

## Numerical Study on Heat Transfer Deterioration in the Initial Heating Section of Supercritical Pressure RP-3 Postprint

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### Abstract

Numerical simulations of convective heat transfer of supercritical pressure RP-3 in vertical circular tubes were performed using the open-source computational fluid dynamics library OpenFOAM, with the research focus on heat transfer deterioration phenomena in the initial heating section. Two low-Reynolds-number turbulence models,  $k-\epsilon$  and  $k-SST$ , were selected for calculations and compared with experimental data, and the predictive capabilities of the two models for heat transfer deterioration under high wall heat flux conditions were discussed. Through analysis of the flow field and temperature field, a mechanistic explanation for the heat transfer deterioration phenomenon in the initial heating section was provided. Finally, the influences of variable thermophysical properties and buoyancy were examined. The results indicate that the  $k-SST$  model cannot simulate heat transfer deterioration, while the  $k-\epsilon$  model can qualitatively describe the rapid increase in inner wall temperature in the initial heating section. Buoyancy effects induced by fluid density variations and gravity are important causes of heat transfer deterioration in the initial heating section.

### Full Text

#### Preamble

**Numerical Study on Heat Transfer Deterioration in the Initial Heating Region of RP-3 under Supercritical Pressure**

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**Abstract:** The open-source computational fluid dynamics toolbox OpenFOAM was employed to simulate convective heat transfer of RP-3 aviation kerosene flowing in a vertical tube under supercritical pressure, with particular emphasis on heat transfer deterioration (HTD) in the initial heating region. Two low-Reynolds-number turbulence models,  $k-\epsilon$  and  $k-SST$ , were implemented and validated against experimental data to evaluate their predictive capabilities for HTD under high wall heat flux conditions. Mechanistic explanations for HTD in the initial heating region were proposed through analysis of the flow and temperature fields, followed by an investigation of the effects of variable properties and buoyancy forces. The results demonstrate that the  $k-SST$  model fails to predict HTD, whereas the  $k-\epsilon$  model can qualitatively capture the rapid rise in inner wall temperature in the initial heating region. Buoyancy forces induced by fluid density variation and gravity constitute a critical factor responsible for HTD in the initial heating region.

**Keywords:** supercritical pressure fluid; convective heat transfer; numerical computation; RP-3

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Scramjet engines represent the core propulsion component of air-breathing hypersonic vehicles, generating extremely high thermal loads due to prolonged, high-intensity supersonic combustion and severe aerodynamic heating [1, 2]. At high Mach numbers, the stagnation temperature of incoming air increases substantially, rendering air-cooling methods ineffective for scramjet thermal protection [3]. Currently, regenerative cooling using onboard hydrocarbon fuel as the coolant is considered one of the most effective active thermal protection strategies for scramjet engines [4].

In regenerative cooling systems, hydrocarbon fuel first flows through millimeter-scale cooling channels in the combustor wall to absorb heat before being injected into the combustion chamber. To enhance heat transfer efficiency and prevent phase change, the pressure within cooling channels exceeds the fuel's critical pressure [5]. The distinctive characteristic of supercritical pressure fluid heat transfer lies in the substantial variation of thermophysical properties with pressure and temperature. Researchers typically define the pseudocritical temperature ( $T_{pc}$ ) as the temperature corresponding to the peak isobaric specific heat ( $C_p$ ) at a given pressure [6]. Within a narrow temperature range near  $T_{pc}$ , the fluid's thermodynamic and transport properties (density, viscosity, isobaric specific heat, thermal conductivity, etc.) undergo dramatic changes. Additionally, buoyancy and thermal acceleration effects caused by density variations influence the flow field. The combined action of these factors renders convective heat transfer of supercritical pressure fluids highly complex [7, 8].

