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# EFFECT DETECTION OF USING A MODIFIED REDLICH-KWONG-AUNGIER EQUATION OF STATE ON THE CALCULATION OF CARBON DIOXIDE FLOW IN A CENTRIFUGAL COMPRESSOR

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*Supercritical $CO_2$ (S-$CO_2$) cycles have found applications in power generation and can achieve high efficiency in a wide range of temperatures and pressures. The Redlich-Kwong-Aungier real gas equation of state is used to describe the thermodynamic properties of the $CO_2$ working fluid. The main problem in its application lies in modeling the phase transition between different states and the region near the critical point of the working fluid.*

*The object of the study is the working process in a centrifugal compressor located in the compression loop with the $CO_2$ working fluid. The proposed mathematical model of the modified Redlich-Kwong-Aungier equation of state allows for a first-order phase transition from the liquid to the supercritical region even near the critical point. A scaling factor was added to the modified equation of state, significantly reducing the error in pressure determination in a wide range of temperatures compared to the original equation of state. The proposed mathematical model can be applied in the pure liquid region, limited to the temperature range from 220 K to 300 K.*

*The mathematical model was used to solve the 3D gasdynamic problem, specifically to determine the thermodynamic and kinematic properties of the flow in a centrifugal compressor in a wide range of operating modes. A comparison of the calculation results with experimental data from the Sandia National Laboratories (USA) report was conducted. A satisfactory agreement of the results at the design point of the compressor characteristic was obtained (less than 5 % discrepancy).*

*Due to the simplicity of the equation of state and the small number (seven) of empirical coefficients, the obtained mathematical model can be used for practical CFD tasks without significant computational time costs*

*Keywords: centrifugal compressor, $CO_2$ pure liquid region, modified Redlich-Kwong-Aungier equation of state, fluid pressure*

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## 1. Introduction

One of the main challenges facing the global community today is the need for energy conservation. With the development of modern market economies, there are requirements for the intelligent use of energy resources, reducing environmental impact, achieving economic viability, etc.

Modern power plants – nuclear, gas, and coal-fired ones – use the Rankine steam cycle to convert generated heat into electricity. In this process, steam systems lose approximately two-thirds of the energy they could potentially generate, as the steam is converted back into water to repeat the cycle.

Instead, in recent years, there have been proposals to utilize a simple recuperated closed Brayton cycle using supercritical carbon dioxide (S-$CO_2$) as the working fluid. It remains in the system and is not released as a greenhouse gas, while it can be heated up much more strongly than steam – up to 700 °C.

Supercritical S-$CO_2$ Brayton cycle and other supercritical cycles are potentially much more efficient in converting thermal energy from power plants into electricity. Unlike traditional Rankine steam cycles or gas (such as helium) superheated Brayton cycles, they have a theoretical conversion efficiency of up to 50 %.

These cycles have great potential to achieve high efficiency over a wide range of cycle outlet temperatures. The high density of the supercritical $CO_2$ working fluid in the system allows for the use of compact energy conversion equipment. In this way, it is possible to reduce significantly the size of the turbine and compressor, which leads to a significant decrease in capital expenditures on turbomachinery.

Carbon dioxide is currently considered one of the most promising gases due to its moderate critical pressure values, as well as its stability over a wide range of temperatures, prevalence, and low cost.

The equations of state for real gases are used to evaluate the thermodynamic properties of the working fluid. Three-parameter equations of state are most commonly used in computational fluid dynamics (CFD) modeling of spatial working fluids due to the simplicity of the equations and high computational speed.

Therefore, the development of a mathematical model of a modified equation of state that allows describing the working range of $CO_2$ in liquid and near-critical regions is a relevant scientific and technical problem.

## 2. Literature review and problem statement

The main advantages of using carbon dioxide as the working fluid in power plants include acceptable efficiency values at relatively low temperatures (up to 700 °C) and the compactness of turbomachinery associated with high pressures in the loop. In [1], conclusions were drawn regarding the potential use of $CO_2$ in nuclear installations, with particular attention given to thermodynamic cycles at supercritical pressures of the working fluid. Several drawbacks of the $CO_2$ supercritical cycle were identified in this work. Compared to ideal gas Brayton cycles, the $CO_2$ supercritical cycle benefits less from increasing the temperature at the turbine inlet and suffers more from increasing the temperature at the compressor inlet. Therefore, special attention should be paid to the design of the pre-cooler and radiator system. It is also worth noting the current absence of a simple and effective means for highly efficient part-load operation of the supercritical $CO_2$ recompression cycle. Since nuclear power plants are economically competitive only at base load conditions, this is not a disqualifying flaw.

In work [2], a series of tests were conducted showing that the centrifugal compressor can effectively compress liquid $CO_2$, even if it was designed to operate near the critical point of $CO_2$. S-$CO_2$ compression systems are ideally suited for liquid metal-cooled reactors (LMRs) and other reactors operating at temperatures in the range from 723 K to 1023 K. This work identifies a supercritical $CO_2$ power cycle that can provide efficiency advantages for LMRs. Gradually increasing the temperature at the outlet of the LMR to 350 °C and using supercritical $CO_2$ systems with reheat in condensing cycles seems more likely to provide short-term reactor power generation and efficiency advantages compared to alternative LMR energy efficiency options. Operating at temperatures above the critical point is very problematic for LMRs due to unfavorable density and heat transfer effects. They occur in the reactor due to the nature of supercritical steam and accelerated corrosion. To avoid some of these problems, concepts are proposed that limit the primary loop to 380 °C at 25 MPa and have a compression cycle efficiency of 37.5 %.

The study [3] provides an overview of recent advances in modified $CO_2$ transcritical refrigeration cycle technologies. A systematic and comprehensive description of new technologies improving basic $CO_2$ refrigeration cycles is presented, including their operating principles, technical characteristics, and performance. In the basic S-$CO_2$ cycle, the transcritical operating principle provides much higher operating pressures than conventional refrigerants, resulting in significantly higher costs and lower system reliability. The work described and solved this problem while simultaneously improved system efficiency by replacing gas evaporation and cooling with absorption and desorption from an absorbent liquid.

In many implementations of the $CO_2$ transcritical cycle, the conditions at the inlet of the compressor or pump are relatively close to the two-phase or liquid region. Fluid acceleration near the compressor inlet may lead to potential condensation or cavitation at the inlet. Despite possible mitigation effects or evidence in the literature, the possibility of operating in the liquid phase is a high-risk condition that cannot be recommended for the high- reliability system design [4]. For compressor operation in the supercritical mode, close to the critical point, there is a hypothesis of the working fluid transitioning to the subcritical mode. This may lead to compressor performance issues if condensation occurs in regions where the liquid falls below the saturation point [5].

Optimal efficiency of the power cycle can be achieved by operating close to the liquid-gas region, where $CO_2$ is a supercritical fluid (S-$CO_2$), as the compression ratio in the main compressor is reduced. However, the S-$CO_2$ cycle and other related $CO_2$ supercritical cycles face significant challenges in compression both mechanically and aerodynamically when dealing with high-density liquid exceeding 70 % of the water density, as demonstrated in [6].

