Thermodynamic properties of CO₂ at up to 200 MPa, including the critical region, calculated by the equation of state with small number of constants

P P Bezverkhii¹*, V G Martynets¹, A B Kaplun² and A B Meshalkin²

¹ Nikolaev Institute of Inorganic Chemistry SB RAS, Lavrentiev ave.3, Novosibirsk, 630090, Russia
² Kutateladze Institute of Thermophysics SB RAS, Lavrentiev ave.1, Novosibirsk, 630090, Russia

*E-mail: ppb@niic.nsc.ru

Abstract. Heat capacities $C_v$, $C_p$ and sound velocity $W$ of carbon dioxide are calculated basing on the new thermal equation of state (EoS) with a small number of regulated constants. This equation includes a new regular EoS with 11 coefficients and scaling EoS with six coefficients and regular transition function containing two adjustable parameters. The results of calculating the thermodynamic properties of CO₂ in the regular behavior range of up to 200 MPa correspond to the accuracy level of the modern reference equations of state. To determine the constants of the calculated equations, only $p, \rho, T$-data for CO₂ were used. The average error in describing the thermal properties of CO₂ does not exceed the error of the available experimental data. The calculated values coincide with the values of the reference data.

1. Introduction

As it is known, to obtain the reference tables on thermodynamic properties of single-component substances, the equations of state (EoS) that contain many terms are used as a rule. The number of adjustable constants in these equations reaches 50–100 or more (e.g., see, [1]). As a rule, in such regular multi-parameter EoS, the critical conditions are not satisfied at the real critical point. On the other hand, the existing crossover scaling EoS are extremely inconvenient because of implicit parametric form and significant difficulties for practical calculations [2].

In recent publications [3–9], the combined equations of state (CES) with a small number of regulated constants, developed by us, have an explicit (nonparametric) form. All thermodynamic properties are calculated using the thermal equation of state obtained during description of $p, \rho, T$-data.

Theoretical grounding of the equation for the scale part of pressure $p_{scal}$ in the explicit form is given in [3, 4]. The presence of regular part $p_{reg}$ in the combined EoS makes it possible to avoid the use of non-asymptotic additional terms that arise in the theory, when the range of scaling application is expanded. The scaling EoS in the explicit form [6–9] are easier to apply for describing of $p, \rho, T$-data and determining the coefficients by approximating these data in comparison with the EoS in parametric form [2, 12]. In [6, 7], the combined EoS, written in the explicit form, includes a regular EoS and scaling EoS in the symmetric [6] and asymmetric form [7].

The known combined EoSs contain a regular part in the form of multi-constant polynomials, where the critical conditions are not satisfied as a rule. Thus, the combined EoS model in the explicit form...
for \( p(\rho, T) \) was applied, for example, in [13]. The scaling-like terms are used in EoS [13], which contains 17 adjustable coefficients. In comparison with [13], the combined EoS [6–9], including the equation proposed in this paper, contain up to 20 adjustable coefficients.

In this paper, a new regular state equation is proposed for \( p_{reg} \) of the CES for calculating the thermodynamic properties in a wider range of CO\(_2\) states at the pressures of up to 200 MPa. This equation has a new form not related to the parameters at the triple point as in regular EoS [6–9].

2. Equations of state and approximation of experimental data

Approximation of existing experimental \( p, \rho, T \) -data for CO\(_2\) by a new combined EoS is carried out in the ranges of their measurements (0 < \( p/\rho_c < 2.217 \) K < \( T < 430 \) K, 0 < \( p \leq 25 \) MPa). For CO\(_2\) a review of experimental \( p, \rho, T \) -data is given in [1]. The approximation array of \( p, \rho, T \) -data (731 points) for CO\(_2\) was formed from the calculated tabular data of [1] in the range of up to 25 MPa, not including the critical region, and experimental \( p, \rho, T \) -data in a wide neighborhood of the critical point in [14,15]. In addition, comparison of results on the pressures (densities) calculated by the combined EoS beyond the approximation ranges with the reference tabular data in the range of up to 200 MPa from [1] showed their coincidence within the data precision. The parameters of the critical and triple points for CO\(_2\) are taken from [1]. The combined EoS has the form of explicit function \( p, T \) and it is written as:

\[
p(p_c) = (1-Y) p_{reg}/p_c + Y p_{scal}/p_c \tag{1}
\]

