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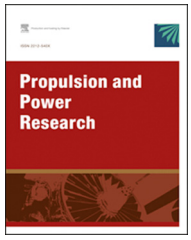

ORIGINAL ARTICLE

Model validation and parametric study of fluid flows and heat transfer of aviation kerosene with endothermic pyrolysis at supercritical pressure

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Abstract The regenerative cooling technology is a promising approach for effective thermal protection of propulsion and power-generation systems. A mathematical model has been used to examine fluid flows and heat transfer of the aviation kerosene RP-3 with endothermic fuel pyrolysis at a supercritical pressure of 5 MPa. A pyrolytic reaction mechanism, which consists of 18 species and 24 elementary reactions, is incorporated to account for fuel pyrolysis. Detailed model validations are conducted against a series of experimental data, including fluid temperature, fuel conversion rate, various product yields, and chemical heat sink, fully verifying the accuracy and reliability of the model. Effects of fuel pyrolysis and inlet flow velocity on flow dynamics and heat transfer characteristics of RP-3 are investigated. Results reveal that the endothermic fuel pyrolysis significantly improves the heat transfer process in the high fluid temperature region. During the supercritical-pressure heat transfer process, the flow velocity significantly increases, caused by the drastic variations of thermophysical properties. Under all the tested conditions, the Nusselt number initially increases, consistent with the increased flow velocity, and then slightly decreases in the high fluid temperature region, mainly owing to the decreased heat absorption rate from the endothermic pyrolytic chemical reactions.

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1. Introduction

In propulsion and power-generation systems, such as the scramjet and advanced gas turbine engines, the combustion chamber is exposed to high heat load from chemical reactions and aerodynamic heating. To ensure engine reliability and durability, the regenerative cooling technology, which uses a hydrocarbon fuel as the coolant, is needed for effective thermal protection [1,2].

During the regenerative cooling process, the engine fuel is circulated in micro cooling channels surrounding the combustion chamber prior to fuel injection and burning, generally under supercritical pressures. As the fuel temperature increases and reaches the trans-critical region, its thermophysical properties experience drastic variations and produce strong influences on the supercritical-pressure fluid flows and heat transfer processes. In addition, as the fuel temperature further rises to around 750 K, thermal cracking of the fuel occurs, a phenomenon known as endothermic pyrolysis, which can further increase the heat-absorbing capacity of a hydrocarbon fuel and benefit the subsequent combustion process [3].

In the open literature, many experimental studies have been carried out on high pressure pyrolysis of hydrocarbon fuels. Yu and Eser [4,5] studied thermal decomposition of C_{10}-C_{14} normal alkanes and their mixture under near-critical and supercritical conditions. A modified free radical mechanism was proposed to explain the product yields, and a first-order reaction mechanism was developed. Zhong et al. [6] conducted experiments to analyze thermal cracking and heat-absorbing capacity of RP-3 at supercritical conditions. Results showed that the chemical heat sink of RP-3 varies with temperature, with a maximum value between 900 K and 960 K, depending on the residence time. Abraham et al. [7,8] developed a real-time quantification infrared method to identify and quantify the pyrolytic products of hydrocarbon fuels. DeWitt et al. [9] studied the effect of fuel type on the pyrolytic reactivity and deposition propensity under supercritical conditions. Jiang et al. [10] recently conducted a series of experiments using an electrically heated micro tube to obtain variations of the local product concentrations and fluid temperature of RP-3. A detailed reaction mechanism consisting of 18 species and 24 chemical reactions was proposed to describe the endothermic fuel pyrolysis.

A number of numerical studies have also been carried out for fundamental understanding of supercritical-pressure fluid flows and heat transfer of hydrocarbon fuels with pyrolysis. Sheu et al. [11] conducted numerical studies on thermal cracking of Norpar-13 under near- and supercritical conditions. A three-step lumped pyrolytic mechanism was employed to account for chemical reactions. Numerical results showed that the endothermic pyrolytic reactions could effectively reduce the fuel and wall temperature. Ward et al. proposed a one-step proportional product distribution (PPD) model for thermal cracking of *n*-decane and *n*-dodecane [12] and investigated pressure effects on fluid flows and heat transfer of *n*-decane with mild thermal cracking [13]. Zhu et al. [14] developed a similar global reaction mechanism of *n*-decane and applied it for numerical studies. Ruan et al. [15] recently simplified the general PPD model proposed by Ward et al. [12] by grouping the high-molecular-weight alkane or alkene species together, and applied the reduced reaction mechanism for efficient numerical simulations of fluid flows and heat transfer of *n*-decane with endothermic pyrolysis.

In these existing studies, since simplified reaction mechanisms were used to account for the endothermic pyrolysis of hydrocarbon fuels, the numerical models are thus only applicable for studying supercritical-pressure heat transfer with mild thermal cracking of the hydrocarbon fuels (generally less than 25% of fuel conversion). The applicability and accuracy of these models need further improvement.

In this paper, a mathematical model has been used to study supercritical-pressure fluid flow and heat transfer of the aviation kerosene RP-3 with endothermic pyrolysis. A complete set of conservation equations of mass, momentum, energy, and species mass fractions are numerically solved, with accurate calculations of thermophysical properties. A detailed reaction mechanism of RP-3, which contains 18 species and 24 elementary reactions [10], is incorporated to account for fuel pyrolysis. Detailed model validations are conducted against a series of experimental data, including the fluid temperature, fuel conversion rate, various product yields, and chemical heat sink. The model is applicable over a wide range of operating conditions and is also capable of providing detailed and accurate numerical results. Comprehensive numerical studies have been carried out to analyze the effects of fuel pyrolysis and inlet flow velocity on the supercritical-pressure fluid flows and heat transfer of RP-3 in a micro cooling tube under a constant wall temperature and at a supercritical pressure of 5 MPa.

2. Mathematical model

2.1. Conservation equations

In the present numerical study of fluid flows and heat transfer of RP-3 with fuel pyrolysis at a supercritical pressure, the following conservation equations of mass, momentum, energy, and species mass fractions are solved:

$$\nabla\bullet\left(\rho\vec{u}\right)=0 \tag{1}$$

$$\nabla\bullet\left(\rho\vec{u}\,\vec{u}\right)=-\nabla p+\nabla\bullet\boldsymbol{\tau} \tag{2}$$

$$\nabla\bullet\left(\rho\vec{u}\,e_t\right)=\nabla\bullet(\lambda\nabla T)-\nabla\bullet\left(p\vec{u}\right) \tag{3}$$

$$\nabla\bullet\left(\rho Y_i\vec{u}\right)=-\nabla\bullet\left(\rho Y_i\vec{u}_{d,i}\right)+S_i \tag{4}$$

The relevant variables are defined in the nomenclature. In these equations, the effect of gravity on fluid flows and heat transfer is neglected because of the small size of the cooling