Extensive research has been conducted to understand convective heat transfer

characteristics of hydrocarbon fuels at supercritical pressure. Zhang et al. [9, 10] experimentally investigated heat transfer characteristics of supercritical pressure RP-3 aviation kerosene in vertically downward-flowing smooth tubes, categorizing the heat transfer process into four stages: initial heating region, normal heat transfer region, heat transfer enhancement region, and heat transfer deterioration region, and developed empirical correlations based on experimental data. Li et al. [11] experimentally studied convective heat transfer of supercritical pressure RP-3 aviation kerosene in vertically upward-flowing tubes, discussing the influence of mass flow rate, heat flux, pressure, and inlet temperature on heat transfer. Liu et al. [12] experimentally investigated convective heat transfer of supercritical pressure n-decane in vertical tubes, examining buoyancy and thermal acceleration effects on heat transfer under two tube diameters (inner diameter 0.95 mm and 2 mm). Zhong et al. [13] numerically studied convective heat transfer of supercritical pressure RP-3 aviation kerosene in horizontal tubes, observing HTD when wall temperature slightly exceeded pseudocritical temperature under high wall heat flux conditions, attributing the phenomenon to turbulent kinetic energy distribution in the near-wall region. Jiang et al. [14] numerically investigated convective heat transfer of supercritical pressure JP-8 aviation kerosene in vertical tubes, evaluating the predictive capabilities of different turbulence models (standard  $k$ - with standard wall functions, RNG  $k$ - with enhanced wall functions, and  $k$ - SST) for HTD, concluding that dramatic viscosity variation with temperature is the primary cause of HTD under high heat flux conditions.

This paper presents a numerical study on convective heat transfer of supercritical pressure RP-3 aviation kerosene in a vertical smooth tube, focusing on HTD in the initial heating region. The predictive capabilities of two low-Reynolds-number RANS turbulence models ( $k$ - $\nu^2$ - $f$  and  $k$ - SST) for HTD in the initial heating region are evaluated. Mechanistic explanations for HTD are proposed through analysis of flow and temperature fields, followed by a discussion of the effects of variable properties and buoyancy forces on heat transfer characteristics in the initial heating region.

### 1.1 Experimental Data Source

Numerical simulation conditions in this study were based on experimental results from Zhang et al. [10] to investigate heat transfer characteristics of supercritical pressure RP-3 aviation kerosene in the initial heating region. In the experiments, aviation kerosene flowed downward through a vertically positioned smooth tube (inner diameter 1.805 mm, outer diameter 2.2 mm). The total tube length was 450 mm, with a 300 mm heated section, preceded by a 90 mm adiabatic upstream section and followed by a 60 mm adiabatic downstream section. Direct electrical heating of the stainless steel tube was employed to achieve approximately uniform wall heat flux conditions. Further experimental details are available in [10]. Simulation parameters are summarized in .

## 1.2 Thermophysical Properties of RP-3

The critical point of RP-3 aviation kerosene is  $T_c = 645.04$  K,  $p_c = 2.33$  MPa [15]. Thermophysical and transport properties were selected following the same approach as in [10]. Density, dynamic viscosity, and isobaric specific heat were obtained from experimental measurements by Zhang et al. [16-18]. Thermal conductivity was calculated using the 10-component surrogate model proposed by Zhong et al. [4] based on the extended corresponding states principle. Thermophysical properties at  $p = 5$  MPa are illustrated in [Figure 1: see original paper].

## 2.1 Governing Equations

Convective heat transfer of aviation kerosene in tubes represents a typical conjugate heat transfer problem, which was solved using a partitioned approach with coupled boundary conditions. The problem was simplified to two-dimensional steady-state due to vertical flow.

The governing equation for heat conduction in the solid domain is Fourier's law, where  $\lambda$  represents solid thermal conductivity and  $\dot{q}$  represents internal heat source.

The governing equations for the fluid domain are as follows:

**Continuity equation:**

**Momentum equation:**

**Energy equation:**

In these equations,  $\rho$  denotes density,  $\mu$  and  $\mu_t$  represent molecular and turbulent viscosity,  $g$  is gravitational acceleration,  $H$  is fluid enthalpy,  $Pr$  and  $Pr_t$  are molecular and turbulent Prandtl numbers ( $Pr_t = 0.85$  in this study), and work done by gravity and viscous dissipation terms are neglected in the energy equation. Definitions of  $\mu_t$  in each turbulence model are presented in the following section.

## 2.2 Turbulence Models

Convective heat transfer of supercritical pressure fluids in tubes is closely related to the near-wall flow field, making accurate prediction of near-wall flow essential. Therefore, selecting appropriate turbulence models is crucial for numerical investigations of supercritical pressure fluid heat transfer. Two low-Reynolds-number RANS turbulence models widely applied in supercritical fluid heat transfer research were selected: the  $k-\epsilon$  model [19] and the  $k-\omega$  SST model [20].

