The degree of dryness is the most important parameter that determines the state of a real gas and the thermodynamic properties of the working fluid in a two-phase region. This article presents a modified Redlich-Kwong-Aungier equation of state to determine the degree of dryness in the two-phase region of a real gas. Selected as the working fluid under study was CO$_2$. The results were validated using the Span-Wanger equation presented in the MINI-REFPROP program, the equation being closest to the experimental data in the CO$_2$ two-phase region. For the proposed method, the initial data are temperature and density, critical properties of the working fluid, its eccentricity coefficient, and molar mass. In the process of its solution, determined are the pressure, which for a two-phase region becomes the pressure of saturated vapor, the volumes of the gas and liquid phases of a two-phase region, the densities of the gas and liquid phases, and the degree of dryness. The saturated vapor pressure was found using the Lee-Kesler and Pitzer method, the results being in good agreement with the experimental data. The volume of the gas phase of a two-phase region is determined by the modified Redlich-Kwong-Aungier equation of state. The paper proposes a correlation equation for the scale correction used in the Redlich-Kwong-Aungier equation of state for the gas phase of a two-phase region. The volume of the liquid phase was found by the Yamada-Gann method. The volumes of both phases were validated against the basic data, and a result in good agreement. The results obtained for the degree of dryness also showed good agreement with the basic values, which ensures the applicability of the proposed method in the entire two-phase region, limited by the temperature range from 220 to 300 K. The results also open the possibility to develop the method in the triple point region (216.59K-220 K) and in the near-critical region (300 K-304.13 K), as well as to determine, with greater accuracy, the basic CO$_2$ thermodynamic parameters in the two-phase region, such as enthalpy, entropy, viscosity, compressibility coefficient, specific heat capacity and thermal conductivity coefficient for the gas and liquid phases. Due to the simplicity of the form of the equation of state and a small number of empirical coefficients, the obtained technique can be used for practical problems of computational fluid dynamics without spending a lot of computation time.

**Keywords:** CO$_2$ two-phase region, saturated vapor pressure, Aungier-modified Redlich-Kwong equation of state, Lee-Kesler and Pitzer method, Yamada-Gann method, degree of dryness.

---

**Introduction**

Equations of state are widely used to assess the thermodynamic properties of working fluids in a two-phase region. The simplest two-parameter equation of state is the van der Waals equation. In this equation, the vapor-liquid equilibrium and the two-phase region were first determined. For more than a hundred years, a significant number of different modifications of the van der Waals equation have been presented, convenient for their form and relative simplicity of calculation. Among the most famous modifications used in computational fluid dynamics, it is worth noting the Redlich-Kwong equation [1], which adequately describes the gas and supercritical regions of pure substances and mixtures. The Soave-Redlich-Kwong modification has found the greatest application for calculating hydrocarbon substances and mixtures [2]. The Peng-Robinson modification [3] improved the prediction of the liquid-phase volume. The equation has been successfully applied to calculate some mixtures in high-pressure regions. However, the success of these modifications is limited to the estimation of vapor pressure. The calculated volumes of saturated liquid do

---

This work is licensed under a Creative Commons Attribution 4.0 International License.

© Hanna S. Vorobieva, 2021
not improve and invariably exceed the data measured [4]. The continuation of the development of the Peng-Robinson equation was the Patel-Teil equation of state, in which the prediction of the thermodynamic properties of matter on the saturation line for polar substances was refined [5]. Work [6] presents a comparison of various equations of state for a binary mixture of CO + CO₂, as well as separately pure CO and CO₂ in the temperature range from 253.15 to 293.15 K. The authors carried out a study using an experimental setup for studying phase equilibrium based on the static-analytical method with liquid phase sampling. The study revealed that the combined Peng-Robinson and Span-Wagner equation of state (PR-WS / NRTL) [7] describes the vapor-liquid equilibrium more accurately compared to other models presented in the work. However, this model requires a large amount of computational time, and is most applicable for binary mixtures with liquid phases. The Peng-Robinson model was also developed for predicting the density of binary mixtures in the liquid phase, and is known as the Volume-translated Peng-Robinson Equation of State [8].

The Aungier modification of the Redlich-Kwong equation made it possible to refine the calculation of the gas phase in a two-phase region through the introduction into the model of the eccentric coefficient and an additional empirical coefficient, which improved the calculation near the critical point [9]. Similar empirical coefficients were previously introduced into the original Redlich-Kwong equation by Soave, Wilson [10] and Barnes-King [11]. All four alternative forms of the Redlich-Kwong equation, described above, were compared in terms of errors in predicting pressure relative to the properties of the working fluid. The smallest error was shown by the model proposed by Aungier [9]. Based on the predictions and validations described in the article, the modifications of Soave and Barnes-King have the $P_r \leq 1$ limitation (where $P_r$ is the ratio of the current pressure to the critical pressure of the working fluid), the Wilson modification has the $P_r > 0.7$ limitation. Moreover, these modifications should not be used for substances with a negative eccentricity coefficient. The original Redlich-Kwong equation and Aungier’s modification do not have such limitations, but the Aungier modification is more accurate in terms of standard deviations by about 50% [9].

