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 hydrocarbons. 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:

\[ \nabla \cdot (\rho \vec{u}) = 0 \]  \hspace{1cm} (1)

\[ \nabla \cdot (\rho \vec{u} \vec{u}) = - \nabla p + \nabla \cdot \tau \]  \hspace{1cm} (2)

\[ \nabla \cdot (\rho \vec{u} e_i) = \nabla \cdot (\lambda \nabla T) - \nabla \cdot \left( \rho \vec{u} \right) \]  \hspace{1cm} (3)

\[ \nabla \cdot (\rho Y_i \vec{u}) = - \nabla \cdot \left( \rho Y_i \vec{u} \frac{d_i}{d} \right) + S_i \]  \hspace{1cm} (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...
tube. The viscous dissipation term is also neglected due to the relatively low flow velocity. The source term, in Eq. (4), results from the endothermic pyrolytic chemical reactions.

The standard $k$-$\varepsilon$ turbulent model, along with an enhanced wall treatment, is employed to handle the turbulent fluid flows. The conservation equations are as follows:

$$\nabla \cdot (\rho \vec{u} \varepsilon) = \nabla \cdot \left( \mu + \frac{\mu_t}{\sigma_t} \nabla k \right) - p \varepsilon + G_k$$ (5)

$$\nabla \cdot (\rho \vec{u} \varepsilon) = \nabla \cdot \left( \mu + \frac{\mu_t}{\sigma_t} \nabla \varepsilon \right) + C_1 \frac{\varepsilon}{k} G_k - C_2 \rho \frac{C_0}{k}$$ (6)

### 2.2. Pyrolytic reaction mechanism

The detailed pyrolytic chemical reaction mechanism of RP-3 proposed by Jiang et al. [10] is used to take into account fuel pyrolysis. It consists of 18 species and 24 elementary reactions. A trace species in the reaction mechanism, styrene, is ignored in the present model due to its negligible mass fraction (less than 1% in weight), and its mass is included in RP-3. Therefore, a total of 16 conservation equations of species mass fractions are numerically solved in the mathematical model.

### 2.3. Thermophysical property calculation

During the fluid flows and heat transfer process, the thermophysical properties of the fuel mixture undergo strong variations at supercritical pressures. Therefore, it’s a prerequisite to accurately calculate the variations with temperature, pressure and species fractions. In our prior numerical studies [16–19], a general framework has been established for this purpose. The extended corresponding states principle is employed to calculate the thermodynamic and transport properties of the fuel mixture, with a pure hydrocarbon fuel, propane, chosen as the reference material. The binary mass diffusivity at high pressures is evaluated in two steps. First the empirical correlation proposed by Fuller [20] is applied to obtain the binary mass diffusivity at low pressures, and then a simple corresponding state method developed by Takahashi [21] is used to take into account the pressure effects.

Surrogate models suggested by Jiang et al. [10] for RP-3 and the lumped products of C$_5$H$_{11}$, C$_5$H$_{13}$, and C$_{10}$H$_{22}$, as listed in Table 1, are used in the present study for property calculations. The critical pressure and temperature of RP-3 are around 2.3 MPa and 646 K, according to experimental measurement [22]. The predicted critical pressure and temperature from the surrogate model are 2.21 MPa and 667 K. The relative errors are -3.9% and 3.6% for the critical pressure and temperature, respectively.

The chemical reaction mechanism and thermophysical property evaluation methods are implemented into the commercial CFD package, Fluent, through its user coding capability, thus establishing a mathematical model and computational software for numerical studying of fluid flows and heat transfer of RP-3 with endothermic pyrolysis at supercritical pressures. More details of the mathematical model can be found in Ref. [23].

