Simulation Methodology of the Screw-Centrifugal Pump for Liquid Hydrogen

A.V. Sulinov, L.S. Shabliy, V.M. Zubanov

Samara National Research University, 34, Moskovskoe shosse, Samara, 443086, Russia

E-mail: waskes91@gmail.com

Abstract. The article describes the basic modeling methods of hydrodynamic processes in screw centrifugal hydrogen pumps using software ANSYS CFD; the variable fluid density is taken into account. Three methods of modeling fluid flow with variable density were proposed in ANSYS CFD. Regression models of variable density were obtained. Regression models characteristics are of the second and fourth order, the pressure range is from 0.09 to 30 MPa and the temperature range is from 18 to 34 K. Regression models were implemented in the method by reference variable density of liquid hydrogen in the form of functional dependence.

1. Introduction
Currently, the major advances in the use of hydrogen technology in energy, transport and other industries were achieved in many developed countries. Hydrogen technologies are also important for rocket and space technology.

The hydrogen as a fuel of the Liquid Propellant Rocket Engine (LPRE) allows one to increase the energy potential of launch vehicles, thereby increasing payload outputted into orbit, also allows solving environmental issues, using environmentally friendly components of rocket fuels [1]. So, the theme of development of the advanced rocket engine using hydrogen as a working fluid has recently increased its relevance.

One of the main units that determines the characteristics and reliability of the LPRE, is a turbopump unit (TPU) [2]. The TPU consists of pumps pumping fuel components and of turbine(s) driving the pumps. A distinctive and important feature of the liquid hydrogen is the strong dependence of its properties not only on temperature, but also on pressure (Fig. 1) [3].

2. Geometric models
CFD-modeling allows one to accelerate research of the LPRE elements [4]. However, in the simulation of the workflow of liquid hydrogen pumps, the ordinary other turbomachinery (complex geometry) [5], unsteadiness of the processes, uncertainty of input data [6, 7]) and a complexity are added. The complexity is associated with the above-described features of the physical properties of hydrogen.

In accordance with the international experience turbomachinery CFD-modeling, and with the authors’ collective experience [2, 8], the processes are modeled as steady-state; the pump geometry is created in a simplified form of sector models of interblade channels. Properties of the working fluid are described additionally because the standard models for liquids with variable density in ANSYS
CFX do not exist.

Figure 1. The dependence of the liquid hydrogen density on the pressure and temperature.

Tasks with dependencies of the working fluid parameters defined by the user, as a rule, are much less stable in comparison with the tasks, where the working fluid has constant parameters. This is due to objective reasons (increasing physical and mathematical complexity of such tasks), and subjective reasons, because such problems increases the number of places where the engineer can make a mistake. To reduce the likelihood of errors when setting complex tasks, the complexity is recommended to increase gradually. Therefore, the solution of the task with variable density depending on pressure and temperature is expedient to perform at several stages.

In this work, the construction of the screw and impeller geometry (Fig. 2) was performed with BladeGen (ANSYS). Geometric modeling of transient passages and the volute was performed with Siemens NX (Fig. 2, c). Mesh models were built using specialized turbo-software ANSYS Turbogrid for blade rows and universal ANSYS Meshing for other elements. The whole model was assembled in ANSYS CFX-Pre.

Figure 2. The screw (a) and impeller (b) models in BladeGen and the scheme of the volute duct model (c) in Siemens NX.
3. CFD-model descriptions and results
First preliminary results were obtained with constant density. The methodology of simulation was based on techniques [8, 9, 10, 11]. There are main parameters of simulation:
- simulation settings are: the type is steady state, turbulence model is k-ε (with inlet turbulence intensity about 5%);
- rotor simulation settings are: rotation speed is 45,000 rpm, interfaces for screw and impeller are "Rotational Periodicity", types of interfaces are "screw-entry", "screw-impeller", "impeller-volute" and "Stage Average Velocity";
- boundary conditions are: total pressure at the pump inlet is 500 kPa, total temperature at the pump inlet is 20 K, mass flow at the pump outlet is 7.429 kg/s;
- properties of liquid hydrogen are: liquid hydrogen density is 76.81 kg/m3, the molar mass is 2.0159 kg/kmol; isobaric heat capacity is 9630 J/(kg · K), dynamic viscosity is 8.6567·10^{-6} Pa·s, thermal conductivity is 0.118 W/(m·K).