Along with the above equations of state, the Aungier modification has been widely used in leading software for modeling the flow of a working fluid, and is also known as the Redlich-Kwong-Aungier equation of state [12]. In this paper, the Aungier modification of the Redlich-Kwong equation will be referred to as the Redlich-Kwong-Aungier equation of state, and will be chosen as the basic one from the point of view of a small number of empirical coefficients and a wide range of applicability.

Among the non-cubic equations of state, known are the combined equations of state that include the regular and scaling parts, describing the P-T data over a wide range of temperatures and pressures. Such equations describe the near-critical region, as well as the region of the liquid phase, with greater accuracy than the cubic equations. Paper [13] proposed an equation representing P-T data near the critical point of vaporization and a crossover transition function that combines two different equations of state. Article [14] uses the Kiselev crossover equation of state, but the results reproduce the properties of the working fluid unsatisfactorily in terms of density, isochoric heat capacity, and speed of sound. Among their disadvantages crossover equations of state have a large number of correction factors, the equations requiring a large amount of computation time.

Taking into account the above, in this paper, the Aungier modification of the Redlich-Kwong equation of state is chosen as the basic one from the point of view of a small number of empirical coefficients and a wide range of applicability for pure CO₂.

**Statement of the Problem and the Purpose of the Study**

The research task of this study is to determine the degree of dryness with the smallest error, in comparison with the experimental data for the CO₂ two-phase region, in a wide temperature range from 220 to 300 K. For the problem presented, it is proposed to use the Redlich-Kwong-Aungier equation of state modified by the author. The modification of the equation of state consists in using a scale correction to determine the gas phase of the two-phase region. To determine the volume of the liquid phase, the author of the study proposes to use the Yamada-Gann method. The volume of saturated vapor in the two-phase region used in the equation of state is proposed to be determined by the Lee-Kesler and Pitzer method.

The purpose of the study is to reduce the error when using the Redlich-Kwong-Aungier equation of state, modified by the author, to find the volume of the gas phase, prove the expediency of using the Yamada-Gunn method to determine the volume of the liquid phase and the Lee-Kesler and Pitzer method to find the saturated vapor pressure, as well as, as a result, reduce the error in determining the degree of dryness in the CO₂ two-phase region in the temperature range from 220 to 300 K.
Description of the Method

Determination of the degree of dryness in the CO\textsubscript{2} two-phase region can be conditionally divided into three stages: finding the pressure of saturated vapor, predicting the volumes of liquid and gas phases, and determining the degree of dryness directly.

Used as the pressure in the two-phase region is the saturated vapor pressure found by the Lee-Kesler method [15]. The advantage of the Lee-Kesler and Pitzer equation is a more accurate solution in a wide range of the two-phase region of pure substances, in comparison with the Clapeyron equation. The equation is simpler, despite the two-parameter correlation form, does not require finding a large number of coefficients, as in the Riedel or Frost-Kalkwarf-Todos equations, and does not have tabular constants, individual for various substances, as in the Antoine equation [15].

Stage 1. The Lee-Kesler and Pitzer method is based on the principle of corresponding states, and consists of the following equations:

\begin{equation}
\ln P_{vpr} = f(0)(Tr) + \omega f(1)(Tr),
\end{equation}

where \(\omega\) is the eccentricity coefficient; \(Tr\) is the reduced temperature, the ratio of the design temperature to the critical one.

The functions \(f(0)\) and \(f(1)\) in the Pitzer expansion (1) are tabulated in wide ranges of reduced temperatures, and are presented by Lee and Kesler in the following analytical form:

\begin{align*}
f(0) &= 5.92714 - \frac{6.09648}{Tr} - 1.28862 \ln Tr + 0.169347 Tr^6; \\
f(1) &= 15.2518 - \frac{15.6875}{Tr} - 13.4721 \ln Tr + 0.435777 Tr^6.
\end{align*}

The reduced pressure of saturated vapor is determined by the Pitzer equation (1). The true value is found as follows:

\begin{equation}
P_{vp} = P_{vp,r} \cdot P_{cr},
\end{equation}

where \(P_{cr}\) is the pressure of the working fluid at the critical point.

Selected as the basic data required to validate the method used were the data from the mini-REFPROP (Reference Fluid Thermodynamic and Transport Properties) program. Mini-REFPROP is a free and abbreviated sample of the full version of the NIST REFPROP software. The program was developed by the National Institute of Standards and Technology (NIST), calculates the thermodynamic properties of only pure substances. For the calculation, the most accurate models close to the experimental data are used. For CO\textsubscript{2}, mini-REFPROP uses the Span-Wagner model [16], which describes the CO\textsubscript{2} operating range with high accuracy.