**$k-\epsilon$  model:**

The  $k$  transport equation:

The  $\epsilon$  transport equation:

where  $P_k$  is the turbulent kinetic energy production term and  $G_k$  is the buoyancy production term constructed using the Generalized Gradient Diffusion Hypothesis (GGDH) [21].

The  $\nu^2$  transport equation:

The elliptic relaxation equation:

Turbulent viscosity in the  $k-\nu^2-f$  model is defined as:

where constants and are detailed in [19].

### **k- SST model:**

The  $k$  transport equation:

The  $\epsilon$  transport equation:

Turbulent viscosity in the  $k$ - SST model is defined as:

Model constants are calculated as:

where and are constants from the  $k$ - and standard  $k$ - models, respectively, detailed in [20].

## **2.3 Numerical Methods**

Numerical simulations were performed using the open-source CFD toolbox OpenFOAM (version 2.4.0) to solve the partial differential equation system. The finite volume method was employed for discretization. The QUICK scheme was used for convection terms in the momentum and energy equations, while first-order upwind scheme was applied for convection terms in other transport equations. The SIMPLE algorithm handled pressure-velocity coupling. Convergence was considered achieved when residuals of all solved variables fell below  $10^{-6}$ .

The computational domain dimensions matched the physical model, with adiabatic sections upstream and downstream of the heated section to ensure fully developed flow at the heated section inlet and numerical stability. Grid refinement was applied near the fluid domain wall to accurately resolve the near-wall flow field. All computational cases satisfied  $y^+ < 0.5$  at the first node near the wall.

Boundary conditions were specified as follows: uniform volumetric heat source in the solid domain to simulate uniform wall heat flux, with adiabatic outer wall and ends; uniform velocity, temperature, and turbulent transport quantities at the fluid domain inlet with zero axial pressure gradient; zero axial gradient for all transport quantities and constant pressure at the outlet. Wall boundary conditions for transport quantities are summarized in .

Grid independence analysis was conducted prior to simulations. The  $k$ - SST model was applied to Case I using three grid configurations with total cell counts

of 72,000, 108,000, and 216,000. Simulation parameters were: pressure 5 MPa, mass flux  $1572.7 \text{ kg/m}^2 \cdot \text{s}$ , inlet temperature 473 K, heat flux  $300 \text{ kW/m}^2$ , vertical downward flow. [Figure 2: see original paper] compares calculated inner wall temperatures with experimental data for the three grids. This case falls in the turbulent regime (mainstream Reynolds number range 14,900–45,000) with monotonically increasing inner wall temperature along the flow direction. The results indicate that 108,000 cells are sufficient for grid-independent solutions, and this configuration was adopted for all subsequent simulations. Good agreement between calculated and experimental wall temperatures validates the present model and numerical methodology.

### 3.1 Prediction of Heat Transfer Deterioration in the Initial Heating Region by Different Turbulence Models

[Figure 3: see original paper] compares inner wall temperatures calculated using the k- SST and k-  $\nu^2$ -f models with experimental data for Cases II-IV. In all subsequent figures,  $x/d = 0$  denotes the start of the heated section. The simulated cases feature relatively low inlet temperature, high density, and low velocity, placing the inlet flow in the transitional regime (inlet Reynolds number 6600). Experimental data reveal a rapid temperature rise with a local peak near the heated section inlet, indicating HTD. Following heat transfer recovery, the inner wall temperature decreases before increasing monotonically along the flow direction. As shown in [Figure 3: see original paper], the k- SST model predicts monotonically increasing inner wall temperature without any local peak, failing to capture HTD. In contrast, the k-  $\nu^2$ -f model shows good agreement with experimental data: inner wall temperature first rises rapidly, then decreases slightly before increasing monotonically, demonstrating its capability to qualitatively describe temperature variation trends in the initial heating region.

The k- SST model assumes isotropic turbulence, whereas the k-  $\nu^2$ -f model employs as the velocity scale to properly represent turbulence attenuation at the wall, partially accounting for turbulence anisotropy. For the present problem, the k-  $\nu^2$ -f model achieves superior performance.

[Figure 4: see original paper] further compares heat transfer coefficients calculated using the k-  $\nu^2$ -f model with experimental data. The model successfully simulates HTD in the initial heating region, and subsequent analysis will be based on its results.