In work [7], the operating characteristics and flow fields of the centrifugal compressor operating with supercritical $CO_2$ were investigated using a three-dimensional CFD software. The geometry considered is based on the main dimensions of the centrifugal compressor installed in the compression loop test stand of the Sandia National Laboratories. All numerical simulations are performed using a recently developed proprietary hybrid CFD solver for compressible fluids, which utilizes both the central processing unit (CPU) and the graphics processing unit (GPU). The thermodynamic properties of the working fluid are calculated using an effective and accurate tabulation technique, the spline-based table lookup (SBTL) method, which is optimized for the applied density-based solution procedure. Numerical results are compared with available experimental data, and the accuracy and computational acceleration potential of the mathematical model combined with SBTL are evaluated in the context of turbomachinery operating in a supercritical $CO_2$ environment. Various challenges arise during the calculation due to significant variation of available experimental data. Sometimes only critical temperature and pressure are known, sometimes pressure, temperature, and volume are provided for the working fluid, and sometimes a complete data set is available. In each case, the data should be fully utilized. It is considered that the relationships discussed in the sections of the study cover the entire range, and the proposed methods do not require an unreasonable amount of time.

In [8], using experimental and CFD data sets obtained from available literature sources, a multifactor regression analysis was conducted to establish correlations that account for the influence of several critical geometric parameters. These correlations demonstrate higher accuracy and universality compared to previous studies and predict thermohydraulic performance within approximately 90 % of existing experimental data and CFD data with an accuracy of ±15 %. The analysis presented in the study allows for conducting only steady-state CFD calculations, which is a significant limitation of the mathematical model.

In work [9], unsteady averaged Reynolds-Navier-Stokes equations are provided for the working process in a scroll compressor operating with transcritical $CO_2$. The influence of the $CO_2$ property tables resolution on numerical modeling is thoroughly investigated. Some phenomena, such as pre-compression and over-compression in the working process, are presented. Finally, the physical mechanisms of asymmetric outflow are identified, taking into account aerodynamics and thermodynamics. The research results indicated that the $CO_2$ property tables resolution has little impact on the simulation results, considering the rapid changes in $CO_2$ properties near the critical point. The research problem lies in the insignificant influence of the $CO_2$ property tables resolution on the simulation results, considering the rapid changes in $CO_2$ properties near the critical point.

The main objective of the work [10] is to present an accurate equation of state that has a simple form and a small number of specific coefficients. The new modification of the Peng-Robinson cubic equation of state (PR-Saali EoS) can reproduce the vapor pressure of various pure components, especially polar ones, and accurately combine pure and mixed components. However, there is a limitation to this modification that should be noted, namely, that the cubic equation of state cannot predict the density of heavy hydrocarbon liquids and hydrogen-bonded systems.

The study [11] presents a unique form of a two-parameter cubic equation of state that uses the critical compressibility factor to solve the problem of unreliable predictions of volumetric phase behavior using conventional two-parameter cubic equations of state. The research problem lies in the inability of accurate modeling of thermodynamic processes near the critical point of the working fluid.

The study [12] presents a mathematical model for determining the basic thermodynamic properties in the two-phase region of carbon dioxide. This mathematical model is based on the modified Redlich-Kwong-Aungier equation of state [13], which can predict the properties of the liquid phase in the two-phase region accurately enough. Equations from [14] were taken as a basis and modified for use in the pure liquid and transcritical regions of $CO_2$. The research problem is the impossibility of modeling the phase transition near the critical point and saturation line in three-dimensional flow during CFD calculations.

Literature review indicates that carbon dioxide is currently considered as one of the most promising gases in supercritical S-$CO_2$ Brayton cycles for power engineering application. To develop new and modernize existing compression loops operating with the S-$CO_2$ cycle, mathematical models are needed to accurately simulate the working process over a wide range of operating modes from the liquid to the supercritical region.

Most S-$CO_2$ cycles operate with maximum efficiency near the critical point of $CO_2$ in the region of pure liquid or in the two-phase region at the compressor inlet. Such boundary conditions necessitate modeling the phase transition between the $CO_2$ working range regions. Several challenges arise during three-dimensional CFD calculations: firstly, the inability to model the phase transition near the critical point and saturation line; secondly, the negligible influence on the simulation results of the $CO_2$ property tables resolution, considering the rapid changes in $CO_2$ properties near the critical point.

The Redlich-Kwong-Aungier real gas equation of state is used in existing mathematical models to describe the thermodynamic parameters of the $CO_2$ working fluid. The main problem when using it lies in modeling the phase transition between different states and the region near the critical point of the working fluid. While this equation provides high accuracy in calculations in the supercritical and gas regions, it is not suitable for modeling the $CO_2$ condensation cycle.

Therefore, it is appropriate to modify the Redlich-Kwong-Aungier equation of state to create a mathematical model based on it that describes the $CO_2$ working range in liquid and near-critical regions.

## 3. The aim and objectives of the study

The aim of the study is to develop and apply a mathematical model based on the Redlich-Kwong-Aungier equation of state that describes the entire working range of $CO_2$ from the liquid to the supercritical region with an acceptable calculation error. This will enable the implementation of the modified equation of state into the AxCFD® CFD software for calculating the parameters of the working fluid in the centrifugal compressor stage in the entire operating range.

To achieve the aim, the following objectives were set:

– analyze the possibility of using a centrifugal compressor in the compression loop for liquid conditions at the compressor inlet;

– modify the standard Redlich-Kwong-Aungier real gas equation of state to describe the entire working range of liquid $CO_2$;

– develop a 3D model of the centrifugal compressor stage in the AxSTREAM® software (USA) and calculate $CO_2$ flow parameters in a centrifugal compressor stage using this model;

– compare the calculation results with experimental data to verify the developed mathematical model.

## 4. Materials and methods of the study

The object of the study is the working process in an industrial centrifugal compressor located in the compression loop, which compresses $CO_2$ in a wide range of operating modes from the liquid to the supercritical region.

The subject of the study is the regularities characterizing the properties of carbon dioxide in the near-critical region and their influence on the compression process characteristics.

Theoretical foundations of the study are based on fundamental laws of thermodynamics and theory of turbomachinery. Flow analysis of the working fluid was conducted using a three-dimensional CFD software (USA) [15] with liquid properties at the inlet and supercritical properties at the outlet. Verification of the obtained calculation results was performed by comparison with publicly available experimental data [2]. The acceptable calculation error compared to the experiment typically should not exceed 5–10 % according to industrial and scientific standards.

The main hypothesis of the study suggests that the use of a scaling factor for pressure in the modified Redlich-Kwong-Aungier equation of state enables the calculation of the centrifugal compressor characteristics in a wide temperature range. This range spans from 220 K to 300 K, in which the working fluid undergoes a first-order phase transition from the liquid to the supercritical region. The mathematical model in the study is limited to this temperature range, which is based on the physical properties of the considered working fluid.

The study was conducted using the parameters of the centrifugal compressor from the experiment reported by Sandia National Laboratories (USA) [2]. The main geometric dimensions of the centrifugal compressor stage are provided in Table 1 [2].