The Span-Wagner equation is successfully used in 1D modeling, for example, to calculate the flow in labyrinth seals [17]. However, the Span-Wagner model has drawbacks for practical application in computational fluid dynamics of 3D calculations: it requires a lot of time to calculate and determine thermodynamic relationships. The technique based on the use of the two-parameter equation of state requires less calculation time and uses fewer auxiliary parameters and coefficients. The saturated vapor pressure in the Span-Wagner model is determined by the Dushek equation [18] from the triple point to the critical one. Figure 1 shows the relative deviation of the saturated vapor pressure values, determined by different equations, from the experimental result. As can be seen from the graphs, the Dushek equation gives the closest to the experimental result. The error increases only near the critical point.
**Stage 2.** Volumes of gas and liquid phases can be found in several simple ways: by determining the volumes of gas and liquid phases from correlation equations based on experimental data; by determining volumes through solving a two-parameter equation of state.

To solve the correlation equations, there is no need to use the values of saturated vapor pressure. For example, in [19], equations are presented for CO₂, whose two-phase density depends only on the reduced temperature

\[
\rho_{\text{liquid}} = (0.466 + 0.466 \cdot (1.9073793 \cdot (1 - T_r)^{0.347} - 0.38225 \cdot (1 - T_r)^{0.667} + 0.42897885 \cdot (1 - T_r)))
\]

\[
\rho_{\text{gas}} = (0.466 + 0.466 \cdot (-1.7988929 \cdot (1 - T_r)^{0.347} - 0.71728276 \cdot (1 - T_r)^{0.667} + 1.7739244 \cdot (1 - T_r))).
\]

Such correlation equations are in good agreement with experimental data, but the empirical coefficients are specific for different substances. A more universal way to find volumes or densities is to use two-parameter equations of state.

The general view of the Redlich-Kwong-Aungier model, written in relation to the volume, is presented in the equation

\[V^3 + a_1V^2 + a_2V + a_3 = 0,\]

where

\[a_1 = -(c + \frac{RT}{P}); \quad a_2 = -(b' b_0 + \frac{RT b_0}{P} - \frac{A(T)}{P}); \quad a_3 = -\frac{A(T) b'}{P}; \quad A(T) = \left(\frac{T_{cr}}{T}\right)^n;\]

\[n = 0.4986 + 1.1735 \omega + 0.475 \omega^2; \quad b_0 = 0.08664 \frac{RT_{cr}}{P_{cr}}; \quad c = \frac{RT_{cr}}{P_{cr}} + b_0 - V_{cr}; \quad b' = b_0 - c,\]

where \(R\) is the gas constant for a particular substance; \(T\) is the current temperature value; \(\omega\) is the eccentricity coefficient; \(P\) is the current pressure value (in the two-phase region, the saturated vapor pressure is used); \(T_{cr}\) is the critical temperature of a substance; \(P_{cr}\) is the critical pressure of a substance; \(V_{cr}\) is the critical volume of a substance.

A cubic equation can be solved by the Cardano-Vieta method. As a result of the solution, three roots of the equation are determined. The largest of them is the volume of the gaseous medium, the smallest one is the volume of the liquid medium. In the database of the mini-REFPROP program, the volume of the gas phase is found from the Span-Wagner equation of state. The Span-Wagner model is based on the definition of the Helmholtz energy, and looks like this:

\[\frac{A(\rho, T)}{(RT)} = \Phi(\delta, \tau) = \Phi'(\delta, \tau) + \Phi''(\delta, \tau),\]

where \(\delta\) is the reduced density; \(\tau\) is the reduced temperature.

The subscripts 0 and \(r\) describe the ideal gas part of the Helmholtz energy function and the residual part, respectively. The Span-Wagner model describes the CO₂ operating range with sufficient accuracy in comparison with the experimental results allowing the model to be used as the basic data for validating the volume of gas and liquid phases obtained from the Redlich-Kwong-Aungier equation. The results of validation are described later in the article.

Two-parameter equations, convenient for practical application in computational fluid dynamics, determine the volume of the liquid phase in the two-phase region with a significant error. In this regard, it was decided to use the Yamada-Gann equation [20] to find the volume of the liquid phase. The equation is the correlating one, but it can be applied to various non-polar and weakly polar substances. The method is in good agreement with the experimental data near and directly at the saturation line

\[V_{\text{liquid}} = V_{cr} \cdot \left(0.29056 - 0.08775 \omega \right) \left(1 - \frac{T}{T_{cr}}\right)^{\frac{3}{2}}.\]

Used as an experimental data base is the mini-REFPROP one where the saturation density for CO₂ is found according to the Dushek equation:
\[ \ln \left( \frac{\rho_{\text{liquid}}}{\rho_{\text{crit}}} \right) = \sum_{i=1}^{4} a_i \left( 1 - \frac{T}{T_{\text{cr}}} \right)^{t_i}, \]

where \( T_{\text{cr}} \) is the critical temperature; \( \rho_{\text{crit}} \) is the critical density; \( a \) is the empirical coefficients \( a_1=1.9245108, a_2=-0.62385555, a_3=-0.32731127, a_4=0.39245142; t \) is the empirical coefficients \( t_1=0.34, t_2=1/2, t_3=10/6, t_4=11/6 \).