### 3.2 Mechanism of Heat Transfer Deterioration in the Initial Heating Region

[Figure 5: see original paper] compares inner wall temperature and convective heat transfer coefficient calculated using the k-  $\nu^2$ -f model with experimental data for Case II. For detailed analysis, four cross-sectional positions were selected along the flow direction: P1-P4 (P1:  $x/d = 8$ , P2:  $x/d = 15$ , P3:  $x/d = 23$ , P4:  $x/d = 40$ ), where P1-P3 are located in the HTD region and P4 is in

the recovery region.

[Figure 6: see original paper] presents axial velocity (a) and temperature (b) distributions at sections P1–P4. In the HTD region (P1–P3), axial velocity within the thermal boundary layer exhibits a parabolic profile. As shown in Figure 6: see original paper, large temperature differences exist between the wall and mainstream fluid, while mainstream temperature changes minimally. This occurs because the thermal boundary layer flow is laminar, impeding heat transfer from the wall to the mainstream. Furthermore, thermal boundary layer thickness increases along the flow direction, continuously increasing thermal resistance and causing HTD. As fluid temperature rises, density decreases and velocity increases, prompting transition from laminar to turbulent flow in the thermal boundary layer (P4). At P4, the temperature difference between wall and mainstream gradually decreases; correspondingly, [Figure 4: see original paper] shows that the convective heat transfer coefficient begins to increase along the flow direction, indicating recovery of heat transfer intensity.

Additional investigation of variable property and buoyancy effects reveals that fluid viscosity variation also contributes to inlet HTD. Fluid heating reduces viscosity, decreasing shear stress in the near-wall viscous layer and deteriorating heat transfer capability. However, this effect is less significant than buoyancy.

[Figure 7: see original paper] compares calculated inner wall temperatures with experimental data when fluid density and viscosity are held constant (at inlet temperature values) and when gravitational acceleration is set to zero ( $g = 0$ ). When density remains constant, no local wall temperature peak appears. When gravity is set to zero, the temperature variation trend closely resembles the constant-density case. When viscosity is held constant, inlet wall temperature rises compared to the constant-density case but remains below actual values. These results demonstrate that buoyancy forces induced by density variation and gravity are the primary cause of HTD in the heated section. This phenomenon resembles laminar mixed convection. In the initial heating region, the boundary layer is laminar. For downward flow, buoyancy acts opposite to the flow direction, reducing near-wall fluid velocity [22]. Consequently, convective energy transport decreases, reducing heat transfer capacity; decreased velocity gradient at the wall reduces shear stress, delaying laminar-to-turbulent transition. The combined effects ultimately lead to HTD.

## 4 Conclusions

This study numerically investigated convective heat transfer of supercritical pressure RP-3 aviation kerosene in a vertical tube using the open-source CFD toolbox OpenFOAM, focusing on HTD in the initial heating region. The main conclusions are:

1. The  $k$ -SST model fails to predict HTD in the initial heating region, whereas the  $k$ - $\epsilon$ -2-f model can qualitatively describe the variation pattern

of inner wall temperature, showing good agreement with experimental data.

2. Buoyancy forces caused by fluid density variation and gravity represent a critical factor responsible for HTD in the initial heating region. The effect of fluid viscosity on inlet heat transfer is less significant than that of buoyancy.