Equation of state (1) includes new regular part \( p_{reg} \) for approximation of \( p, \rho, T \) -data in the liquid and gas states beyond the critical region, singular scale part \( p_{scal} \) for the critical region, and transition (crossover) function

\[
Y = \omega[(1 - \omega/\omega_o)^2/(1 - 1/\omega_o)^2] \text{erfc}(\sqrt{\lambda} |\tau|) \exp(-\mu(\Delta p)^2),
\]

where \( \tau = t - 1, \Delta p = \omega - 1 \) are the relative "distances" from the critical points, \( t = T/T_c, \omega = \rho/\rho_c, \lambda \) and \( \mu \) are adjustable constants that determine the region of \( p_{scal} \) influence, \( \text{erfc}(\sqrt{\lambda} |\tau|) \) is the Laplace error function.

2.1. Regular equation of state

In contrast to \( p_{reg} \) with 13 constants in [8], we suggest a new type of equation for \( p_{reg} \) with 11 adjustable constants, not related to the parameters of the triple point (\( z_c \) is the sign for \( z_c/p_c \pi T_c = 0.274588 \)):

\[
p_{reg}/p_c = (\alpha t/\Delta t)(1 + A_1(\epsilon^{1/2} - 1 - 2/t)\omega[1 - \omega/\omega_c] + A_2(\omega - t - A_3(\epsilon^{1/2} - 1))
+A_4(\epsilon^{1/2} - 1 - 3/t)\omega[1 - \omega/\omega_c] + A_5(\epsilon^{1/2} - 5/t)\omega[2 - 5\omega/\omega_c]
+A_6/\omega + A_7/\omega^2 + A_8/\omega^3 + A_9/\omega^4 + A_{10}/\omega^2).
\tag{2}
\]

In the equation (2), \( x = 1 - z_c \omega, \varphi(\omega) = EXP(-\omega/(1 - z_c \omega)) \). The temperature functions contained in certain terms with \( A_i \) are related to the form of applied intermolecular potential [10, 16]. Constants \( A_5, A_6 \) and \( A_{11} \) were calculated by the formulas following from the conditions at the critical point,

\[
(p_{reg}(p_c, T_c))_{calc} = p_c^{exp}, \quad [(\partial(p_{reg}/p_c)/\partial \omega)_{calc} = 0, \quad [(\partial^2(p_{reg}/p_c)/\partial \omega^2)_{calc} = 0, \quad
\]

and by the values of other \( A_i \). These formulas are cumbersome and not given here.

2.2. Scaling equation of state

Singular part \( p_{scal} \) in (1) includes values \( p_c, \rho_c, T_c \), adjustable constants \( q, k, M_a p, C_1, b, a_p \) and it is chosen with consideration of asymmetry using the form [8]:

\[
p_{scal}/p_c = 1 - k q_p - q_y \Delta \rho \Delta \rho^{1/2} - [1 + \delta \cdot \Delta \rho] + (\tau + q_p) |\Delta \rho|^{1/2} (\Delta \rho + \Delta \rho^{1/2}) - k \int x(\tau + q_p) |\Delta \rho|^{1/2} dx + (M - a_p)/(1 - a_p) - \Delta \rho \Delta \rho^{1/2} h_1,
\tag{3}
\]

In the equation (3), \( k \) is the compressibility coefficient in asymptotic dependence \( p_c K_c = \tau^\gamma/k \) along the critical isochore. Value \( q \) in (3) is a coefficient in the asymmetric form of the boundary curve.
(binodal) $\Delta \rho_{\text{bin}} = \pm (\text{q}^0 + B_1 (\text{q})^2)$. $B_1 = -bk \cdot 2.531412 / q, \rho_p = 4.0015q [4, 9]$. Values of $q = 0.14796, B_1 = -0.8104$ were obtained by approximating the experimental binodal of CO$_2$ [1]. The critical indexes were equal to $\beta = 0.3255, \gamma = 1.239, \alpha = 0.11 [17]$. $C_r = k \beta \gamma B(\alpha - 1, 2\beta) / q^2$, $B(\alpha - 1, 2\beta) = 2.6396$ represent the Euler beta function, $\delta = (\gamma + \beta) / \beta$, $\alpha$ is the heat capacity index in temperature dependence of $C_v$ along the critical isochore $\rho = \rho_c, M-a_p = s_c(T_c/p_c - a_p, s_c$ is the critical entropy per unit volume, $q_0$ is the constant of Pokrovsky transformation [18]. It is obvious that the asymmetry coefficient $b$ in EoS (3) is directly related to the asymmetric term in the expression for binodal ($bk = -0.22881173$).