### 3. Results and discussion

#### 3.1. Model validations

Detailed model validations are conducted in this section against two sets of experimental data of Jiang et al. [10]. As shown in Figure 1, the turbulent fluid flows and heat transfer of RP-3 with endothermic pyrolysis in a micro cooling tube are numerically simulated using the previously developed mathematical model and computational software. In the calculations, the tube diameter is 1 mm, with two tube lengths of 0.635 m and 0.870 m used in test 1 and test 2, respectively. A constant heat flux is imposed on the tube surface. The constant fuel temperature, mass flow rate, and operating pressure are specified at the tube inlet. Outflow
boundary conditions are specified at the tube outlet. The other operating parameters are listed in Table 2, consistent with the experimental set-ups in Ref. [10]. Two computational meshes of $2540 \times 50$ for test 1 and $3480 \times 50$ for test 2 in the $x$- and $r$- directions, respectively, are chosen for the present studies, based on our previous numerical work [15].

Figure 2 shows variations of the calculated bulk fluid temperature in the heated section for the two different cases. The bulk fluid temperature is defined as

$$T_b = \frac{\int_A \rho \bar{u} c_p T dA}{\int_A \rho \bar{u} c_p dA}$$ (7)

The fluid temperature initially increases rapidly, but the increasing rate slows down in the high temperature region, due to the endothermic chemical reactions. The numerical results are compared with experimental data [10], showing very good agreements. The maximum relative errors are only 5.5% and 2.2% for the two test cases, respectively.

Figure 3 shows variations of the predicted fuel conversion rate, along with the measured experimental data. The fuel conversion rate is defined as:

$$Y_b = 1 - \frac{\int_A \rho \bar{u} Y_{RP-3} dA}{\int_A \rho \bar{u} dA}$$ (8)

Thermal cracking of RP-3 mainly occurs at around $x = 300$ mm for case 1 and $x = 450$ mm for case 2. At both locations, the bulk fluid temperature reaches around 750 K, as shown in Figure 2. The calculated results match the experimental data very well. At the thermal exit, the relative errors between the calculated and experimental data are only 5.9% and 3.08% for the two test cases, respectively.

Detailed species yields from the endothermic pyrolysis of RP-3 are shown in Figure 4. Mass fractions of the light products, such as methane and ethane, increase monotonically along the heated section. Mass fractions of the heavy products, such as $C_5^+$ and $CC_5^{++}$, initially increase with fuel pyrolysis, but then decrease as more fuel is thermally cracked. This is caused by the secondary chemical reactions in the detailed pyrolytic chemical reaction mechanism. Excellent matches between the numerical results and experimental data can be clearly observed in Figure 4(a)-(d) for the light species, but relatively larger deviations occur between the two sets of data for the two lumped species, $C_5^+$ and $CC_5^{++}$, mainly in the transition regions.
the pyrolytic chemical reaction mechanism of RP-3 [10], since C5+ and CC5+ are used to represent two groups of relatively heavy species, the chemical reactions for them are simplified and thus may not be very accurate.

The numerically calculated heat sink, which directly indicates the potential cooling capacity of RP-3, is compared with the analytical result in Figure 5. The heat sink initially increases linearly with temperature, but once the bulk fluid temperature exceeds 800 K, it shows a rapid rise, attributable to the extra heat absorbing capacity of the hydrocarbon fuel through endothermic chemical reactions in the high temperature region. Again, the calculated values are consistent with the analytical data [10].

In this section, detailed model validations have been carried out against a series of experimental data, including the bulk fluid temperature, fuel conversion rate, various product yields, and chemical heat sink, fully verifying the accuracy and reliability of the mathematical model.