Table 1

Main dimensions of the centrifugal compressor stage

| Geometric parameter | Value |
|---|---|
| Impeller geometry | |
| Number of full blades | 6 |
| Number of splitter blades | 6 |
| Impeller inlet radius at the hub | 2.537585 mm |
| Impeller inlet radius at the shroud | 9.372047 mm |
| Impeller outlet radius | 18.68170 mm |
| Blade angle of the impeller leading edge at the hub | 17.88 degrees |
| Blade angle of the impeller leading edge at the middle radius | 37.13 degrees |
| Blade angle of the impeller leading edge at the shroud | 50.00 degrees |
| Blade angle of the impeller trailing edge | –50.00 degrees (backward) |
| Angle between streamlines and the shaft at impeller inlet | 0 degrees |
| Angle between streamlines and the shaft at impeller outlet | 90 degrees |
| Full blade length | 25.0 mm |
| Splitter blade length | 12.5 mm |
| Axial length of the impeller | 15.9 mm |
| Blade thickness at the impeller leading edge | 0.762 mm |
| Blade thickness at the impeller trailing edge | 0.762 mm |
| Blade height at the impeller leading edge | 1.7 mm |
| Clearance gap at the impeller tip | 0.254 mm |
| Vaned diffuser geometry | |
| Number of vanes | 17 |
| Diffuser inlet radius | 18.5 mm |
| Diffuser outlet radius | 26.0 mm |
| Blade angle at the diffuser inlet | 71.50 degrees |
| Blade angle at the diffuser outlet | 42.44 degrees |
| Blade height at the diffuser inlet | 1.8 mm |
| Blade height at the diffuser outlet | 1.8 mm |
| Diffuser blade-to-blade channel length | 10.6 mm |
| Blade thickness at the diffuser inlet | 0.0 mm |
| Blade thickness at the diffuser outlet | 3.35 mm |

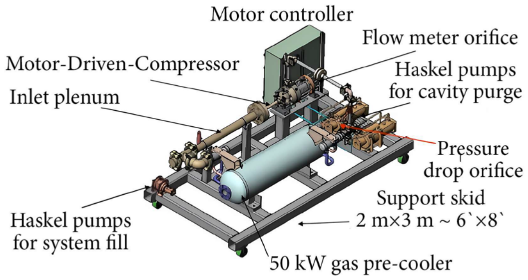
Fig. 1 depicts the schematic (*a*) and a photo (*b*) of the compression loop test stand with supercritical $CO_2$ (S-$CO_2$) working fluid, undergoing a phase transition from liquid to supercritical region [16]. One of the main components of this stand is the centrifugal compressor. Its maximum rotational speed is 65,000 rpm, the mass flow rate of the working fluid is 4.1 kg/s, and the pressure ratio is 1.65, with $CO_2$ density at the compressor inlet approximately 70 % of water density. The compression loop turbo-compressor in the experiment [2] operated on both the liquid and vapor sides of the saturation curve, very close to the critical point, above the critical point, and even on the saturation curve. The compressor operating modes varied from near-choking to rotating stall.

For the numerical experiment, software products developed by SoftInWay Inc. (USA) [15] were used in the study. Specifically, the AxSTREAM® software was utilized for creating a 3D model of the computational domain and conducting one-dimensional calculation of the working fluid parameters in the centrifugal compressor stage and its characteristics. This best-in-class software provides an integrated and rational approach to turbomachinery design, analysis, and optimization. Encompassing the entire design process of radial, axial, and mixed turbomachinery, it includes gas and steam turbines, compressors, blowers, pumps, fans, rotors, bearings, secondary flows, and cooling systems.

The AxCFD® software was used to calculate the spatial flow in the centrifugal compressor stage. It enables the numerical computation of fluid flow in turbomachinery blade-to-blade channels for individual blade rows, stages, or the entire turbomachine, including elements such as ducts, etc.

Thanks to the integrated architecture such parameters as geometry, boundary conditions, radial clearance values, number of blades, rotational speed, etc. are automatically transferred from the AxSTREAM® software to AxCFD®. There is the capability to edit these parameters as desired to explore different effects. Periodicity conditions, as well as flow inlet and outlet surfaces are automatically generated based on the geometry from AxSTREAM®.

In the AxCFD® software, various types of mesh generation are available, which can be refined in each direction, in the boundary layer, and in rotating zone blocks.



*a*

*b*

Fig. 1. Compression loop test stand with supercritical $CO_2$ working fluid [16]: *a* — schematic; *b* — photo

Different boundary conditions can be assigned depending on whether the user wants to calculate pressure values (at inlet or outlet) or the mass flow rate of the turbomachinery. Viscosity and various turbulence models (k-ε, k-ω, k-ε RNG, k-ω SST) can be used for new calculations or for updating existing ones. Heat exchange between the blades and the fluid can be accounted for along with surface roughness of the material. Each calculation can be performed for a specified width (radial cross-section), for an axisymmetric cross-section, or for the entire 3D geometry of the turbomachinery.

The parameters of the working fluid and the centrifugal compressor, which are specified as boundary conditions for flow calculations, are taken from the Sandia National Laboratories report [2]:

– total enthalpy at the inlet – 295.29 kJ/kg;

– total pressure at the inlet – 7.32 MPa;

– static pressure at the outlet – 9 MPa;

– mass flow rate – 1.5 kg/s;

– rotational speed – 40,000 rpm.

The $CO_2$ working fluid is described by the properties required for the selected equation of state, including:

– parameters at the critical point: pressure, temperature, and density (7.377 MPa; 304.13 K; 467.6 kg/m$^3$);

– acentric factor (0.224);

– molar mass (44.01 kg/kmol);

– polynomial coefficients $A_1$–$A_5$ (functions of $Cp_0(T)$) [18];

– parameters at the reference point: temperature, pressure, internal energy and entropy (last two parameters taken at 500K and 1 MPa from mini-RefPROP [17]);

– the scaling factor for the liquid region of $CO_2$ from the modified Redlich-Kwong-Aungier model [14].

To verify the calculation results of $CO_2$ parameters, data from the mini-REFPROP software were used. This program is a free short version of the full version of the NIST REFPROP software, developed by the National Institute of Standards and Technology (NIST) (USA), which computes the thermodynamic properties of pure substances only [17]. The mini-REFPROP calculations use the most accurate models, close to experimental data. For calculating $CO_2$ parameters in the mini-REFPROP program, the Span-Wagner model is used, which accurately describes the $CO_2$ entire range.

The study was conducted in the following sequence:

– the possibility of using a centrifugal compressor in the compression loop for liquid conditions at the inlet to the compressor was analyzed;

– a modification of the standard Redlich-Kwong-Aungier real gas equation of state was made by introducing a scaling factor for pressure to describe the entire working range of liquid $CO_2$;

– a 3D model of the centrifugal compressor stage was created, based on which the $CO_2$ flow parameters in the centrifugal compressor stage were calculated in the AxSTREAM® and AxCFD® software (USA) [15];

– a comparison of the computational results with experimental data from the Sandia National Laboratories report [2] was made.

