CFD-calculation of influence of impurities on the characteristics of a helium turboexpander

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Abstract. The process of expanding of two-component gaseous mixture was studied in a stage of a turboexpander unit in three-dimensional unsteady setting with use of methods of computer fluid dynamics. The calculation method used in this work made it possible to study the turboexpander unit in a single calculation model but not in parts due to the use of sliding interfaces. Based on the distribution of the supersaturation ratio, assumption was made about the possible localization of phase transitions in the flow part of the stage of the turboexpander unit, confirmed by the characteristic impeller damage.

1. Introduction
Turbo-expander units (TEU) are vane type cryogenic expansion machines. They are designed to solve a wide range of problems: receiving cold, cleaning and liquefying gases for storage and transportation, and generation of electricity in turbine expanders-generators.

In real conditions, the working medium in the turboexpander contains a certain amount of impurities that affect the flow characteristics, the resulting temperature at the outlet of the TDA, and the life time of the flow part of the unit. The presence of impurities often causes erosion of the impeller blades due to droplet bombardment of the resulting condensate. The aim of this study is to refine the methodology for calculating the expansion of multicomponent mixtures in the flow part of the turboexpander stage, to modernize the calculation package with additional equations, namely, considering the supersaturation ratio, as a first approximation for further studies of bulk condensation in the flow part.

2. Formulation of the problem
A two-component flow was considered, which expands in the flow part of the stage of a turboexpander unit in a three-dimensional formulation. The solution was carried out by methods of computer fluid dynamics.

2.1. Mathematical description
The mathematical description includes a system of equations consisting of the Navier – Stokes equations for a compressible gas averaged by Reynolds and Favre [1], equations of state, and turbulence equations for closing the system. Shock waves were not modelled; therefore, bulk viscosity was not considered in the equations of motion [2].

In equations for a compressible gas, the density, pressure and heat flux are averaged according to Reynolds: \( \rho = \bar{\rho} + \rho' \), \( p = \bar{p} + p' \), \( q_i = q_i + q_i' \); and velocity, enthalpy, energy and temperature are
averaged according to Favre: \( u_i = \bar{u}_i + u_i^* \), \( h = h + h^* \), \( e = \bar{e} + e^* \), \( T = T + T^* \). This ultimately gives a system of equations for a compressible gas, including the equations of continuity, motion, and energy:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho \bar{u}_j) &= 0; \\
\frac{\partial}{\partial t} (\rho \bar{u}_j) + \frac{\partial}{\partial x_j} (\rho \bar{u}_j \bar{u}_j) &= -\frac{\partial P}{\partial x_j} + \frac{\partial}{\partial x_j} \left[ \bar{\tau}_{ji} + \bar{\tau}_{j,j} \right]; \\
\frac{\partial}{\partial t} \left[ \rho \left( \bar{e} + \frac{\bar{u}_j^2}{2} \right) \right] + \frac{\partial}{\partial x_j} \left[ \rho \bar{u}_j \left( h + \frac{\bar{u}_j^2}{2} \right) \right] &= \frac{\partial}{\partial x_j} \left[ u_i \left( \tau_{ji} + \tau_{j,j} \right) \right];
\end{align*}
\]

(1)

where \( \rho \) is density; \( \bar{u} \) is velocity; \( p \) is pressure, \( \tau_{ji} \) is viscous stress tensor, \( \bar{\tau}_{j,j} = -\rho \bar{u}_i^* \bar{u}_i^* \) is turbulent stress tensor, \( q \) is heat flux, \( \bar{q}_{ij} = -\rho \bar{u}_i^* h^* \) is turbulent heat flux, \( e \) is internal energy, \( h \) is enthalpy, \( T \) is temperature, and \( k \) is kinetic energy of turbulence. The term \( \bar{\tau}_{ji} u_i^* - \rho \bar{u}_i^* u_i^* / 2 \) in the energy equation considers the molecular and turbulent transfer of kinetic energy of turbulence. In the system of equations (1), the method of silent summation using a twice-repeated index is used.