Evaluation of the accuracy of the Dushek method in comparison with the experimental data is presented in figure 2.

As can be seen from the dependencies in the figure, the Dushek method is in good agreement with the experimental values, and can be used in the future to validate the Yamada-Gann method.

**Stage 3.** Determination of the CO\(_2\) dryness degree in the two-phase region in the temperature range from 220 to 300 K.

The degree of dryness can be easily found using the volumes of gas and liquid phases, determined in step 2

\[
\text{Quality} = \frac{\rho_{\text{gas}}}{\rho_{\text{gas}}} - \frac{\rho_{\text{liquid}}}{\rho_{\text{gas}}} - \frac{\rho_{\text{liquid}}}{\rho_{\text{gas}}},
\]

where the densities of the gas and liquid phases are determined as

\[
\rho_{\text{liquid}} = \frac{1}{V_{\text{liquid}}}, \quad \rho_{\text{gas}} = \frac{1}{V_{\text{gas}}}. \tag{3}
\]

**Results and Discussion**

Below are the results of validation of the method described in the previous section.

**Results for stage 1. Determination of the CO\(_2\) saturated vapor pressure**

A numerical comparison of the basic saturated-vapor pressure values taken from mini-REFPROP and obtained by the Lee-Kesler and Pitzer method in the two-phase region shows that they are in good agreement (relative error less than 1%), and is shown in figure 3 and in table 1.

**Table 1. Numerical comparison of the results for the saturated vapor pressure determined by the Lee-Kesler and Pitzer method and from the mini-REFPROP database**

| Temperature \( T, \text{K} \) | mini-REFPROP, Saturated vapor pressure, Pa | Lee-Kesler and Pitzer method, Saturated vapor pressure, Pa | Relative error, % |
|-------------------------------|---------------------------------------------|-------------------------------------------------|-----------------|
| 216.60                        | 518140                                      | 519104.66                                       | 0.186           |
| 226.60                        | 783110                                      | 783726.06                                       | 0.079           |
| 236.60                        | 1138200                                     | 1137680.18                                      | -0.046          |
| 246.60                        | 1600400                                     | 1597345.16                                      | -0.191          |
| 256.60                        | 2187400                                     | 2180354.74                                      | -0.322          |
| 266.60                        | 2918400                                     | 2906419.44                                      | -0.411          |
| 276.60                        | 3814300                                     | 3798655.70                                      | -0.410          |
| 286.60                        | 4900000                                     | 488532.28                                       | -0.295          |
| 296.60                        | 6208400                                     | 6203605.78                                      | -0.077          |
| 300.00                        | 6713100                                     | 6712583.40                                      | -0.008          |
| 304.12                        | 7375900                                     | 7375792.32                                      | -0.001          |

**Results for stage 2. Determination of the volume of gas and liquid phases in the CO\(_2\) two-phase region**

A numerical comparison of the gas phase volumes determined from the Redlich-Kwong-Aungier equation of state and the basic values obtained from the mini-REFPROP database is shown in figure 4 and in table 2.
As it is seen from table 2, the error between the basic data and the values determined from the Redlich-Kwong-Aungier equation of state increases with approaching near-critical region. Temperature ranges from the triple point ($T=216.59 \text{ K}$) to $220 \text{ K}$ and from $300 \text{ K}$ to the critical point ($T=304.13 \text{ K}$) will not be considered in this work. To refine the gas-phase volume values in the entire temperature range under study, a scale correction $n_{2p}$ was introduced into the equation of the coefficient $A(T)$ of the Redlich-Kwong-Aungier model. The distribution of the scale correction values for the temperature range from $220$ to $300 \text{ K}$ is shown in figure 5. The modified equation of the coefficient $A(T)$ is presented below

$$A(T) = a \left( \frac{T - T_a}{T} \right) \left( n_{2p} \right) ,$$

where the scale correction $n_{2p}$ is given in the form of a correlation equation, and has the form

$$n_{2p} = -3.416687 + 0.029098 \cdot T + 0.0002418 \cdot T^2 - 2.86799 \cdot 10^{-6} \cdot T^3 + 9.3607 \cdot 10^{-9} \cdot T^4 - 1.0205347 \cdot 10^{-11} \cdot T^5 .$$

A numerical comparison of the basic data for the gas phase volumes with the modified Redlich-Kwong-Aungier equation of state is presented in table 3. The estimation of the change in the errors in the temperature range under study is given in figure 6 for the original and modified Redlich-Kwong-Aungier equations of state.