Figure 4 Variations of species yields from fuel pyrolysis. (a) CH₄, (b) C₂H₄, (c) C₂H₆, (d) C₃H₆, (e) C₅+, and (f) CC₅+.
3.2. Effects of fuel pyrolysis and inlet velocity

In this section, the model is applied to study effects of the fuel pyrolysis and inlet flow velocity on fluid dynamics and heat transfer characteristics of RP-3 in a micro cooling tube at a supercritical pressure of 5 MPa. The tube diameter is 1 mm, with a total length at 800 mm. An inlet section of 150 mm is thermally insulated to ensure a fully developed flow before heat transfer starts, and an outlet section of 150 mm is also thermally insulated to avoid effects of the outflow boundary conditions on numerical results. The middle section with a tube length of 500 mm is heated with a constant wall temperature of 950 K for the purpose of fundamental studies. Results calculated using different thermal boundary conditions are discussed in Ref. [23]. In the present study, the flow velocity, varying from 0.5 m/s to 4 m/s, is prescribed at the tube inlet. The detailed operating parameters are listed in Table 3.

Figure 6 shows variations of the bulk fluid temperature calculated with and without consideration of fuel pyrolysis. The inlet flow velocity is 0.5 m/s. At the thermal exit, the endothermic pyrolytic chemical reactions lead to around 40 K decrease in the bulk fluid temperature. In this case, the fuel conversion rate at thermal exit is approximate 80%, as discussed later in this section.

Variations of the surface heat flux, with and without consideration of fuel pyrolysis, are shown in Figure 7. In the current case with a constant wall temperature, it is more appropriate to use the surface heat flux to elucidate the effects of fuel pyrolysis on the convective heat transfer [15]. Because of the endothermic chemical reactions, the surface heat flux is significantly increased. Particularly at the thermal exit, at which point 80% of RP-3 is thermally cracked, the surface heat flux with fuel pyrolysis increases nearly 10 times, comparing with that without fuel pyrolysis. It should also be noted that the sudden increase of the surface heat flux from \( x/D = 150 \), as clearly observable in Figure 7, is caused by strong variations of thermophysical properties of the cracked fuel mixture in the trans-critical region when the fluid temperature rises from a subcritical to supercritical state. More detailed discussion is provided in Ref. [23].

The effects of inlet flow velocity on fluid flows, fuel pyrolysis, and heat transfer are further analyzed. Figure 8 shows variations of the bulk fluid temperature and surface heat flux at different inlet flow velocities. As the inlet velocity increases, the bulk fluid temperature and surface heat flux decreases, while the surface heat flux increases significantly. This physical phenomenon is attributable to the improved heat transfer performance at a high flow velocity.

Figure 9 presents variations of the fuel conversion rate along the heated section at different inlet flow velocities. The thermal decomposition of RP-3 weakens as the flow velocity increases. At the thermal exit, the fuel conversion rate drops from 80% to 13% as the inlet flow velocity

<table>
<thead>
<tr>
<th>Table 3 Operating parameters used for parametric study.</th>
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<tr>
<td>Parameters</td>
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<tr>
<td>Inlet pressure, ( p_0/\text{MPa} )</td>
</tr>
<tr>
<td>Wall temperature, ( T_w/\text{K} )</td>
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<tr>
<td>Inlet temperature, ( T_0/\text{K} )</td>
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<td>Inlet velocity, ( u_0/(\text{m/s}) )</td>
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increases from 0.5 m/s to 4 m/s. This is mainly due to the decreased fluid temperature, as shown in Figure 8(a).

Variations of the volumetric heat absorption rates from fuel pyrolysis at different inlet flow velocities are presented in Figure 10(a). The general trend is that the endothermic value initially increases significantly with the increase of the fluid temperature, and then it starts to decrease in the high temperature region, caused by the decrease of RP-3 concentration [23]. It is observed that the maximum value of the volumetric endothermic value increases as the inlet flow velocity increases, because of the increased mass flow rate.

To quantitatively compare the endothermic heat absorption rate with the total surface heat flux at the tube wall, an equivalent endothermic surface heat flux can be defined [15]. Variations of the equivalent endothermic surface heat flux at different inlet flow velocities are shown in Figure 10(b). By directly comparing the results in Figures 10(b) and 8(b), it is found that the surface heat flux from the endo-
thermic pyrolytic chemical reactions amount to more than 60% of the total wall heat flux in the high fluid temperature region for all the cases. Therefore, fuel pyrolysis plays a dictating role in supercritical-pressure heat transfer in the high fluid temperature region.