2.3. Approximation of experimental data
The root-mean-square error $\sigma_r$ in approximating the $p, \rho, T$ -data of CO$_2$ by pressure (1) was 0.95%, average absolute deviation of calculated pressure was AAD = 0.63%, and for calculated density, it was $\sigma_\rho = 0.78$% and AAD = 0.51%. The technique used to minimize the quadratic functional is described in detail in [6]. The coefficients of CES (1) are as follows: $A_1 = 0.032949433; A_2 = 1.255070529$; $A_3 = 2.151878473; A_4 = -0.0097640765; A_5 = -0.0025982647$ (calculation); $A_6 = -0.0662254823$ (calculation); $A_7 = 0.4125148619; A_8 = 0.051723040; A_9 = 0.0025736756; A_{10} = -0.0002731598; A_{11} = 0.0078325775$ (calculation); $M-a_p = 7.2470764; q = 0.14796; k = 9.321165; \lambda = 370.528; \mu = 24.567; C_1 = -19.50; a_p = 0.2444, b = -0.0245475$.

2.4. Calculation of heat capacities $C_v, C_p$ and sound velocity $W$
Coefficients of CES (1) are used to calculate heat capacity $C_v$ by the well-known ratio of thermodynamics, which includes derivative $[\partial^2 / \partial t^2]_0$:

$$C_v = C_{v,\text{reg}} - zRt^4 \left[ 2 - (\partial^2 / \partial t^2) \right]_0 \omega^2 d\omega + 2 \left[ (\partial^2 / \partial t^2) \right]_0 \omega^2 d\omega + \frac{\partial^2 (\partial^2 / \partial t^2) \omega^2 d\omega}{(\partial (\partial^2 / \partial t^2) \omega^2 d\omega)}, (4)$$

where $C_{v,\text{reg}} = (p_{\text{cal}} - p_{\text{reg}}) / p_c$.

Integrals in (4) are not expressed in elementary functions and calculated numerically. In equation (4) $C_{v,\text{reg}}$ is calculated by constants $A_1, A_3, A_4, A_5, A_6$ according to expression:

$$C_{v,\text{reg}} = C_{v,\text{id}} R [A_4 (\omega^2 / t^2) \partial^2 (\partial^2 / \partial t^2) \omega^2 d\omega + A_4 \partial^2 (\partial^2 / \partial t^2) \omega^2 d\omega + 25 A_5 \omega^2 \partial^2 (\partial^2 / \partial t^2) \omega^2 d\omega], (5)$$

where $C_{v,\text{id}}$ is contribution of the heat capacity of rarefied gas, calculated for CO$_2$, using formula in [1].

To calculate $C_v$ (4) near and far from the critical point, the expressions for calculating the integrals in $\partial (\partial^2 / \partial t^2) / p_c$ and $(\partial^2 (p_{\text{cal}} / p_c) / \partial t^2) / p_c$ were replaced by rapidly convergent series of the different shapes at $\tau < 0$ and $\tau > 0 [6, 9]$. Calculations of $C_v$ by (4) along isotherms in the liquid state region ($\omega > 1$) revealed an insufficient decrease in integral contributions to $C_v$ (4) with increasing $\omega (\Delta \rho > 0.5)$. These integrals contain $\partial (\partial^2 / \partial t^2) / \partial t$ and give a certain remainder at numerical integration, when passing through the critical region, up to $\omega_p = 2.520381$. Therefore, when calculating $C_v$ in the liquid region, we used a special procedure of replacing the value of $T_c$ in the crossover function $Y(\tau, \Delta \rho)$ and its temperature derivatives in (4) by the values of spinodal temperature of liquid $T_c$ corresponding to the density, at which $C_v$ is calculated. Temperature $T_c$ was calculated by the value of $\omega$ equal $\omega_0$ at the upper limit of integrals in (4) according to formula $\Delta \rho = \pm (-\text{q}^0 + B_2 (\text{q})^2)$, where $\tau_c = T_c / T$, $q_c = 2.4196q, B_2 = -bk \beta [q_p - q_c]^{-4} (1 - \omega^2)^{1 - 4} + 2.6396q^2] = -2.20853939 \cdot bk [4]$. In the critical region, the values of $T_c$ are close to $T_p$, and for $\omega > 1$ and $T > T_c$ the temperature factor in $Y(\tau, \Delta \rho)$ with new $\tau = (T - T_c) / T_c$ extinguishes rapidly the contribution of the critical region to $C_v$. For region $\omega > 1$ and $T < T_c$, the $T_c$ values obtained for the “mirror” reflection of the liquid branch $\tau_c (\Delta \rho)$ of spinodal...
relative to line $T = T_c (\tau = 0)$ were applied. To calculate $C_v$ along the isochores in the liquid state region at $T < T_c (\tau < 0)$, we used an additional procedure of excluding the singular contribution to integrals of (4) at numerical integration over the density at $-0.01 < \tau < 0$ (corresponding to the range of $-0.15 < \Delta \rho_{\text{bin}}$ on the binodal for a given temperature were within this range). This allows us to "cut off" the singular contribution to $C_v$ at $\Delta \rho > 0.5$.