As it is seen from table 3 and figure 6, the introduction of the scale correction $n_{2p}$ into the Redlich-Kwong-Aungier equation significantly reduced the error over the entire temperature range under study, which will further reduce the error in determining the dryness coefficient.

| Temperature $T$, K | mini-REFPROP, Gas phase volume, m$^3$/kg | Redlich-Kwong-Aungier, Gas phase volume, m$^3$/kg | Relative error, % |
|-----------------|---------------------------------|---------------------------------|-----------------|
| 220             | 0.06322                         | 0.06324                         | 0.03            |
| 240             | 0.03003                         | 0.03005                         | 0.04            |
| 260             | 0.01552                         | 0.01553                         | 0.03            |
| 280             | 0.00821                         | 0.00821                         | 0.01            |
| 300             | 0.00372                         | 0.00373                         | 0.05            |
Let us now proceed to the assessment of the volume of the liquid phase of the CO₂ two-phase region in the temperature range from 220 to 300 K. In Table 4, compared are the values determined from the original and modified Redlich-Kwong-Aungier equations and the basic data from mini-REFPROP. The scale correction values are the same for the gas and liquid phases.

The modification of the Redlich-Kwong-Aungier equation of state made it possible to reduce the error in determining the volume of the liquid phase; however, the tendency for the error to increase when approaching the near-critical region remained. The selection of a new scale correction for the liquid region is not advisable, since this will lead to the addition of new coefficients and complication of the Redlich-Kwong-Aungier model. As described in the Statement of the Problem and the Purpose of the Study and Description of the Method sections, to determine the volume of the liquid phase in a two-phase region, the Yamada-Gann equation can be used. Table 5 shows the comparative results for this method.

Figure 7 compares the results for the liquid-phase volumes determined by the original and modified Redlich-Kwong-Aungier equations, using the Yamada-Gann method. The calculated results are validated against the basic values obtained in mini-REFPROP. The Yamada-Gann method provides the best matching with the basic values.

Thus, to find the gas phase volume in a two-phase region, it is preferable to use the modification of the Redlich-Kwong-Aungier equation of state, and to find the liquid phase volume, the Yamada-Gann method. In other words, when solving the modified cubic Redlich-Kwong-Aungier equation, the value of the largest root will correspond to the gas phase volume, and the Yamada-Gann method will be used directly for the liquid phase volume.

**Results for stage 3. Determination of the degree of dryness in the CO₂ two-phase region**

The method for determining the degree of dryness is described in the Statement of the Problem and the Purpose of the Study and Description of the Method sections.
by equations (2), (3). Below are graphs of the distribution of the degree of dryness depending on the density for the entire temperature range under study. Figure 8 shows the values of the degree of dryness, which were determined using the original Redlich-Kwong-Aungier equation of state (to find the volumes of the gas phase) and the Yamada-Gunn method (to determine the volumes of the liquid phase).

Figure 9 shows the values of the degree of dryness, which were determined using the modified Redlich-Kwong-Aungier equation of state (to find the volumes of the gas phase) and the Yamada-Gunn method (to determine the volumes of the liquid phase). The calculated results are in good agreement with the basic values obtained from mini-REFPROP for the entire temperature range under study.

For a more detailed analysis, let us consider the distribution of errors for the method using the modified Redlich-Kwong-Aungier equation of state and the Yamada-Gunn method, depending on density (Fig. 10). Figure 10 demonstrates a small error for densities from 40 to 800 kg/m³ for the temperature range from 220 to 280 K. The error increases as CO₂ approaches the saturation line (the degree of dryness tends to zero and the degree of humidity, to 1, respectively), especially for temperatures close to the temperature of the triple point (220 K) and for the near-critical temperature (300 K). The saturation line is a first-order phase transition, and requiring a more precise description than that proposed in the methodology of this paper. The error for a temperature of 300 K has a tendency which is different from the others presented in the graph. This behavior can be explained by the effects occurring in the near-critical region, near a second-order phase transition. As for the saturation line, the near-critical region should be described more accurately than it is proposed in the methodology of this paper. It should be noted, however, that the method proposed in this paper describes a large part of the temperature range in a wide range of densities with sufficient accuracy.

**Conclusions**

The method proposed for determining the degree of dryness in the CO₂ two-phase region, which uses, as a basis, the modified Redlich-Kwong-Aungier equation of state and the Yamada-Gunn method, makes it possible to obtain the values of the volumes of gas and liquid phases with good accuracy in comparison with the basic values. The results obtained for the degree of dryness showed good agreement with the basic values, which ensures the applicability of the proposed technique in the entire two-phase region, limited by the temperature range from 220 to 300K. The results also open up an opportunity to develop the technique in the triple point region (216.59–220 K) and in the near-critical region (300–304.13 K). Due to the simplicity of the form of the equation of state and a small number of empirical coefficients, the obtained technique can be used for practical problems of computational fluid dynamics without spending a lot of time for computation.