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## References

- [1] Powell O A, Edwards J T, Norris R B, et al. Development of Hydrocarbon-Fueled Scramjet Engines: The Hypersonic Technology (HyTech) Program[J]. *Journal of Propulsion and Power*, 2001, 17(6): 1170-1176.
- [2] Fry R S. A Century of Ramjet Propulsion Technology Evolution[J]. *Journal of Propulsion and Power*, 2004, 20(1): 27-58.
- [3] Edwards T. Liquid Fuels and Propellants for Aerospace Propulsion: 1903-2003[J]. *Journal of Propulsion and Power*, 2003, 19(6): 1089-1107.
- [4] Zhong Fengquan, Fan Xuejun, Yu Gong, et al. Heat Transfer of Aviation Kerosene at Supercritical Conditions[J]. *Journal of Thermophysics and Heat Transfer*, 2009, 23(3): 543-550.
- [5] Hua Yixin, Wang Yazhou, Meng Hua. A Numerical Study of Supercritical Forced Convective Heat Transfer of n-Heptane Inside a Horizontal Miniature Tube[J]. *The Journal of Supercritical Fluids*, 2010, 52(1): 36-46.
- [6] He S, Kim W S, Bae J H. Assessment of Performance of Turbulence Models in Predicting Supercritical Pressure Heat Transfer in a Vertical Tube[J]. *International Journal of Heat and Mass Transfer*, 2008, 51(19-20): 4659-4675.
- [7] Pioro I L, Duffey R B. Experimental Heat Transfer in Supercritical Water Flowing Inside Channels (Survey)[J]. *Nuclear Engineering and Design*, 2005, 235(22): 2407-2430.
- [8] He S, Kim W S, Jackson J D. A Computational Study of Convective Heat Transfer to Carbon Dioxide at a Pressure Just Above the Critical Value[J]. *Applied Thermal Engineering*, 2008, 28(13): 1662-1675.
- [9] Zhang Bin, Zhang Chunben, Deng Hongwu, et al. Heat Transfer Characteristics of Hydrocarbon Fuel at Supercritical Pressure in Vertical Circular Tubes[J]. *Journal of Aerospace Power*, 2012, 27(03): 595-603.
- [10] Zhang Chunben, Xu Guoqiang, Gao Lin, et al. Experimental Investigation on Heat Transfer of a Specific Fuel (RP-3) Flows Through Downward Tubes at Supercritical Pressure[J]. *The Journal of Supercritical Fluids*, 2012, 72(0): 90-99.

- [11] Li Wei, Huang Dan, Xu Guoqiang, et al. Heat Transfer to Aviation Kerosene Flowing Upward in Smooth Tubes at Supercritical Pressures[J]. International Journal of Heat and Mass Transfer, 2015, 85: 1084-1094.
- [12] Liu Bo, Wang Xi, Zhu Yin Hai, et al. Experimental Investigation of Convection Heat Transfer of n-Decane at Supercritical Pressures in a Micro/Mini Vertical Tube[J]. Journal of Engineering Thermophysics, 2014, 35(01): 114-118.
- [13] Dang Guoxin, Zhong Fengquan, Chen Lihong, et al. Numerical Investigation on Flow and Convective Heat Transfer of Aviation Kerosene at Supercritical Conditions[J]. Science China Technological Sciences, 2013, 56(2): 416-422.
- [14] Jiang H, Ervin J, West Z, et al. Turbulent Flow, Heat Transfer Deterioration, and Thermal Oxidation of Jet Fuel[J]. Journal of Thermophysics and Heat Transfer, 2013, 27(4): 668-678.
- [15] Deng Hongwu, Zhang Chunben, Xu Guoqiang, et al. Visualization Experiments of a Specific Fuel Flow Through Quartz-glass Tubes Under both Sub- and Supercritical Conditions[J]. Chinese Journal of Aeronautics, 2012, 03(03): 372-380.
- [16] Deng Hongwu, Zhang Chunben, Xu Guoqiang, et al. Density Measurements of Endothermic Hydrocarbon Fuel at Sub- and Supercritical Conditions[J]. Journal of Chemical & Engineering Data, 2011, 56(6): 2980-2986.
- [17] Deng Hongwu, Zhang Chunben, Xu Guoqiang, et al. Viscosity Measurements of Endothermic Hydrocarbon Fuel from (298 to 788) K under Supercritical Pressure Conditions[J]. Journal of Chemical & Engineering Data, 2012, 57(2): 358-365.
- [18] Deng Hongwu, Zhu Kun, Xu Guoqiang, et al. Isobaric Specific Heat Capacity Measurement for Kerosene RP-3 in the Near-Critical and Supercritical Regions[J]. Journal of Chemical & Engineering Data, 2011, 57(2): 263-268.
- [19] Lien F-S, Kalitzin G. Computations of Transonic Flow with the v2-f Turbulence Model[J]. International Journal of Heat and Fluid Flow, 2001, 22(1): 53-61.
- [20] Menter F R. Two-Equation Eddy-Viscosity Turbulence Models for Engineering Applications[J]. AIAA Journal, 1994, 32(8): 1598-1605.
- [21] Daly B J, Harlow F H. Transport Equations in Turbulence[J]. Physics of Fluids, 1970, 13(11): 2634-2649.
- [22] Kim W S, He S, Jackson J D. Assessment by Comparison with DNS Data of Turbulence Models Used in Simulations of Mixed Convection[J]. International Journal of Heat & Mass Transfer, 2008, 51(5-6): 1293-1318.

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