The value of $C_p$ was calculated in agreement with the general formula of thermodynamics:

$$C_p = C_v + z_c R \omega^{-2} \left[ \frac{\partial (p / p_c)}{\partial \omega} \right] / \left[ \frac{\partial (p / p_c)}{\partial \omega} \right],$$

where

$$\left[ \frac{\partial (p / p_c)}{\partial \omega} \right] = \frac{\partial (p_{\text{reg}} / p_c)}{\partial \omega} \frac{\partial \omega}{\partial \tau} = \frac{\partial (p / p_c)}{\partial \omega} \frac{\partial \omega}{\partial \tau} = \frac{\partial (p_{\text{reg}} / p_c)}{\partial \omega} \frac{\partial \omega}{\partial \tau}.$$

When substituting expressions for the derivatives, formula (6) takes form

$$C_p = C_v + R z_c \frac{\partial \omega}{\partial \tau} \left( C_{p3} + C_{p2} + C_{p1} \right) \frac{1}{(C_{p6} + C_{p5} + C_{p4})},$$

where $C_{p1} = \frac{\partial (\Delta p_{\nu})}{\partial \omega} \frac{\partial \omega}{\partial \tau}$, $C_{p2} = \frac{\partial (\Delta p_{\nu})}{\partial \omega} \frac{\partial \omega}{\partial \tau}$, $C_{p3} = \frac{\partial (p_{\text{reg}} / p_c)}{\partial \omega} \frac{\partial \omega}{\partial \tau}$, $C_{p4} = \frac{\partial (p_{\text{reg}} / p_c)}{\partial \omega} \frac{\partial \omega}{\partial \tau}$, $C_{p5} = \frac{\partial (\Delta p_{\nu})}{\partial \omega} \frac{\partial \omega}{\partial \tau}$, $C_{p6} = \frac{\partial (p_{\text{reg}} / p_c)}{\partial \omega} \frac{\partial \omega}{\partial \tau}$.

Equilibrium adiabatic sound velocity $W$ is calculated by the standard formula, written in the dimensional form, when using expressions for the derivatives:

$$W = \left( \frac{p_c}{R} \right)^{0.5} \left[ C_{p4} + C_{p5} + C_{p6} + (C_{p3} + C_{p2} + C_{p1}) \right] \frac{1}{(C_{p6} + C_{p5} + C_{p4})} \sqrt{z_c t/(\omega^2 C_v)}.$$  

### 3. Calculation results on heat capacity and sound velocity

We should note that the experimental and tabular data on $C_v$ [19–23] and sound velocity $W$ [1, 24–27] for CO$_2$ on isochores and isotherms (with the exception of the approximation formula for $C_v,_{\text{id}}$) were used only for comparison with the $C_v$ and $W$ values obtained through calculation by formulas (4–7).

Good agreement of calculated $C_v$ curves along the experimental isotherms at $T > T_c$ is shown in figure 1 in comparison with the available data [22, 23] at $\omega > 1$ ($\Delta \rho > 0$), lines $5$ and $6$ show the isotherms of regular contribution of $C_v,_{\text{reg}} (5)$ in the distance (323.087 K) and near (304.14 K) $T_c$.

Calculation of $C_v (\tau)$ along the critical isochore by equation (4) showed complete agreement with experimental data on the near-critical isochores [19, 20] (figure 2). The dashed line shows the course of the regular part $C_v,_{\text{reg}}$.

**Figure 1.** Calculated curves of heat capacity $C_v$ along isotherms at $T > T_c$. Experiment: ●, 323.087 K; □, 308.092 K, [22]; ○, 305.092 K, [23]; calculation: 1 – 323.087 K, 2 – 308.092 K, 3 – 305.092 K, 4 – 304.14 K; 5, 6 – $C_v,_{\text{reg}} (5)$ at $T = 323.087$ K (dashed line) and 304.14 K (thin line).