**References**

1. Redlich, O. & Kwong, J. N. S. (1949). On the thermodynamics of solutions. V. An equation of state. Fugacities of gaseous solutions. Chemical Reviews, vol. 44, iss. 1, pp. 233–244. https://doi.org/10.1021/cr60137a013.
2. Soave, G. (1972). Equilibrium constants from a modified Redlich-Kwong equation of state. Chemical Engineering Science, vol. 27, iss. 6, pp. 1197–1203. https://doi.org/10.1016/0009-2509(72)80096-4.

3. Peng, D. Y. & Robinson, D. B. (1976). A new two-constant equation of state. Industrial & Engineering Chemistry Fundamentals, vol. 15, iss. 1, pp. 59–64. https://doi.org/10.1021/i160057a011.

4. Haghtalab, A., Mahmoodi, P., & Mazloumi, S. H. (2011). A modified Peng–Robinson equation of state for phase equilibrium calculation of liquefied, synthetic natural gas, and gas condensate mixtures. The Canadian Journal of Chemical Engineering, vol. 89, iss. 6, pp. 1376–1387. https://doi.org/10.1002/cjce.20519.

5. Thamanavat, K., Sun, T., & Teja, A. S. (2009). High-pressure phase equilibria in the carbon dioxide+ pyrrole system. Fluid Phase Equilibria, vol. 275, iss. 1, pp. 60–63. https://doi.org/10.1016/j.fluid.2008.09.019.

6. Chapoy, A., Ahmadi, P., de Oliveira Cavalcanti Filho, V., & Jadhawar, P. (2020). Vapour-liquid equilibrium data for the carbon dioxide (CO2)+ carbon monoxide (CO) system. The Journal of Chemical Thermodynamics, vol. 150, paper 106180. https://doi.org/10.1016/j.jct.2020.106180.

7. Renon, H. & Prausnitz, J. M. (1968). Local compositions in thermodynamic excess functions for liquid mixtures. AIChE Journal, vol. 14, iss. 1, pp. 135–144. https://doi.org/10.1002/aic.690140124.

8. Abudour, A. M., Mohammad, S. A., Robinson Jr, R. L., & Gasem, A. M. (2013). Volume-translated Peng-Robinson equation of state for liquid densities of diverse binary mixtures. Fluid Phase Equilibria, vol. 349, pp. 37–55. https://doi.org/10.1016/j.fluid.2013.04.002.

9. Aungier, R. H. (1995). A fast, accurate real gas equation of state for fluid dynamic analysis applications. Journal of Fluids Engineering, vol. 117, iss. 2, pp. 277–281. https://doi.org/10.1115/1.2817141.

10. Wilson, G. M. (1966). Calculation of enthalpy data from a modified Redlich-Kwong equation of state. Advances in Cryogenic Engineering, vol. 11, pp. 392–400. https://doi.org/10.1007/978-1-4757-0522-5_43.

11. King, C. J., Foss, A. S., Grens, E. A., Lynn, S., & Rudd, D. F. (1973). Chemical process design and engineering. Chemical Engineering Education, vol. 7, iss. 2, pp. 72–74.

12. ANSYS FLUENT 12.0 User’s Guide https://www.ansys.com/products/fluent/products/12.0.

13. Bezverkhy, P. P., Martynets, V. G., & Matizen, E. V. (2009). Equation of state for 3He, including a regular and a scalar part. Low Temperature Physics, vol. 35, iss. 10, pp. 945–955. https://doi.org/10.1063/1.3253391.

14. Rykov, S. V. & Bagautdinova, A. Sh. (2009). Chishlemny analiz krossovernogo uravnienia sostoyaniya [Numerical analysis of the crossover equation of state]. Nauchny zhurnal NIU ITMO. Seriya: Khokolchina tekhnika i konditsionirovaniye Scientific Journal NRU ITMO. Series: Refrigeration and Air Conditioning, no. 1, pp. 1–24 (in Russian).

15. Lee, B. I. & Kesler, M. G. (1975). A generalized thermodynamic correlation based on three-parameter corresponding states. AIChE Journal, vol. 21, iss. 3, pp. 510–527. https://doi.org/10.1002/aic.690210313.

16. Span, R. & Wagner, W. (1996). A new equation of state for carbon dioxide covering the fluid region from the triple-point temperature to 1100 K at pressures up to 800 MPa. Physical of Chemical Reference Data, vol. 25, iss. 6, pp. 1509–1596. https://doi.org/10.1063/1.555991.