## 5. Results of the study of the centrifugal compressor working process using the modified Redlich-Kwong-Aungier equation of state

### 5. 1. Analysis of the possibility of using a centrifugal compressor in the compression loop for liquid conditions at the compressor inlet

In the experiment [2], the Sandia compression loop was used, demonstrating that the centrifugal compressor can effectively "pump" liquid $CO_2$, even if its impeller was designed to operate near the critical point rather than on the liquid side of the saturation curve.

The "Temperature-Entropy" diagram corresponding to this experiment is presented in Fig. 2 [2], where the compressor inlet is indicated by point 1, the compressor outlet by point 2, and the state points after expansion by point 3. These state points are marked in green.

The experiment started the cycle with a high-density liquid at the compressor inlet (1), then $CO_2$ was compressed along a line of nearly constant entropy (1→2). Subsequently, the liquid $CO_2$ was forced through a flow restriction, causing an almost isenthalpic pressure drop onto the saturation curve (2→3) before being cooled in the cooler back to subcritical liquid (3→1).

As shown in Fig. 2, the compression and pressure drop segments in the proposed scheme are almost vertical, providing only a little or no margin for transitioning into the two-phase region at point 3.

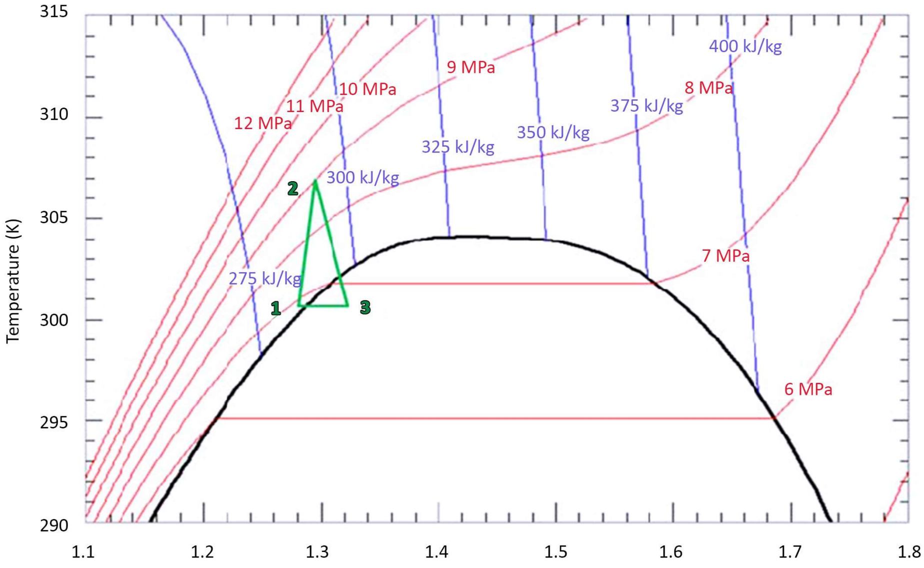


Fig. 2. The "Temperature-Entropy" diagram for the compressor operating on liquid $CO_2$ [2]

During this experiment pressure and temperature of the working fluid were maintained nearly constant, although a slight increase in both parameters was observed. In later experiments, a PID controller was employed to keep $CO_2$ liquid state points unchanged. The liquid $CO_2$ at the compressor inlet had temperature of 85 °F (303 K) and pressure of 1,020 psia (7.32 MPa), with mass flow rate of 3.4 lb/s (1.5 kg/s). The compressor outlet pressure was 1,300 psia (9 MPa), resulting in a pressure ratio of 1.27 (Fig. 3) [2].

If the working fluid from the experiment is described using the Redlich-Kwong-Aungier equation of state model, it will be insufficiently accurate for the liquid, two-phase, and near-critical regions of the centrifugal compressor operation. This model accurately describes the properties of the fluid in the supercritical and gas regions.

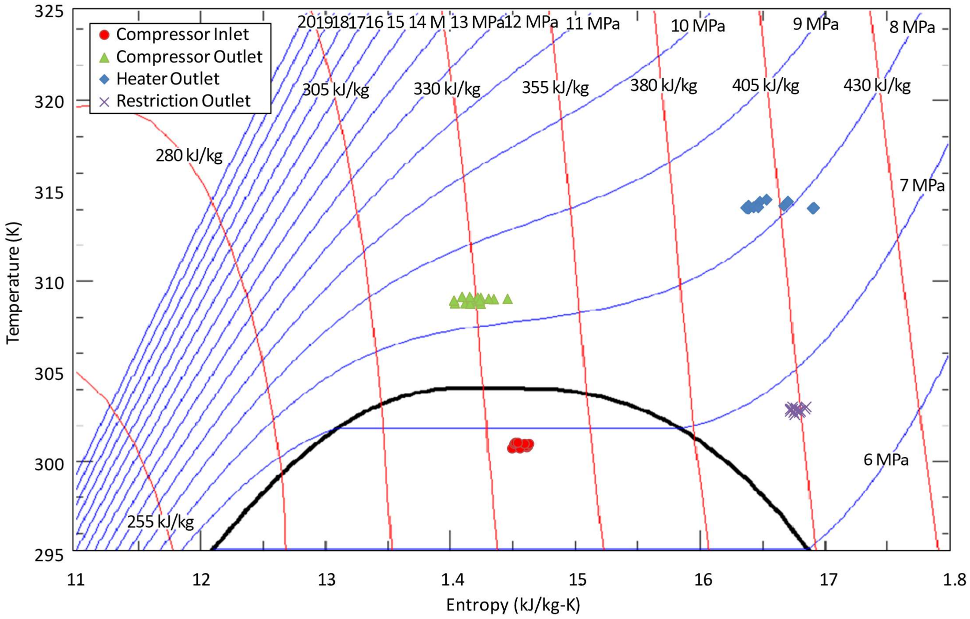


Fig. 3. "Temperature-Entropy" diagram of S-$CO_2$ compression loop with liquid $CO_2$ (303 K) at the compressor inlet

### 5. 2. Modification of the standard real gas equation of state to describe the entire working range of liquid $CO_2$

Equations of state for real gases are used to describe the thermodynamic properties of the working fluid. The main problem when using these equations is modeling the phase transition between different states and the critical point region of the working fluid.

For modeling the $CO_2$ condensation cycle, the Redlich-Kwong-Aungier equation of state was selected, which provides high accuracy in calculations in the supercritical and gaseous regions. The theoretical approach to its modification is described in [13]. In the critical point region, where phase transition occurs, significant fluctuations in thermodynamic parameters such as pressure, temperature, and density are observed. This leads to difficulties in achieving convergence in 3D AxCFD® calculations and reliability of the obtained results, up to the complete impossibility of obtaining a convergent calculation.

The fluid pressure can be found using the Redlich-Kwong-Aungier equation of state. The original form of this two-parameter equation of state is as follows [14]:

$$P=\frac{R\cdot T}{V-b+c}-\frac{A(T)}{V\cdot(V+b)}, \tag{1}$$

where

$$A(T)=a\cdot\left(\frac{T_{cr}}{T}\right)^{n},\quad b=0.08664\cdot R\cdot T_{cr}/P_{cr},$$

$$c=\frac{R\cdot T_{cr}}{P_{cr}+\dfrac{a}{V_{cr}\cdot(V_{cr}+b)}}+b-V_{cr}.$$

Here, $R$ is the gas constant for the specific working fluid; $T$ and $P$ are the current temperature and pressure values; $T_{cr}$, $P_{cr}$, $V_{cr}$ are the critical temperature, critical pressure and critical volume of the working fluid correspondingly.