**Figure 2.** The heat capacities $C_v$ for CO$_2$ along near-critical isochores. Experiment: ●, 468.57 kg/m$^3$, Beck at al. [19]; □, 467.5 kg/m$^3$, Δ, 470.1 kg/m$^3$, ×, 461.2 kg/m$^3$, Abdulagatov et al. [20]. Calculation of $C_v (4)$: ——, 470.1 kg/m$^3$; ——, 467.5 kg/m$^3$; ——, $C_v,_{\text{reg}} (5)$ at $\rho = \rho_c$.
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Figure 3. Heat capacity $C_v$ on isochores in the region of liquid state of CO$_2$ at $\rho > \rho_c$. Experiment: ○ - 549.79 kg/m$^3$, [19]; ▲ - 533.6 kg/m$^3$, ● - 615.4 kg/m$^3$, [21]; calculated curves: 1 - 549.79 kg/m$^3$, 2 - 533.6 kg/m$^3$, 3 - 615.4 kg/m$^3$.

Figure 4. Single-phase heat capacity $C_v$ along binodal of CO$_2$: ----, calculation by (4), this work; --, values calculated by EoS [1]; ---, calculation by (4) using CES with 8 - constant regular part [7]; × - liquid, Δ - gas, the data [24]; ●, [21].

Figure 5. Behavior of sound velocity $W$ (7) (-----) on the branches of boundary curve in comparison with reference data (-----) of [1].

Figure 6. Sound velocity $W$ vs. pressure (up to 100 MPa). Calculated curves: 1 - 373.15 K; 2 - 348.15 K; 3 - 323.15 K; 4 - 304.25 K; 5 - 298.15 K. Experiment: Δ - [25]; ○ - [26]; + - [27].

The calculated $C_v$ (4) curves along the isochores at $\rho > \rho_c$ are compared with the available data from [19, 21] in figures 3. A more rapid increase in experimental $C_v$ as compared to the calculation, when $\tau$ approaches zero, may be caused by the beginning of phase separation due to the temperature difference necessary for $C_v$ measurement.

The behavior of calculated $C_v$ (4) along the experimental CO$_2$ binodal [1] is shown in figure 4 in comparison with tabulated data on $C_v$ of Span and Wagner [1]. The difference in the behavior of curves is observed in the binodal region adjacent to the critical point, which is caused by inclusion of the singular contribution to $C_v$ by the scaling theory in comparison with calculation by multi-constant regular EoS [1].

Sound velocities $W$, calculated by (7) along the gas and liquid branches of the boundary curve (figure 5, solid lines), show a complete coincidence on the gas branch and a slight difference from the reference data [1] on the liquid branch in the regular region (thin lines). The solid lines in figure 6 show the results of calculating $W$ as a function of pressure by (7) along isotherms, for which the experimental data are available in relatively narrow pressure ranges [25–27].

It is obvious that the calculated and experimental values coincide both for $p$ of up to 10 MPa and for $p > 50$ MPa, the calculation is also performed in the range of 10 MPa < $p$ < 50 MPa, where there is
no data on the sound velocity. Curve 4 represents calculation at $T = 304.25 \text{ K}$ (near $T_c$), where experimental data are absent. At $T = 298.15 \text{ K}$ (below $T_c$, curve 5), the calculated curve ends at the points on the branches of the boundary curve. At that, data of [25–27] were not involved to obtain the coefficients of CES (1).

4. Conclusion
We propose a new approach that allows us to calculate the thermodynamic properties from a combined EoS with a small number of adjusting constants, for which only $p$, $\rho$, $T$-data are needed, in contrast to the known multi-constant crossover equations of state, which require all available data to determine their parameters. Using the thermal combined EoS the unified description of the thermal and caloric properties of CO$_2$ is proposed. The $p,\rho,T$-data were described in gas and liquid states from the triple point to supercritical temperatures with a pressure error of $\sim 0.9\%$. Heat capacity $C_v$ and sound velocity in a wide range of parameters in single-phase state, including the critical region, were calculated. The calculated curves of heat capacity $C_v$, show good agreement with experimental data, with deviations in the range of 5% - 8% in different areas of the state. The calculated sound velocity coincides within the experimental error with the known data. The proposed combined EoS makes it possible to develop the reference tables on the thermodynamic properties of CO$_2$.

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