations. The applicability of these simplified pyrolytic reaction mechanisms is, however, limited to mild fuel pyrolysis with the fuel decomposition less than 25%, and they are incapable of predicting the surface coking phenomenon.

Recently, Jiang et al. conducted a series of experiments on thermal decomposition of the aviation kerosene RP-3 and developed a detailed pyrolytic chemical reaction mechanism, which contains 18 species and 24 elementary reactions and is applicable over a wide range of operating conditions with fuel conversion up to approximately 90%, at a supercritical pressure of 5 MPa [27]. Based on further experimental and analytical studies, a kinetic model is also proposed to predict carbon deposition on the cooling channel surface within 20 min after the surface coking reactions start [28]. This detailed pyrolytic chemical reaction mechanism of RP-3 has recently been implemented into a computational fluid dynamics (CFD) model for fundamental studies of the effect of fuel pyrolysis

on the supercritical-pressure turbulent heat transfer of RP-3 in engine cooling channels [14].

In this paper, based on the model previously developed and validated in [14] for studying fluid flows and heat transfer of RP-3 with a detailed consideration of fuel pyrolysis, the kinetic model obtained in [28] for predicting the initial surface coking of RP-3 on cooling channel surface has been tested, modified, and implemented. The new model is thus capable of treating both fuel pyrolysis and surface coking in the regenerative cooling process. It is further validated and then applied to examine the turbulent heat transfer of RP-3 in a circular cooling tube. Effects of two key influential parameters, the surface heat flux and inlet flow velocity, on fluid flows, heat transfer, fuel pyrolysis, and carbon deposition at a supercritical pressure of 5 MPa are analyzed in the present study. This work has fundamental importance and practical implication for the development of the regenerative cooling technology in the advanced air-breathing propulsion systems.

2. Theoretical formulation

2.1. Conservation equations

In the present study, the following steady-state Favre-averaged conservation equations of mass, momentum, energy, and species mass fractions are numerically solved:

$$\nabla \cdot (\bar{\rho} \tilde{\mathbf{u}}) = 0 \quad (1)$$

$$\nabla \cdot (\bar{\rho} \tilde{\mathbf{u}} \tilde{\mathbf{u}}) = -\nabla \bar{p} + \nabla \cdot \tilde{\boldsymbol{\tau}} \quad (2)$$

$$\nabla \cdot (\bar{\rho} \tilde{\mathbf{u}} \tilde{e}_t) = \nabla \cdot (\lambda \nabla \tilde{T}) - \nabla \cdot (\bar{p} \tilde{\mathbf{u}}) \quad (3)$$

$$\nabla \cdot (\bar{\rho} \tilde{Y}_i \tilde{\mathbf{u}}) = -\nabla \cdot (\bar{\rho} \tilde{Y}_i \tilde{\mathbf{u}}_{d,i}) + \tilde{S}_i \quad (4)$$

The standard k - ε turbulent model with an enhanced wall treatment, which solves a one-equation Wolfstein model in the near wall region, is employed to treat the turbulent fluid flows.

$$\nabla \cdot (\bar{\rho} \tilde{\mathbf{u}} \tilde{k}) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla \tilde{k} \right] - \bar{p} \tilde{\varepsilon} + \tilde{G}_k \quad (5)$$

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