Parameters are distributed (pressure, temperature, velocity) through the flow pass (Fig. 3) and pump integral parameters were obtained. Some of calculation results are shown in Table 1, and a comparison of some project data is given.

### Table 1. The results of the simulation of the workflow in a pump with constant density

| Parameter                        | Project value | CFD-result |
|----------------------------------|---------------|------------|
| The pressure at the inlet of RK, MPa | 1.068         | 1.081      |
| The pressure at the outlet of RK, MPa | 6.458         | 7.493      |
| The pressure at the pump outlet, MPa | 9.761         | 10.96      |
| Outflow angle of the screw, deg.     | 5.209         | 11.41      |
| Outflow angle of the RK, deg.        | 1.486         | 5.611      |

As has been mentioned above that the described CFD-calculation was performed without taking into account the changing of density due to changes of pressure and temperature. Pressure between the pump inlet and the outlet varies from 0.1 to 15 MPa (Figure 3), and the temperature - from 20 to 25 K. The above-mentioned factors influence the density change in different directions, but its combined effect leads to density increasing by 15%, from 70 kg/m$^3$ at the input to 80 kg/m$^3$ at the output (Fig. 1).

4. Methods for density variation simulation
In this work, the options of accounting changes of liquid hydrogen density in the CFD-calculation were proposed. ANSYS CFX allows one to set any constant and variable parameters. Three variants of the variable density modeling were considered:
1. the built-in Peng-Robinson model for a state equation.
2. setting of the density variation in a tabular form.
3. setting of the density variation in an algebraic function form.

4.1. Setting the variable density via Peng-Robinson model
The ANSYS CFX library has a section with the components properties that are set by the equation «Materials-pengrob.ccl». It includes a group of "wet" components «Wet Peng Robinson», which contain hydrogen with the Peng-Robinson state equation. The model parameters are left by default, changes were only in the temperature limiter: «Lower Cp0(T) Temperature Limit» was changed from 100 K to 14 K, and «Upper Cp0(T) Temperature Limit» was changed from 1000 K to 100 K.

CFD-results in Table 2 show a significant difference of parameters obtained using the Peng-Robinson model from the results at constant density. However, the level difference was much larger than expected. The change of density in the range of 75...80 kg/m$^3$ according to experts should change the parameters by no more than 5-10%, with respect to the calculation with constant average density. Detailed analysis revealed that the density calculated with the Peng-Robinson model was at the level...
of 40...45 kg/m³ and remained virtually unchanged for the flow part despite the change in pressure and temperature.

Table 2. CFD-results of the pump workflow with density predetermined by the Peng-Robinson model

| Parameter                          | Constant density | Peng-Robinson model |
|------------------------------------|------------------|---------------------|
| The pressure at the inlet of RK, MPa | 1.081            | 0.5689              |
| The pressure at the outlet of RK, MPa | 7.493            | 4.113               |
| The pressure at the pump outlet, MPa | 10.96            | 6.882               |
| An outflow angle of the screw, deg. | 11.41            | 17.14               |
| An outflow angle of the RK, deg.    | 5.611            | 6.972               |

So, this study reveals the impossibility to apply the default model of Peng-Robinson taken from the ANSYS CFX library, for easy modeling of the flow of liquid hydrogen in the pump.

4.2. Setting the density variation in a tabular form

The most obvious way is to set a variable density as primary table data from reference [3]. There is a tool “User Function” in the ANSYS CFX for parameters dependence description in a tabular form.