17. Zhu, Y., Jiang, Y., Liang, S., Guo, C., Guo, Y., & Cai, H. (2020). One-dimensional computation method of supercritical CO2, labyrinth seal. Applied Sciences, vol. 10, iss. 17, paper 5771. https://doi.org/10.3390/app10175771.

18. Gilgen, R., Kleinrahm, R., & Wagner, W. (1992). Supplementary measurements of the (pressure, density, temperature) relation of carbon dioxide in the homogeneous region at temperatures from 220 K to 360 K and pressures up to 13 MPa. The Journal of Chemical Thermodynamics, vol. 24, iss. 12, pp. 1243–1250. https://doi.org/10.1016/S0002-9614(05)80264-2.

19. Anwar, S. & Carroll, J. J. (2016). Carbon dioxide thermodynamic properties handbook: Covering temperatures from -20 °C to 250 °C and pressures up to 1000 bar. John Wiley & Sons, 608 p. https://doi.org/10.1002/9781119083948.

20. Yamada, T. & Gunn, R. D. (1973). Saturated liquid molar volumes. Racket equation. Journal of Chemical and Engineering Data, vol. 18, iss. 2, pp. 234–236. https://doi.org/10.1021/je60057a006.

Received 07 September 2021
Результаты проведены за дополняемого рівняння Спана-Вансера, наведенного у програме mini-REFPROP та най-більш наближеного до експериментальних даних у двофазній області CO2. Для запропонованого методу відносних даними є температура і густину, критичні властивості робочого тіла, його коефіцієнт аеродинамічності, а так-ож молярна маса. У процесі його розв'язання знаходяться тиск, який для двофазної області стає тиском наси-ченої пари, об'ємі газової і рідкої фаз двофазної області, густини газової і рідкої фаз, а також ступінь сухості. Тиск насищеної пари визначено методом Лі-Кеслера і Пінтера, результати досі збігаються з експериментальними даними. Об'єм газової фази двофазної області знайдено за модифікованим рівнянням стану Редліха-Квонга-Анг’єс. У статті запропоновано корекційні рівняння для масштабної поправки, що використовуються в рівнянні стану Редліха-Квонга-Анг’єс для газової фази двофазної області. Об'єм рідкої фази знайдено методом Ямада- Гінна. Об'єми обох фаз були визначені з базовими даними і досі збігаються. Отримані рівняння для ступені сухості також показали хороший збіг з базовими значеннями, що забезпечує можливість застосування запропонованої методики у всіх двофазних областях, обмеженою температурним діапазоном від 220 до 300 К. Ре- результати також відкривають можливість для розвитку методики в області потрійної точки (216,59–220 К) і в навколокритичній області (300–304,13 К) та для визначення з більшою точністю основних термодинамічних па- раметрів CO2 в двофазній області, таких, як енергія, втрати, зв'язок, коефіцієнт стиснення, питома теплопровідність і коефіцієнт теплопровідності для газової і рідкої фаз. Завдяки простоті форми рівняння стану і неве- ликої кількості емпіричних коефіцієнтів відмінну методику можна використовувати для практичних задач об- числювальної гідродинамики без великої затрати часу на обчислень.

Ключові слова: двофазна область CO2, тиск насищеної пари, рівняння стану Редліха-Квонга-Анг’єс, метод Лі-Кеслер і Пінтера, метод Янмада-Гінна, ступінь сухості.

Література

1. Redlich O., Kwong J. N. S. On the thermodynamics of solutions. V. An equation of state. Fugacities of gaseous solutions. Chem. reviews. 1949. Vol. 44. Iss. 1. P. 233–244. https://doi.org/10.1021/cr60137a013.

2. Soave G. Equilibrium constants from a modified Redlich-Kwong equation of state. Chem. eng. sci. 1972. Vol. 27. Iss. 6. P. 1197–1203. https://doi.org/10.1016/0009-2509(72)80006-4.

3. Peng D. Y., Robinson D. B. A new two-constant equation of state. Industrial & Engineering Chemistry Fundamentals. 1976. Vol. 15. Iss. 1. P. 59–64. https://doi.org/10.1021/i160057a011.

4. Haghtalab A., Mahmoodi P., Mazloumi S. H. A modified Peng–Robinson equation of state for phase equilibrium calculation of liquefied, synthetic natural gas, and gas condensate mixtures. The Canadian J. Chem. Eng. 2011. Vol. 89. Iss. 6. P. 1376–1387. https://doi.org/10.1002/jcde.20519.

5. Thamanavat K., Sun T., Teja A. S. High-pressure phase equilibria in the carbon dioxide+ pyrrole system. Fluid Phase Equilibria. 2009. Vol. 275. Iss. 1. P. 60–63. https://doi.org/10.1016/j.fluid.2008.09.019.

