Simulation of heat transfer in a flow of over-critical nitrogen and oxygen in a horizontal circular tube

S V Borodkin\textsuperscript{1,3}, I L Bataronov\textsuperscript{2}, A V Ivanov\textsuperscript{1} and V I Ryazhskikh\textsuperscript{2}

\textsuperscript{1}Military Scientific Educational Center of Military-Air Forces “N.E. Zhukovsky and Ju.A. Gagarin Military-Air Academy”, Voronezh, Russian Federation
\textsuperscript{2}Voronezh State Technical University, 394026, Voronezh, Moskovsky prospekt, 14, Russian Federation

\textsuperscript{3}E-mail: borodkinstanislav@yandex.ru

Abstract. In the framework of the $k$-$\varepsilon$ turbulence model with enhanced wall treatment, heat transfer in a flow of over-critical nitrogen and oxygen in a horizontal circular tube with heat boundary conditions of the third kind in the pressure range of 20\textendash{}40 MPa, mass flow rates of 0.03\textendash{}0.12 kg/s, and heat transfer coefficients to the environment of 500\textendash{}2000 W/(m\textsuperscript{2}K) is simulated. The distributions of the bulk temperature, calculated as the thermodynamic temperature of the average mass enthalpy of the supercritical fluid flow, are obtained. Analysis of the heat transfer coefficient of the flow showed that at pressures less than three times the critical one, a reduced heat transfer mode appears, so the near-critical region is not recommended for use in oxygen and nitrogen gasifiers. In the framework of the multiplicative model for the Nusselt number, insignificant simplices of thermophysical properties are established and correlations for oxygen and nitrogen in the over-critical region are constructed, which agree with the result of the computational experiment with an average relative accuracy of 1\textendash{}1.5\%. On the basis of the one-dimensional heat transfer equation, the adequacy of the obtained correlations is shown. It is established that when using the bulk temperature based on the mass average enthalpy, a separate account of the initial heat transfer section is not required.

1. Introduction

High-pressure nitrogen and oxygen are widely used in the power and life support systems of aerospace aircraft. The production of these materials from cryogenic liquid is carried out by gasification using on-board or ground installations [1]. Optimization of the gasification process in the supercritical fluid state (SCF) requires the use of the heat transfer coefficient between the SCF and the heating system [2–5]. For ordinary liquids and gases, universal dependences for calculating this coefficient are obtained [3, 5], while for SCF there are a large number of theoretical and experimental studies [6–8], which give very heterogeneous results for the Nusselt number, depending on the type of substance and experimental conditions. At the same time, data on nitrogen is very limited, and on oxygen is practically absent. In the near-critical region, which is characterized by a sharp change in the thermophysical properties of SCF with temperature, processes occur that lead to reduced heat transfer [5]. Therefore, for gasification, an over-critical region of SCF states is usually recommended, in which the change in properties is fairly smooth. In this case, sufficiently reliable results on the local heat transfer coefficient can be obtained by calculating the turbulent heat and mass transfer in the framework of approved models [9–11].
2. Problem statement
To calculate the conjugate heat and mass transfer in a turbulent flow, $k-\varepsilon$ turbulence models [10, 11], based on the Reynolds-averaged transport equations (RANS), are currently most widely used, including for the SCF [12–15].

To simplify the computational problem, we will neglect the buoyancy effects and the swirling of the flow in the heat exchanger. These effects can be accounted for by the corresponding correction factors [2, 3]. Then the problem becomes axially symmetric. The use of an axially symmetric formulation makes it possible to significantly reduce the numerical dimension of the problem, which is important for performing calculations in a long, thin tube.

As shown by experimental observations and theoretical calculations [12-15], the pressure drop in the SCF-flow in the evaporator is less than 0.1% of the operating pressure, so the influence of the pressure change in the SCF flow on the thermophysical properties can also be ignored in the calculation.

The standard $k-\varepsilon$ model with enhanced wall treatment, which has higher accuracy [12–15], is adopted for the simulation.

The numerical computations were performed using ANSYS CFD FLUENT software.

The region of solution of the problem was the longitudinal section of the circular tube of radius $R = 5$ mm and length $L = 4$ m. To exclude the influence of boundary effects at the inlet and outlet of the tube, buffer regions with a length of 20 mm were added at the ends with the condition of thermal insulation of the tube surface (figure 1).

In accordance with the selected geometry, the following boundary conditions were set on the lines $\Gamma_i$ (figure 1).

1) On the line $\Gamma_1$ of the input flow of SCF: uniform temperature distribution $T(r) = T_{in}$ and self-similar distribution of the velocity of the turbulent flow. Using this self-similar profile reduces the size of the input buffer zone required to relax the input distributions of variables.