During the supercritical-pressure heat transfer process, as the fluid temperature increases and many low-molecular-weight products are produced, the thermophysical properties of the fluid mixture exhibit strong variations. Figure 11 shows variations of the fluid density, constant-pressure heat capacity, and fluid viscosity at different inlet flow velocities. These properties are calculated using the bulk fluid temperature. The fluid density experiences drastic decrease at various inlet flow velocities. The constant-pressure heat capacity reaches a maximum value in the trans-critical region when the fluid temperature transits from the subcritical to supercritical state.

The decrease in fluid density along the heated section leads to the significantly increased flow velocity, as shown in Figure 12, in which detailed velocity distributions in the flowfield and velocity variations in the axial and radial directions are provided. In the case with an inlet flow velocity at 4 m/s, the maximum velocity at the thermal exit can reach more than 40 m/s. The corresponding variations of the Reynolds number at different inlet flow velocities are presented in Figure 13. The Reynolds number is quite small at the tube inlet. For example, with an inlet flow velocity at 0.5 m/s, the Reynolds number is only 286 at the inlet of the heated section, but it rapidly increases in the heat transfer process prior to fuel pyrolysis. This is caused by the combined effects of the increased flow velocity and the significantly decreased fluid density and viscosity (Figure 11(a) and (c)). Therefore, the fluid flow and heat transfer process transits from the laminar to turbulent state.

Figure 14 presents variations of the heat transfer coefficient, the Nusselt number, at various inlet flow velocities. This parameter initially increases, consistent with the increased flow velocity and thus enhanced heat transfer, but it slightly decreases in the high fluid temperature region, mainly owing to the decreased heat absorption rate from fuel pyrolysis, as shown in Figure 10. As discussed early in this section, a supercritical-pressure heat transfer process of RP-3 is dictated by the endothermic pyrolytic chemical reactions in the high fluid temperature region.

4. Conclusions

In this paper, a mathematical model has been used to examine fluid flows and heat transfer of the aviation kerosene RP-3 with endothermic pyrolysis at a supercritical pressure. 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, containing 18 species and 24 elementary reactions, is incorporated to account for endothermic decomposition of the hydrocarbon fuel. The model is applicable over a wide range of operating conditions.

Detailed model validations have been carried out against a series of experimental data, including the fluid temperature, fuel conversion rate, various product yields, and heat sink. Good matches between the numerical and experimental results clearly verify the accuracy and reliability of the mathematic model.

Effects of the endothermic fuel pyrolysis and inlet flow velocity on fluid flows and heat transfer of RP-3 in a circular cooling tube have been investigated under a constant surface temperature of 950 K and at a supercritical...
Figure 12  Detailed distributions of velocity magnitude at inlet velocities of (a) 0.5 m/s and (b) 4 m/s, (c) velocity variations along axial direction at $r=0$ mm and (d) velocity variations along radial direction at $x/D=500$.

Figure 13  Variations of Reynolds number at different inlet velocities.

Figure 14  Variations of Nusselt number at different inlet velocities.
pressure of 5 MPa. Results reveal that the endothermic pyrolytic chemical reactions significantly improve the heat transfer process, particularly in the high temperature region. The equivalent surface heat flux from the endothermic fuel pyrolysis amounts to more than 60% of the total wall heat flux at the thermal exit under all the tested conditions. During the supercritical-pressure heat transfer process, the flow velocity significantly increases, and the corresponding Reynolds number also increases but mainly prior to fuel pyrolysis. This is caused by the drastic variations of various thermophysical properties. As a result, the fluid flow and heat transfer process transits from the laminar to turbulent state. The heat transfer coefficient, 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 fuel pyrolysis.

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