Constants $a$ and $b$ are related to the gas critical pressure and critical temperature. Constant $c$ is a correction to eliminate a known deficiency of the Redlich-Kwong model at the critical point, where it predicts a compressibility factor of 1/3. The optimal value for the parameter $n$ is correlated by Aungier:

$$n=0.4986+$$
$$+1.1735\cdot\omega+$$
$$+0.4754\cdot\omega^{2}. \tag{2}$$

To reduce the difference between the isotherms, the Redlich-Kwong-Aungier equation of state was modified using a scaling factor $n\_liquid$. The scaling factor is incorporated into the coefficient $A(T)$ and allows for decreasing the difference between the Redlich-Kwong-Aungier equation of state isotherm and the reference data isotherm. The modified coefficient $A(T)_{liquid}$ can be calculated as follows:

$$A(T)_{liquid}=a\cdot\left(\frac{T_{cr}}{T}\right)^{\left(n\_liquid/n\right)}. \tag{3}$$

The values of the scaling factor $n\_liquid$ are determined over a wide temperature range in the pure liquid region, from the minimum temperature of carbon dioxide, 216.59 K, to the vicinity of the critical temperature, 300 K, with a step of 20 K. The distribution of the scaling factor $n\_liquid$ is presented in Fig. 4.

The dependence of the modified parameter $A(T)_{liquid}$ on temperature maintains a similar trend as the similar dependence of the original parameter $A(T)$ does (Fig. 5).

The optimal value of the scaling factor $n\_liquid$ can be determined for any temperature from 216.59 K to 300 K using an empirical function:

$$n\_liquid=a_0+a_1\cdot T+a_2\cdot T^{2}+$$
$$+a_3\cdot T^{3}+a_4\cdot T^{4}+a_5\cdot T^{5}+a_6\cdot T^{6}, \tag{4}$$

where:

$a_0$=–3.80666E+03; $a_1$=6.59754E+01;

$a_2$=–3.92603E–01; $a_3$=6.11597E–04;

$a_4$=2.74395E–06; $a_5$=–1.18587E–08; $a_6$=1.26942E–11.

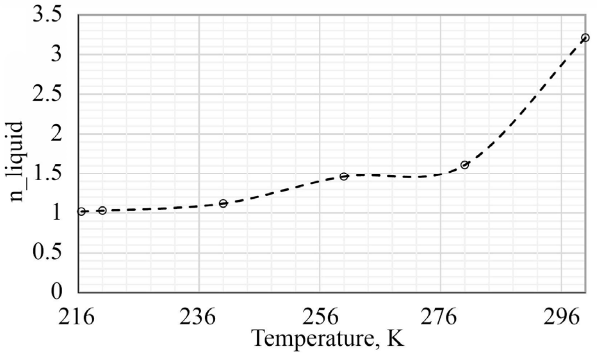


Fig. 4. Distribution of the scaling factor *n_liquid*

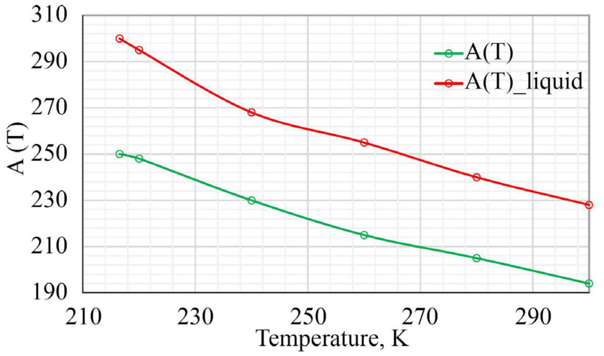


Fig. 5. Dependence of the modified parameter $A(T)_{liquid}$ and the original parameter $A(T)$ on temperature

### 5. 3. Creating a 3D model and conducting flow parameter calculations in the centrifugal compressor stage using AxSTREAM® and AxCFD® software

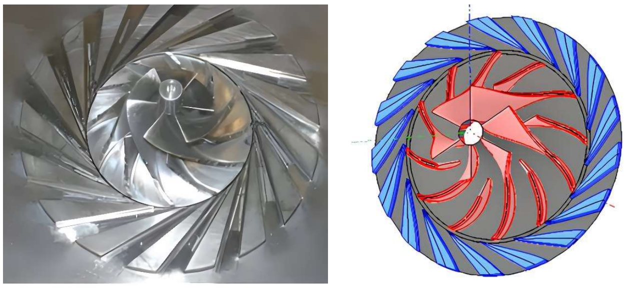
Based on the main geometric dimensions provided in Table 1 [2], a 3D model of the centrifugal compressor stage was created in the AxSTREAM® software [15]. It consists of an impeller with splitter blades and a wedge-shaped vaned diffuser.

Fig. 6 shows three-dimensional models of the centrifugal compressor stage taken from the experiment [2] (*a*) and developed in AxSTREAM® (*b*). From the figure, it can be seen that the 3D model accurately reproduces the geometry of the centrifugal compressor stage used in the experiment [2].

Next, the 3D model of the compressor stage was imported into 3D AxCFD® [15] for further numerical analysis of the flow in the region of liquid $CO_2$ at the inlet to the compressor and in the supercritical region at the compressor outlet.

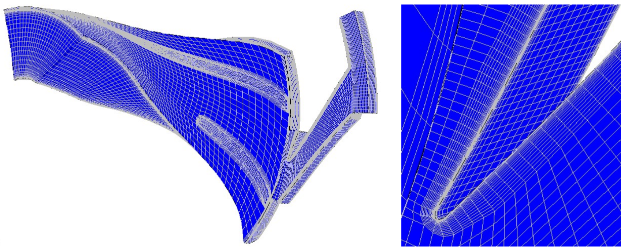
Fig. 7, *a* presents a structured hexagonal mesh for the entire computational domain. In the boundary layer zone near the domain walls, mesh cells should be densified, as shown in the example of the leading edge of the impeller blade in Fig. 7, *b*.

The k-ε model was selected as the turbulence model, with a turbulence intensity of 1 %. The parameter Y+ for this model should not be less than 120 on the walls of the computational domain, and its distribution in the computational domain is presented in Fig. 8.