2) On line $\Gamma_4$ of the SCF output flow: no conductive heat transfer and uniform pressure distribution $p(r) = P_{out}$. The exact conditions at the output from the heat exchange zone are not known in advance, so usually a buffer zone is introduced without heat exchange with a coolant of such length that at the exit from it the flow can be considered stable, that is, such that the formulated conditions are fulfilled. Then, at the actual boundary of the output from the heat transfer zone, natural boundary conditions will automatically be obtained. The length of the required buffer zone is determined by the selection in the computational experiment.

3) On the line $\Gamma_3$ of heat exchange with the environment, the Newton-Richman condition with a given heat transfer coefficient $\alpha_0$ is used:
\[ \lambda \frac{\partial T}{\partial r}(R, z) = \alpha_0 \cdot (T_{\text{ex}} - T_w(z)). \]  

(1)

Here \( \lambda \) is the thermal conductivity coefficient of SCF, \( T_{\text{ex}} \) is the temperature of the environment, \( T_w \) is the temperature of the flow of SCF on the wall \( \Gamma_2 \). Usually, the theoretical calculation of convective heat transfer is made for one of two modes: constant heat flow through the wall and constant wall temperature [5]. However, in a real technical device, none of these conditions are fulfilled, and the physical conditions of heat exchange are closer to the general condition of heat balance (1). For practical purposes, it is sufficient to study a problem with a constant heat transfer coefficient \( \alpha_0 \), which, thereby, becomes an additional variable parameter of the model.

4) On the lines \( \Gamma_3 \) of the buffer zones, a thermal isolation condition is applied to ensure the stabilization of the input and output SCF flows.

The functions of the temperature dependence of the thermophysical parameters were used in the form of specially constructed approximations [16].

For the correct solution of the problem near the wall, a boundary mesh was used, consisting of 8 layers of thin rectangular elements with a decreasing thickness, formed in automatic mode (figure 1). The rest of the solution area was covered with triangular elements with a maximum size of 0.4 mm.

The constructed grid contained about 200,000 finite elements, the number of degrees of freedom is about 820000, the time to solve one problem on a 6-core processor with a frequency of 3.6 GHz was 25 minutes.

3. Computational experiment for calculating heat transfer in a one-dimensional SCF-oxygen flow

The computational experiment was carried out for the following parameter values covering the operating modes of the gasifiers:

- Input temperature \( T_{\text{in}} = 90 \) K.
- Output pressure \( P_{\text{out}} = 20\div40 \) MPa.
- Environment temperature \( T_{\text{ex}} = 333 \) K.
- Mass flow rate SCF \( G = 0.03\div0.12 \) kg/s.
- Heat transfer coefficient \( \alpha_0 = 500\div2000 \) W/(m²s).

The bulk temperature \( T_h \) was calculated on the basis of the integral energy balance equation:

\[ \Delta h(z) = \frac{2\pi R \alpha_0}{G} \int_0^5 (T_{\text{ex}} - T_w(z')) dz'. \]  

(2)

where \( \Delta h(z) \) is the change in the average mass enthalpy of the SCF flow from the input section to the section with the \( z \)-coordinate. Based on the thermodynamic dependence of the change in the specific enthalpy on the temperature at constant pressure, an approximating formula \( T - T_{\text{in}} = \Theta(\Delta h) \) was constructed, using which the bulk temperature was calculated:

\[ T_h(z) = T_{\text{in}} + \Theta(\Delta h(z)). \]  

(3)

The calculation is also performed by calculating the increment of the average mass specific enthalpy in a given flow section with respect to the value at the input to the heat exchange zone according to the formula:

\[ \Delta h(z) = \frac{2\pi}{G} \int_0^\pi h(r, z) v_z(r, z) \rho(r, z) r dr - h_0. \]  

(4)
Here \( h(r, z) \) is the local value of the specific enthalpy of SCF, \( v_z (r, z) \) is the \( z \)-component of the local flow rate of SCF, \( \rho (r, z) \) is the local value of the density of SCF. Then the temperature value \( T_h \) was calculated using the formula (3).

Within the limits of the error of the computational experiment and the error of the physical model, both calculated values of the bulk temperature coincided with each other up to the value of the viscous dissipation, which was insignificant in this experiment. This also justifies the neglect of viscous dissipation in calculating the bulk temperature, commonly used in SCF-flow simulation [12–15].