Additional equation is required for multicomponent flows. This is equation of diffusion, which is the law of mass conservation for each component of the mixture [3]:

\[
\frac{\partial \rho_k}{\partial t} + \frac{\partial}{\partial x_j} (\rho_k \bar{u}_j) + \frac{\partial j_{k,j}}{\partial x_j} = 0,
\]

(2)

where \( \rho_k \) is the density of the \( k \)th component of the mixture, \( j \) is diffusion mass flux of the \( k \)th component. Diffusive mass flux is determined according to Fick's law and can be represented in the following form:

\[
j_{k,j} = -\rho D \frac{\partial C_k}{\partial x_j},
\]

(3)

where \( D \) is the diffusion coefficient, \( C_k \) is the mass fraction of the \( k \)th component.

The next important step is to describe the interconnections between the thermodynamic characteristics (density, pressure and temperature) of the working fluid. To a first approximation, the ideal gas equation of state was used, however, according to the results of comparison with experimental data, a discrepancy was found that was resolved by applying the Redlich-Kwong equation of state of real gases is used [4], which has the following form:

\[
p = \frac{RT}{V_m - b} - \frac{a}{\sqrt{T}V_m(V_m + b)},
\]

(4)

where \( R \) is the universal gas constant, \( V_m \) is the molar volume, \( a \) and \( b \) are constants depending on a particular substance, determined through critical parameters:

\[
a = \frac{0.42748R^2T_{cr}^{2.5}}{p_{cr}}
\]

\[
b = \frac{0.086664RT_{cr}}{p_{cr}}
\]

(5)

Here, \( T_{cr} \) is the critical temperature, \( p_{cr} \) is the critical pressure.

The Redlich – Kwong equation (4) can be used in the range of pressures and temperatures for which \( p/p_{cr} < 0.5T/T_{cr} \). In this paper, calculations were carried out for pressures and temperatures in the
region of applicability. If the ideal gas equation of state is used, then difference between results of
calculation and experimental data is significantly higher in comparison with use of the Redlich –
Kwong equation.

Due to that the relationship between the turbulent components of the stress tensor \( \mathbf{T}_{ij} \) and the heat flux vector \( \mathbf{q}_j \) with the parameters of the averaged flow is unknown and needs to be determine
d, system (1) turns out to be open. To close the system of equations, one of the turbulence models must be used.
In this work, we use the standard \( k-\omega \) turbulence model, since it showed the best stability for
compressible flows [5]. The equations of this model in general form are written as follows:

\[
\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_i}\left(\Gamma_k \frac{\partial k}{\partial x_i}\right) + G_k - Y_k
\]

(6)

\[
\frac{\partial}{\partial t}(\rho \omega) + \frac{\partial}{\partial x_i}(\rho \omega u_i) = \frac{\partial}{\partial x_i}\left(\Gamma_\omega \frac{\partial \omega}{\partial x_i}\right) + G_\omega - Y_\omega
\]

where \( k \) is the kinetic energy of turbulence, \( \omega \) is the energy dissipation rate, \( G_k, \ G_\omega \) are the terms
responsible for the generation of \( k \) and \( \omega \), \( \Gamma_k, \Gamma_\omega \) are the diffusion coefficients, \( Y_\omega, \ Y_k \) are the attenuation
coefficients. In this paper, for simplicity of presentation, the computations for the terms \( G_k, \ G_\omega, \ \Gamma_k, \ \Gamma_\omega, \)
and \( Y_\omega, \ Y_k \) are not presented.

To localize areas in which phase transitions are possible, an equation is needed for the supersaturation
ratio, which is calculated in each cell of the computational grid, is added to the calculation packet and is determined as follows:

\[
s = \frac{p_i}{p_s(T)}
\]

(7)

where \( p_i \) is the vapor pressure, \( p_s \) is the saturation pressure.

Supersaturation is a necessary, but not always sufficient condition for bulk condensation. Nucleation
rate of droplets depends on supersaturation ratio strongly, but it is close to zero at small supersaturation
ratio. Intensity of bulk condensation increases with increase of supersaturation ratio. For example, in
our previous paper [6], the flow of a vapor – gas mixture in supersonic part of Laval nozzle was studied.
It was shown that there are no droplets at small supersaturation ratio, intensive nucleation begins when
supersaturation ratio reaches a certain value. In [6] the kinetic equation for the droplet size distribution
function was solved numerically. In the framework of the present study, it is planned to use similar
approach for description of the bulk condensation process, both in a guiding apparatus, which, in fact,
is a set of nozzle channels, and in a diffuser and impeller.