6. Chapoy A., Ahmadi P., de Oliveira Cavalcanti Filho V., Jadhawar P. Vapour-liquid equilibrium data for the carbon dioxide (CO2)+ carbon monoxide (CO) system. The J. Chem. Thermodynamics. 2020. Vol. 150. Paper 106180. https://doi.org/10.1016/j.jct.2020.106180.

7. Renon H., Prausnitz J. M. Local compositions in thermodynamic excess functions for liquid mixtures. AICHe J. 1968. Vol. 14. Iss. 1. P. 135–144. https://doi.org/10.1002/aic.690140124.

8. Abudour A. M., Mohammad S. A., Robinson Jr R. L., G asem A. M. Volume-translated Peng–Robinson equation of state for liquid densities of diverse binary mixtures. Fluid Phase Equilibria. 2013. Vol. 349. P. 37–41. https://doi.org/10.1016/j.fluid.2013.04.002.

9. Augnier R. H. A fast, accurate real gas equation of state for fluid dynamic analysis applications. J. Fluids Eng. 1995. Vol. 117. Iss. 2. P. 277–281. https://doi.org/10.1115/1.2817141.

10. Wilson G. M. Calculation of enthalpy data from a modified Redlich-Kwong equation of state. Advances in Cryogenic Eng. 1966. Vol. 11. P. 392–400. https://doi.org/10.1007/978-1-4757-0522-5_43.

11. King C. J., Foss A. S., Greens E. A., Lynn S., Rudd, D. F. Chemical Process Design and Engineering. Chem. Eng. Education. 1973. Vol. 7. Iss. 2. P. 72–74.

12. ANSYS FLUENT 12.0 User’s Guide https://www.ansys.com/product/fluency/docs Fluent/html/ug/main_pre.htm.

13. Безверхий П. П., Мартынчук В. Г., Матяшен Э. В. Уравнение состояния "Не", включающее регулярную и касейлинговскую части. Физика высоких температур. 2009. Т. 35. № 10. С. 947–955.

14. Рыков С. В., Бацукова И. Ш. Численный анализ кроссоверного уравнения состояния. Науч. журн. НИУ ИТМО. Сер. Холодильная техника и кондиционирование. 2009. Т. 1. С. 1–24.

15. Lee B. I., Kessler M. G. A generalized thermodynamic correlation based on three-parameter corresponding states. AICHe J. 1975. Vol. 21. Iss. 3. P. 510–527. https://doi.org/10.1002/aic.690210313.

16. Span R., Wagner W. A new equation of state for carbon dioxide covering the fluid region from the triple-point temperature to 1100 K at pressures up to 800 MPa. J. Phys. and Chem. Reference. 1996. Vol. 25. Iss. 6. P. 1509–1596. https://doi.org/10.1016/1.555991.
The main issues associated with the development of two-phase mechanically pumped loops (2φ-MPL) for thermal control systems of spacecraft with large heat dissipation were formulated back in the early 80s. They have undeniable advantages over single-phase loops with mechanical pumping and two-phase capillary pumped loops at power more than 6 kW and heat transfer distance more than 10 meters. Intensive research and development of such systems started in the USA together with European, Canadian and Japanese specialists due to plans to build new high-power spacecraft and the Space Station Freedom project. In the 90’s, S. P. Korolev Rocket and Space Corporation Energia (Russia) was developing a 2φ-MPL for the Russian segment of the International Space Station with the capacity of 20...30 kW. For this purpose, leading research organizations of the former Soviet Union were involved. In the last two decades, interest in two-phase heat transfer loops has significantly increased because of high-power stationary communications satellites and autonomous spacecraft for Lunar and Martian missions. The paper presents a retrospective review of worldwide developments of 2φ-MPLs for thermal control systems of spacecraft with large heat dissipation from the early 80’s to the present. The participation of scientists and engineers of the Ukrainian National Aerospace University “KhAI” and the Center of Technical Physics is considered. The main directions of research, development results, and scientific and technical problems on the way to the practical implementation of such system are considered. Despite a large amount of research and development work done, there were no practically implemented projects of spacecraft with the high-power thermal control system until recent days. The first powerful stationary satellite with the 2φ-MPL was SES-17 satellite on the NEOSAT platform by Thales Alenia Space - France. The satellite was successfully launched into space on October 24, 2021 by onboard an Ariane 5 launcher operated by Arianespace from the Europe’s Spaceport in Kourou, French Guiana.

Keywords: spacecraft; thermal control system; two-phase mechanically pumped loop.

Introduction

The progress of space technology leads to an increase in the power equipment of spacecraft, the power of which is up to tens of kW. The problem of heat dissipation from equipment and devices into space is acute for such spacecrafts.

This work is licensed under a Creative Commons Attribution 4.0 International License.
© Gennadiy O. Gorbenko, Pavlo H. Gakal, Rustem Yu. Turna, Artem M. Hodunov, 2021

DOI: https://doi.org/10.15407/pmach2021.04.027