Using the equations (2) and (3), from the numerical solution of the problem for a given set of values of the parameters \( G, \alpha_0, P_{\text{out}} \), the distributions of the bulk temperature and the wall temperature along the flow length, selectively presented in figure 2, were calculated. For each set of parameters, the temperatures are represented by curves of the same type: the lower curve is the bulk temperature, the upper curve is the wall temperature.

\[
q(z) = \alpha_0 \left( T_{\text{ex}} - T_w(z) \right).
\]

(5)

For comparison, a calculation was also made with a pressure of \( P_{\text{out}} = 10 \, \text{MPa} \) from the near-critical region, the result of which is shown in figure 2(a) by a dotted line. As can be seen, in this area there is a significant decrease in the intensity of heat transfer and an increase in the temperature factor.

On the distribution of the wall temperature, a characteristic initial section of thermal stabilization with a length of about 30 cm is observed. However, this section is not visually detected on the distribution of the bulk temperature. Therefore, the further analysis was carried out only for data from the heat-stabilized zone.

As can be seen from figure 2, the change in SCF pressure slightly affects the difference between the bulk temperature and the wall temperature, as well as the character of the change in these temperatures along the tube. However, an increase in the heat transfer coefficient leads to a significant change in the temperature profile and an increase in the output temperature. In turn, the change in the mass flow rate of SCF has a similar, but inverse, effect on the temperature profile.

4. Correlation of the heat transfer coefficient of SCF-oxygen

To calculate the local heat transfer coefficient of SCF, the heat flow density through the wall was used, which is found from the equation (1):

\[
\alpha(z) = \frac{q(z)}{T_w(z) - T_h(z)} = \frac{T_{\text{ex}} - T_w(z)}{T_w(z) - T_h(z)}.
\]

(6)
Note that here the heat transfer coefficient is determined relative to the bulk temperature (3), so, generally speaking, it may not coincide with the values found from other correlations.

The local Nusselt number was determined on the basis of equation (6) by the formula

\[
\text{Nu} = \frac{2R\alpha}{\lambda(T_h)}.
\] (7)

This value was also determined for the thermal conductivity coefficient taken at the bulk temperature.

As a result, for each combination of parameters, a table \((\text{Nu}, T_h, \alpha, P\)) is found for the dependence of the Nusselt number on the flow temperatures of the SCF and the wall, the pressure of the SCF, and the environment heat transfer coefficient. Some results of processing the computational experiment according to equations (6), (7) are presented in figure 3. A comparison is also made with the calculation of heat transfer in the near-critical region (figure 3(a), curve 10 MPa). As can be seen from the comparison, the exit to the near-critical region leads to a significant irregular decrease in the heat transfer coefficient. Therefore, the operating mode of the pacificators should be selected in such a way that the working area of the evaporator remains in the over-critical pressure region \((P \geq 3P_c\)) where \(P_c\) is the critical pressure.

**Figure 3.** Temperature dependence of the heat transfer coefficient and the Nusselt number in SCF-oxygen at different pressure (a), mass flow rate (b), and heat transfer coefficient to the environment (c).

To obtain the correlation, a multiplicative model was used, in which all commonly used factors were included:

\[
\text{Nu}(T, P) = a_0 \Pr^{a_1} \text{Re}^{a_2} \left( \frac{\mu}{\mu_w} \right)^{a_3} \left( \frac{\lambda}{\lambda_w} \right)^{a_4} \left( \frac{c_p}{c_{pw}} \right)^{a_5} \left( \frac{\rho}{\rho_w} \right)^{a_6} \left( \frac{c_p}{c_{pw}} \right)^{a_7} \frac{2R\alpha_0}{\lambda} \Pr^{a_8},
\] (8)

where \(\bar{\alpha} = \frac{h_w - h}{T_w - T_h}\) is the average integral heat capacity of SCF, \(\Pr = \frac{\mu c_p}{\lambda}\) is the Prandtl number in SCF, \(\bar{\Pr} = \frac{\mu c_p}{\lambda}\) is the average heat capacity of the Prandtl number, often used [5, 6, 8] in constructing the correlations for SCF, \(c_p, \rho, \mu\) are the specific heat capacity, density, and dynamic viscosity of SCF, which
are functions of pressure and temperature [16]. The “w” index means the calculation of the value at the wall temperature $T_w$.

The coefficients $a_i$ were determined by regression analysis of the linearized model obtained by logarithm of equality (8). The analysis showed that the coefficients $a_1$ and $a_9$ are strongly correlated, with the coefficient $a_1$ having less significance in the model. Also, the coefficients $a_3$, $a_4$ and $a_8$ were essentially insignificant. As a result of filtering out these coefficients, the model was reduced to the form

$$\text{Nu}(T, P) = 0.0292 \Pr^{0.542} \Re^{0.773} \left( \frac{\rho_w}{\rho} \right)^{0.464} \left( \frac{c_p}{c_p} \right)^{0.663} \left( \frac{c_p}{c_{pw}} \right)^{0.357}.$$  \hspace{1cm} (9)

In this model, all the coefficients showed a high level of significance, and the relative error in determining the natural (not logarithmic) values of the Nusselt number was: the maximum value is 3%, the average value is 1%.