*a* *b*

Fig. 6. Centrifugal compressor stage: *a* – experiment; *b* – 3D model developed in AxSTREAM®



*a* *b*

Fig. 7. Computational structured mesh: *a* – entire computational domain; *b* – boundary layer near the leading edge of the impeller blade

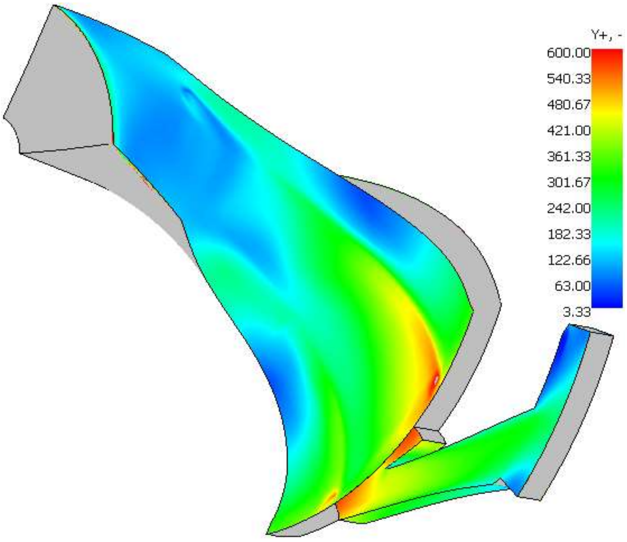


Fig. 8. Distribution of the Y+ parameter in the rotor and stator domains

As seen in Fig. 8, the distribution of the Y+ parameter corresponds to the specified condition, ensuring proper modeling of the boundary layer and consideration of fluid viscosity in the calculations.

### 5. 4. Results of the working fluid calculation in the centrifugal compressor stage with the modified equation of state and their verification

The results of the flow calculation in the AxCFD® software can be presented as visualizations of pressure, temperature, velocity, Mach number isolines, etc. at any location in the computational domain. The export of numerical results allows for comparing the calculated parameters of the working fluid with experimental data.

The distribution of the main flow parameters in the centrifugal compressor stage is shown in Fig. 9–14.

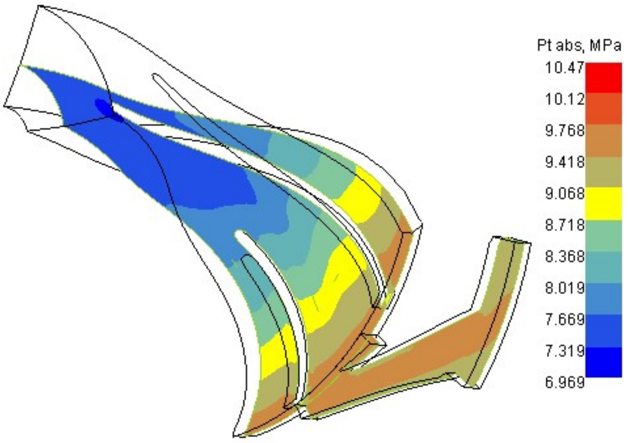


Fig. 9. Total pressure distribution (50 % from the hub)

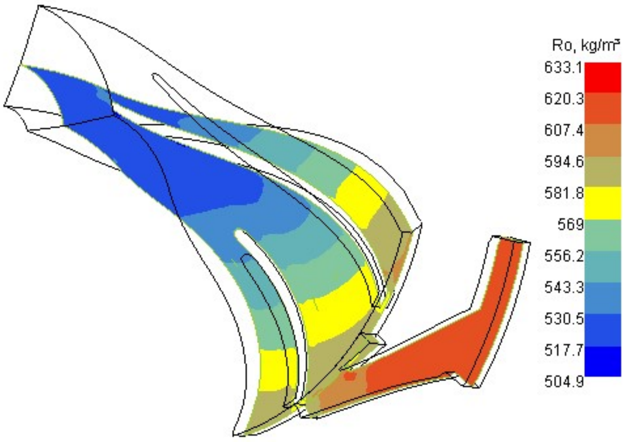


Fig. 10. Density distribution (50 % from the hub)

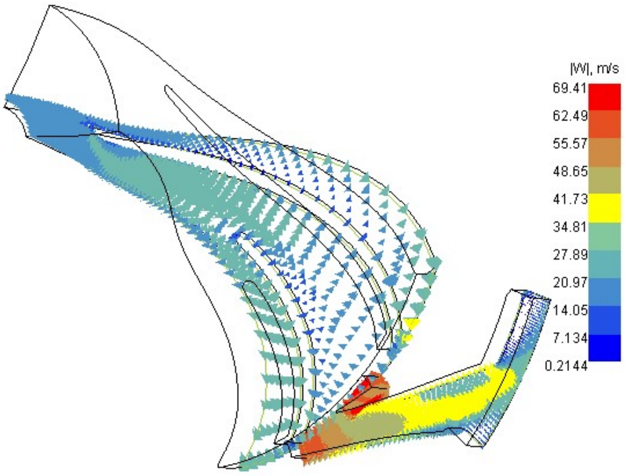


Fig. 11. Relative velocity vectors distribution (10 % from the hub)

In the AxSTREAM® software [15], a numerical investigation of the one-dimensional flow of the working fluid was conducted to determine its parameters and calculate the compressor characteristic, as shown in Fig. 15 with the broken line. Additionally, Fig. 15 includes a comparison of the centrifugal compressor stage characteristic with the design point calculated in 3D AxCFD® software and the design point taken from the experiment.

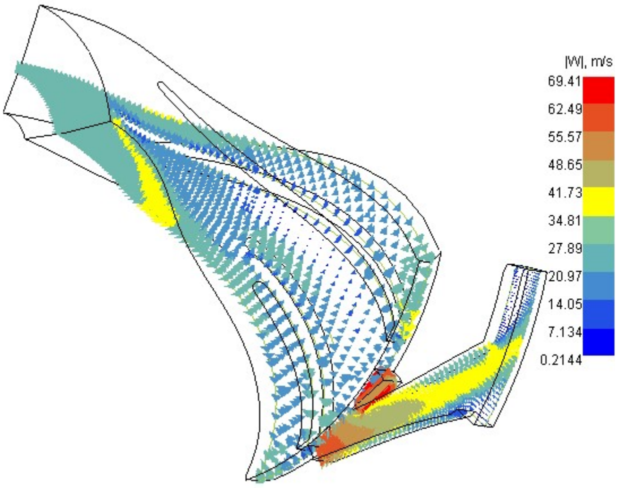


Fig. 12. Relative velocity vectors distribution (50 % from the hub)

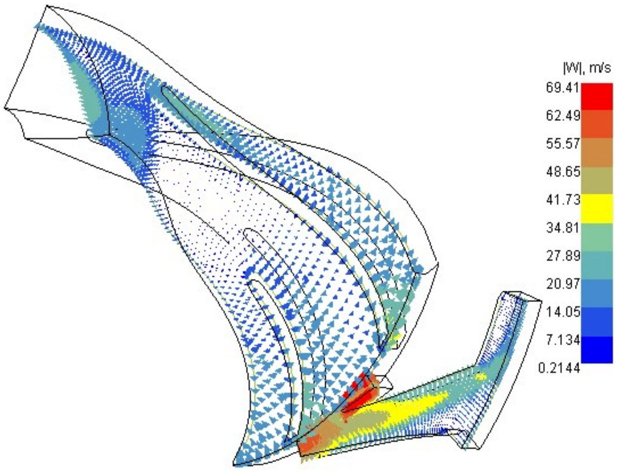


Fig. 13. Relative velocity vectors distribution (80 % from the hub)

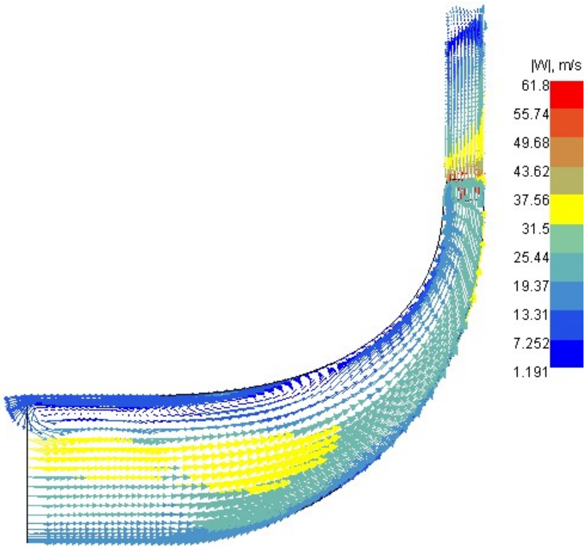


Fig. 14. Relative velocity vectors distribution on meridional view

The characteristic of the centrifugal compressor stage is presented as a dependence of the total pressure ratio on the mass flow rate. The experimental point is taken from the work [2].