Since the extrapolation of parameters is performed automatically, two methods have been proposed to prevent the parameters scattering out of the range given in the table. The first is the adding in the table of the fictitious values bounding the inner ones. The values provide the constancy of extreme values of the function even in the arguments (pressure and temperature) going out of the main range due to calculation fluctuations that can be non-physical (for example, the negative pressure value). Verification shows that this method is insolvent: pressure extrapolation beyond the physical range of 0,09-10 MPa, so the density may be very different from the limit value (Fig. 4). The cause of this phenomenon probably lies in the incorrect extrapolation algorithm of three-dimensional user-defined functions in ANSYS CFX.

The second method implies the explicit restriction of argument values and functions of the mathematical expression of the form:

$$\rho[\text{min-max}] = \min\{\rho_{\text{max}} ; \max \{\rho(p,T) ; \rho_{\text{min}}\}\},$$
where \( \rho(p,T) \) - a table function of density calculation, the values of which are outside the boundaries \([\rho_{\text{min}}; \rho_{\text{max}}]\). The values of \( p \) and \( T \) arguments may also be previously limited in a similar manner.

### 4.3. Setting the density variation in the algebraic function form

Parameters dependencies can be set as explicit two-parameteric function \( \rho = f(p,T) \) written on CFX Expression Language (CEL). However, the expression of tabular dependencies via the functional expression needs a regression model. The regression model was obtained in two variants: second-order and fourth-order.

The second-order model is slightly cheaper, but less accurate. To estimate complexity difference we can compare two half-models of density dependency on pressure:

\[
\begin{align*}
\rho_{\text{lo} \ T=34\text{K}} &= -0.0003p^4 + 0.0188p^3 - 0.5043p^2 + 6.4977p + 38.666, \\
\rho_{\text{2o} \ T=34\text{K}} &= -0.0752p^2 + 2.7633p + 49.156.
\end{align*}
\]

Figure 5 shows graphs of approximating the density change when the temperature is constant and the pressure varies from 0.09 to 15 MPa. The second difficulty is to approximate the two-parameter dependence. In this case, it is easy to see that the coefficients of all one-parameter dependencies change monotonically following the change of the second parameter - temperature; the character of these relationships is close to the line (Fig. 6).

![Figure 5](image1.png)

**Figure 5.** Graphs of approximating the density change when the temperature is at constant and pressure varies from 0.09 to 15 MPa.

![Figure 6](image2.png)

**Figure 6.** The dependence of the coefficients in the one-parameter equations of the temperature.

The fourth-order model is more complex but more accurate:

\[
\begin{align*}
\rho &= (-0.0000002T^2 + 0.0001T - 0.0014)p^3 + (0.0001T^2 - 0.0044T + 0.0495)p^3 + \\
&+ (-0.0024T^2+0.0954T-1.0112)p^2 + (0.0243T^2-0.933T+10.129)p - 0.0984T^2 + 2.9881T + 101.62.
\end{align*}
\]

These models describe the liquid hydrogen density variation in the pressure variation range from 0.01 to 30 MPa and the temperature variation range from 16 to 34 K.

### 5. Conclusion

The following main conclusions can be drawn from the study results of hydrodynamic processes modeling techniques in ANSYS CFX:

1. ANSYS CFX can be applied to the qualitative assessment of the results of design calculations by the working fluid modeling at constant average density.
2. Three methods of liquid hydrogen flows of modeling variable density ANSYS CFX are proposed.
3. Perceptivity of applying the setting variable density method of liquid hydrogen in the form of functional dependence for modeling the workflow of the screw centrifugal hydrogen pump in ANSYS CFX is justified.

4. Regression models of liquid hydrogen variable density of the second-order and fourth-order were received in the pressure range from 0.09 to 30 MPa and in the temperature range from 18 to 34 K.

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