5. Computational experiment and correlation for the heat transfer coefficient of SCF-nitrogen

The second series of calculations was performed for SCF-nitrogen with the same set of parameters as for oxygen. The results of processing the computational experiment according to equations (2)–(7) showed that the effect of pressure, mass flow rate of SCF and heat transfer coefficient for SCF-nitrogen qualitatively coincides with similar results obtained for SCF-oxygen.

To approximate the dependence of the Nusselt number in nitrogen, the model (8) was also used, but the coefficients $a_i$ were considered linear functions of pressure. In the framework of the regression analysis, the same insignificant coefficients were established as in the case of oxygen, and an additional insignificant coefficient $a_5$ was established. In addition, the coefficient $a_7$ found a significant dependence on pressure. The resulting correlation for nitrogen has the form:

$$\text{Nu}(T, P) = 0.03862 \Pr^{0.500} \Re^{0.745} \left( \frac{\rho_w}{\rho} \right)^{0.442} \left( \frac{c_p}{c_{pw}} \right)^{0.223} \left( \frac{P}{P_c} \right)^{1.392},$$  \hspace{1cm} (10)

where $P_c$ is the critical nitrogen pressure (3.4 MPa). For equation (10), the relative error in determining the natural values of the Nusselt number was the maximum value of 5%, the average value of 1.5%.

6. Discussion

In the high-temperature limit, the last three factors in the left side of equations (9), (10) tend to one, and $\text{Pr} \rightarrow \text{Pr}_c$, as a result, equations (9), (10) show good agreement with the classical Dittus-Boelter correlation, which is important for calculations in a wide temperature range. This also confirms the validity of equations (9), (10). The difference in the numerical coefficients is due to the fact that for the Reynolds numbers under consideration, the Dittus-Boelter correlation itself is inaccurate [5], and our correlations are also constructed for a range of high pressures.

The criterion equations (9), (10) do not explicitly include the factor of the environment heat transfer coefficient, its influence is automatically taken into account through the self-consistent formation of the wall temperature in the process of heat transfer. This means that a self-similar mode of heat transfer from SCF is formed in the considered over-critical region, which allows using universal dependences of the form (9, 10) for a wide range of pressures and mass flow rates.

To verify equations (9), (10), the bulk temperature distribution was calculated in the framework of a one-dimensional model of heat transfer in the flow [4]

$$Gc_p \frac{dT_h}{dz} = \pi \frac{T_{ex} - T_h}{R(T_h, T_w)}; \quad R(T_h, T_w) = \frac{1}{2R_G} + \frac{1}{2R_G(T_h, T_w)}.$$  \hspace{1cm} (11)
Here $R_t$ is the thermal resistance between the SCF and the environment. To determine the wall temperature, we use the ratio following from the equation (6):

$$T_w = \frac{\alpha_0 T_{cx} + \alpha(T_h, T_w) T_h}{\alpha_0 + \alpha(T_h, T_w)}.$$  \hspace{1cm} (12)

Equation (12) forms a rapidly convergent scheme of simple iterations for determining the wall temperature at a given bulk temperature. The result of solving the system (11), (12) with equations (7), (9) for the heat transfer coefficient in SCF-oxygen is shown in figure 4.

![Figure 4](image)

**Figure 4.** Solution of the one-dimensional equation (11) (lines) in comparison with the result of a computational experiment (circles).

Similar results are obtained for equation (10).

Figure 4 shows that the correlations (9) and (10) allow us to obtain an adequate distribution of the volume temperature of the flow of supercritical nitrogen and oxygen in the gasifier evaporator. It should be noted that equations (9) and (10) are constructed without taking into account the initial heat transfer section. However, the solution obtained with these equations coincides with the result of a computational experiment, in which this section is automatically taken into account. Hence, it can be concluded that when using the bulk temperature, determined by the average mass enthalpy, in the heat transfer equation (11), a separate account of the initial heat transfer section is not required.

Figure 4 also shows an example of calculating the bulk temperature distribution at a pressure of 10 MPa, which is located in the near-critical region and does not fall into the pressure range for which equations (9) and (10) are constructed. Nevertheless, even in this case, a good agreement is obtained with the result of the computational experiment. However, this fact needs to be experimentally verified [5].

Correlations (9), (10) were used to analyze and optimize the operation of the gasification unit SGU-7KM-U and showed results that are in good agreement with experimental observations.

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