The numerical results of the calculation in comparison with the experimental data are shown in Table 2.

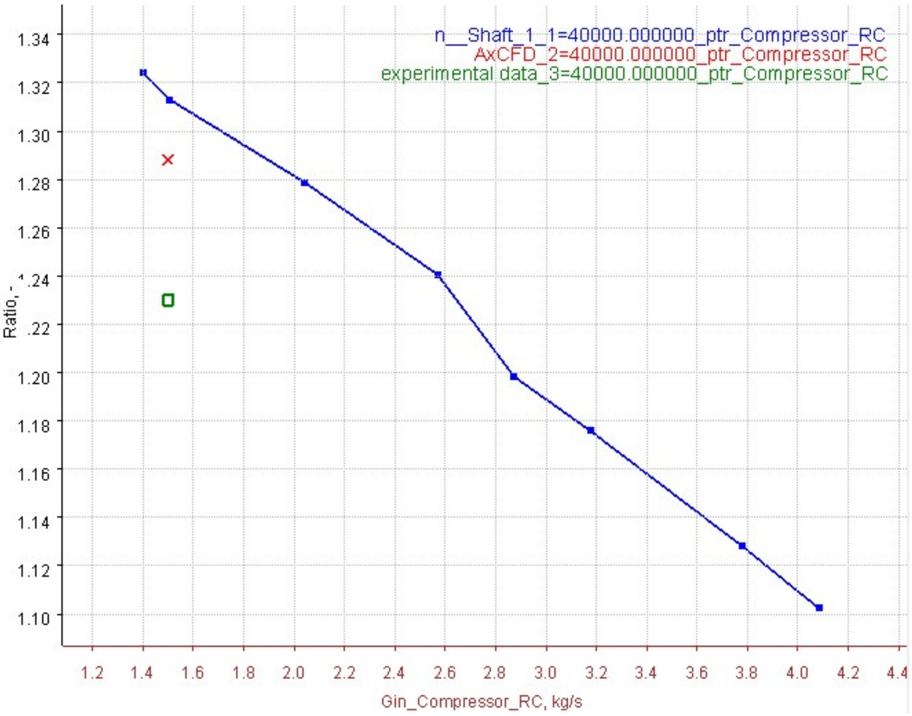


Fig. 15. Centrifugal compressor stage characteristic

Table 2

Comparative analysis of 3D CFD calculation results and experimental data

| Parameters | Units | 3D AxCFD | Experimental data | 1D AxSTREAM | Critical properties of $CO_2$ |
|---|---|---|---|---|---|
| Compressor inlet | | | | | |
| *Pt* | MPa | 7.32 | 7.32 | 7.32 | 7.377 |
| *It* | kJ/kg | 295.29 | 295.29 | 295.29 | – |
| *Tt* | K | 288.14 | 303 | 302.99 | 304.13 |
| Phase | – | liquid | liquid | liquid | – |
| Compressor outlet | | | | | |
| *Pt* | MPa | 9.43 | 9 | 9.61 | 7.377 |
| *It* | kJ/kg | 299.28 | 303.4 | 299.76 | – |
| *Tt* | K | 309.9 | 308.15 | 306.48 | 304.13 |
| Phase | – | supercritical gas | supercritical gas | supercritical gas | – |
| Compressor parameters | | | | | |
| Mass flow rate | kg/s | 1.5 | 1.5 | 1.5 | – |
| *ptr* | – | 1.288 | 1.23 | 1.313 | – |
| Error *ptr* | % | 4.778 | – | 6.748 | – |

Here *Pt*, *It*, *Tt* – total pressure, total enthalpy and total temperature of the working fluid, respectively, *ptr* – total pressure ratio of the working fluid in the centrifugal compressor stage.

## 6. Discussion of the calculation results of the working fluid in the centrifugal compressor stage with the modified equation of state

Based on the conducted analysis, it is shown that the centrifugal compressor, located in the compression loop, can be effectively used for working with liquid carbon dioxide. The "Temperature-Entropy" diagrams of the S-$CO_2$ compression cycle with liquid $CO_2$ (303 K) at the compressor inlet are presented in Fig. 2 and Fig. 3. They demonstrate that the working fluid $CO_2$ can exist in different phases in the cycle depending on temperature and pressure.

The considered working fluid can be calculated using the mathematical model of the Redlich-Kwong-Aungier equation of state (1). This model accurately describes the properties of the working fluid in the supercritical and gaseous regions but is not precise enough for the liquid, two-phase, and near-critical regions.

In this study, a mathematical model of the modified Redlich-Kwong-Aungier equation of state was developed, allowing for the description of the $CO_2$ working range in the liquid and near-critical regions. To reduce the difference between the isotherms, the scaling factor *n_liquid* (3) is introduced into the coefficient $A(T)$ of equation (1). Its value can be determined for temperatures from 216.59 K to 300 K using the empirical function (4). Comparison of the dependencies of the original coefficient $A(T)$ and the modified coefficient $A(T)_{liquid}$ on temperature shows a similar trend in Fig. 5.

The presented modified Redlich-Kwong-Aungier equation of state provides better accuracy in predicting the pressure of the liquid phase compared to the original forms of the cubic equation of state. On the other hand, the modified equation has a simpler form and fewer parameters for fitting compared to scaling equations of state.

The mathematical model was validated over a wide temperature range from 220 K to 300 K in the pure liquid region for carbon dioxide. The calculation results were compared with the Span-Wagner model from the mini-REFPROP software [17], which accurately describes the entire $CO_2$ operating range. While the Span-Wagner model is successfully used in one-dimensional modeling, it has limitations for practical application in 3D computational fluid dynamics – it requires a significant amount of time for calculation and determination of thermodynamic dependencies. Comparative analysis showed satisfactory agreement between the calculation results and the Span-Wagner model. The relative calculation error ranged from 3 to 25 % and showed a significant tendency to decrease from the saturation line to the high-pressure region compared to using the original form of the Redlich-Kwong-Aungier equation of state.

The modified Redlich-Kwong-Aungier equation of state demonstrates satisfactory agreement with experimental data over a wide range of temperatures in the supercritical and gas regions (relative calculation error ranging from 3 to 25 %). For gas, this range extends from 220 K to 300 K (the minimum temperature of the $CO_2$ operating range being 216.59 K, and the critical temperature being 304.13 K). For the supercritical region, the temperature range is from 305 K to 405 K.