2.2. Model description

The three-dimensional model of the stage of the turboexpander unit is shown in figure 1. The principle
of operation of the turboexpander stage is well known: the gas through the inlet 1 enters the guiding
apparatus 2, after that it expands and rotates the impeller 3 with a certain frequency, and then through
the diffuser 4 it enters the outlet 5 and then into the main (not shown).

On the basis of a three-dimensional model, a model of the flow part was built, which was divided
into elementary volumes, from which a three-dimensional computational grid is formed. In contrast to
the calculations presented in the literature [7], in which each part of the turbine stage is considered
separately, we used the partition of the flow part into zones with common sliding interfaces, which made
it possible to carry out calculations of the complete model.

Thus, the final calculation model consists of four zones: a guide apparatus, an impeller, a gap between
the diffuser and the impeller, and a diffuser.
Figure 1. Three-dimensional model of the stage of a turboexpander apparatus.

2.3. **Boundary conditions**

Figure 2 shows the model of the flowing part and the computational grid of the turboexpander stage, the grid is constructed of joined polyhedra, the boundary layer is considered by the grid.

![Figure 2](image)

Figure 2. Boundary conditions and the computational grid of the turboexpander stage.

A pressure-inlet condition was imposed on the inlets 1, the pressure $P_{in}$ and the inlet temperature $T_{in}$ were set. The pressure-outlet condition was imposed on the outlet 2, the pressure in the outlet line $P_{out}$ was set, and the temperature at the outlet of the diffuser $T_{out}$ was a calculated parameter. For each design point, the impeller speed was set.

In this paper, we considered the flow of a two-component mixture, helium and nitrogen, mass fraction of nitrogen was 5% at the entrance to the TEU. The design regimes were chosen so that the values of pressures and temperatures are in the range from 60.15 K to 126 K. These temperatures are triple point and critical point of nitrogen, respectively.

3. **Result and discussion**

During the calculation, the distribution of the volume fraction of the components of the mixture was obtained, which is illustrated in figure 3 for the component of the nitrogen mixture. It can be seen that
nitrogen is distributed fairly evenly in the flow, does not form large accumulation areas in the flow part, thus, no separation of the mixture is observed.

![Figure 3](image3.png)

**Figure 3.** Distribution of the volume fraction of nitrogen in the cross section of the TUE flow part.

In figure 4 the distribution of the supersaturation ratio in the cross section of the guide vane is shown. It can be seen that there are areas in which the supersaturation ratio reaches high values, substantially greater than 1. In view of this, we can assume that in these areas active condensation of the condensing component (nitrogen) is possible. Assuming that condensate droplets are actively forming in these areas, it is easy to see that they are likely to create areas of erosive wear on the edges of the impeller, flying into it at high speed. The results obtained are in qualitative agreement with the typical localization of erosion wear due to bombardment by condensate droplets. For example, in [8] the characteristic places are shown for impeller vanes destruction coinciding with the assumed trajectories of droplets formed due to phase transitions.

![Figure 4](image4.png)

**Figure 4.** Distribution of the supersaturation ratio in the cross section of the guide vane.

4. **Conclusions**
Using methods of computer fluid dynamics, study was made of the process of expanding of two-component mixture in a stage of a turboexpander unit in a three-dimensional unsteady setting. Methodology was developed for calculating the expansion of multicomponent mixtures in the flow part
of the turboexpander stage, the calculation package was modernized with additional equations, namely, considering the supersaturation ratio, as a first approximation for further studies of volume condensation in the flow part. It was shown that the components of the mixture are distributed fairly evenly, without explicit separation of impurities. Areas of high supersaturation ratio, which qualitatively coincide with the characteristic places of destruction of the impeller blades, along the trajectories of potentially formed droplets due to phase transitions, are revealed.

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