In the modified Redlich-Kwong-Aungier equation of state, there is a coefficient $A(T)_{liquid}$, to which equation (3) a scaling factor *n_liquid* is added. The dependence of *n_liquid* on temperature is shown in Fig. 4. It is defined over a wide temperature range in the region of pure liquid, from the minimum temperature of carbon dioxide 216.59 K to close to the critical temperature of 300 K.

The inclusion of this scaling factor in equation (1) significantly reduces the error in pressure determination over a wide temperature range compared to the unmodified equation of state. In regions of high density, the pressure determination error increases, leading to inaccuracies in the calculation of other thermodynamic parameters such as enthalpy, entropy, specific heat capacity, etc.

The scaling factor can be selected not only for the liquid region but also for near-critical regions to obtain accurate results near the critical point.

The modified equation of state preserves the original form of the Redlich-Kwong-Aungier model, and its modified form can be used without excessive computational time.

A three-dimensional model of the compressor stage from the Sandia National Laboratories report [2] was developed in AxSTREAM®, and the result of comparison with the physical object is presented in Fig. 6. Subsequently, the model was imported into 3D AxCFD® for further analysis of the working fluid in the liquid $CO_2$ region at the compressor inlet and in the supercritical region at the compressor outlet. The working fluid is $CO_2$ with properties taken from mini-REFPROP [17]. For further calculations in 3D AxCFD®, a working fluid described by the mathematical model of the modified Redlich-Kwong-Aungier equation of state was created.

An automated structured hexagonal mesh, specific to turbomachinery, was used to partition the computational domain. Hexahedra are used to create the structured mesh in the main region of the computational domain (Fig. 7, *a*), while prisms are used to create the boundary layer near the domain walls (Fig. 7, *b*).

The turbulence model is the k-ε model. For preliminary calculations, this turbulence model is sufficient since it does not require a detailed description of the boundary layer, which is replaced by algebraic dependencies. For proper boundary layer modeling, the parameter Y+ for this turbulence model should not be less than 120 on the walls of the computational domain, as shown in Fig. 8.

The main boundary conditions for the calculation are temperature and density, allowing the use of a density-based mathematical model for CFD solvers. Additional boundary conditions include the properties of the working fluid and certain empirical coefficients, which can be obtained from reference literature.

After conducting the numerical experiment, the calculation results are obtained in the form of visualization of isolines of the main flow parameters at any location within the computational domain (Fig. 9–14) and in the form of the characteristic of the centrifugal compressor stage (Fig. 15).

The distributions of total pressure (Fig. 9) and density (Fig. 10) of the working fluid at the mid-span height of blade-to-blade channels of the centrifugal compressor stage reflect the physical distribution of these parameters within the compressor. Total pressure increases in the impeller due to the mechanical energy supplied to the flow and decreases in the vaned diffuser due to losses. The density of the flow increases from the inlet to the outlet of the stage due to compression in both blade rows.

The impeller clearance gap significantly influences the flow structure at the blade relative height from 50 % to 90 %, as shown in Fig. 14. The clearance gap value is 0.254 mm at an overall blade height of 6.83 mm at the inlet and 1.7 mm at the outlet. The flow passing through the clearance gap forms a vortex, which dissipates only at 50 % of the blade relative height. It is also noteworthy that there are no flow separations from the rotor and stator blades (Fig. 11–13).

A comparison was made between the characteristic of the centrifugal compressor stage calculated with 1D AxSTREAM® and the design points calculated with 3D AxCFD® and obtained from the experiment.

As can be seen in Fig. 15, the design point calculated in 3D AxCFD® aligns well with the experimental design point (with less than 5 % discrepancy).

The results of the working fluid flow calculation were obtained over a wide temperature range (from 220 K to 300 K) in the centrifugal compressor stage. Additionally, there is satisfactory agreement between numerical and experimental data (relative error ranging from 3 % to 25 %). Therefore, the modified Redlich-Kwong-Aungier equation of state is suitable for calculating the flow of the working fluid not only in supercritical and gas regions but also in liquid, two-phase, and near-critical regions.

A significant advantage of using this mathematical model in three-dimensional CFD problems is the ability to obtain a steady physical solution with acceptable error under boundary conditions that are close to the saturation line or in close proximity to the critical point. The use of the original equation of state in most cases prevents obtaining a steady physical solution and further analysis of results under similar boundary conditions.

The mathematical model in the study is limited by the temperature range chosen according to the physical properties of the considered working fluid (from 220 K to 300 K). The melting point, sublimation temperature (triple point), and critical temperature (critical point) constrain the working range of the mathematical model.

The limitation of the study lies in the fact that the mathematical model of the modified equation of state can only be used for $CO_2$. For other working fluids, the mathematical model will produce incorrect results.

The development of the study has several directions:

1. The mathematical model can be improved for phase transitions across the saturation line to further reduce the error of the calculation results in comparison with experimental data.

2. The developed mathematical model can be extended so that the scaling factor *n_liquid* for any other pure liquid is selected automatically.

3. The developed mathematical model can be expanded for calculating gas mixtures.

## 7. Conclusions

1. On the basis of the research from the Sandia National Laboratories report, the potential of using a centrifugal compressor in a compression loop for liquid conditions at the compressor inlet were analyzed. It is demonstrated that an industrial centrifugal compressor can effectively operate with $CO_2$ as the working fluid on the liquid and vapor sides of the saturation curve, very close to and above the critical point, and even on the saturation curve itself. The $CO_2$ working fluid can exist in different phases depending on temperature and pressure. Additionally, the working fluid can undergo phase transition inside the compressor.

2. The Redlich-Kwong-Aungier equation of state was modified to describe the entire working range of liquid $CO_2$. An additional parameter, the scaling factor for pressure, was introduced into the original Redlich-Kwong-Aungier equation of state. The equation for this parameter is presented in a convenient form, describing the entire temperature range of the liquid from 220 K to 300 K for isotherms from minimum to maximum liquid volumes corresponding to each temperature.

3. A 3D model of the centrifugal compressor stage was created in the AxSTREAM® software (USA) based on geometric parameters from the Sandia National Laboratories report. Using this model, calculations of one-dimensional and three-dimensional flows of $CO_2$ in the centrifugal compressor stage were conducted employing the developed mathematical model of the modified Redlich-Kwong-Aungier real gas equation of state. The modified equation of state for calculating the working fluid in the centrifugal compressor stage was implemented into the AxCFD® software (USA) for three-dimensional CFD simulations.

4. The obtained results of the $CO_2$ flow parameters calculations in the centrifugal compressor stage were compared with experimental data to verify the developed mathematical model. The discrepancy between numerical and experimental results does not exceed 5 % at the design point of the centrifugal compressor stage characteristic.

## Conflict of interest

The authors declare no conflict of interest regarding this study, including financial, personal, authorship, or any other interests that could influence the study and its outcomes presented in this article.

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## Data availability

The manuscript has no associated data.

## Use of artificial intelligence tools

The authors confirm that they did not use artificial intelligence technologies in creating the presented article.

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