AN ACCURATE EQUATION OF STATE FOR CARBON DIOXIDE

FENG-HSIN HUANG, MENG-HUI LI, LLOYD L. LEE
AND KENNETH E. STARLING
School of Chemical Engineering and Materials Science,
University of Oklahoma, Norman, Oklahoma 73019, U.S.A.
FRANK T. H. CHUNG
National Institute of Petroleum and Energy Research,
Bartlesville, Oklahoma 74005, U.S.A.

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An equation of state for carbon dioxide is developed here that yields high accuracy in P-V-T calculations over wide ranges of temperatures (216–423 K) and pressures (to 310.3 MPa). It is particularly accurate around the critical region due to the use of “nonanalytical” terms to model the critical isotherm. Thus it is suited to applications in supercritical states. The density calculation is reliable to within 0.1–0.2% outside the critical region, and to within 1% near the critical point. The equation has also been tested for vapor pressure and enthalpy calculations (with deviations less than 0.06%, and 2–5 J/g, respectively). Comparison with a number of existing equations of state shows that the present equation is more dependable.

Currently, carbon dioxide is extensively used in enhanced oil recovery, food industry, and refrigeration processes. It is daily transmitted by pipelines over broad geographical areas. The large-scale use of CO₂ has prompted more careful examination of existing methods of predicting its physical properties. For efficient process design and engineering calculations better and more accurate correlations of P-V-T and thermal properties are needed. Different processing needs (e.g. refrigeration, natural gas processing and beverage carbonation) put different emphases on the state conditions and properties of CO₂ required. The cryogenic conditions are important for refrigeration, while the critical region is important for supercritical extraction. Pipeline transmission requires accurate high-pressure properties. And carbonation processes need good solubility data. It is desirable to have a single equation covering all these regions and at the same time giving accurate predictions.

No simple equation in the literature has been able to describe the entire fluid regime of CO₂ with high accuracy, especially in the critical region. Some of the most used equations are the Bender equation and Altunin-Gadetski equation (IUPAC). There are a few caveats that must be noted in advance before developing such an equation. First, the behavior of gases in the critical region is nonclassical, i.e. no analytic function exists that is able to follow the critical fluctuations. Secondly, the equation developed cannot be more accurate than the available experimental data. If the best available data are in error by (±)0.1%, the equation developed cannot exceed this accuracy. There is an extensive review of the experimental information up to 1976 in IUPAC. We list the sources of experimental data used in this work in Table 1. They have been evaluated at the University of Oklahoma. These data were used in the development of the present equation of state.

Our equation is a combination of an analytical part, similar to the form used by Bender, and a nonanalytical part, in the form of Wagner's functions:

\[ Z = \frac{P}{\rho RT} = 1 + b_2 \rho^2 + b_3 \rho^3 + b_4 \rho^4 + b_5 \rho^5 + \frac{b_7 \rho^6}{\exp[-c_21(A T)^2]} + \frac{b_8 \rho^8}{\exp[-c_21(A T)^2]} + \frac{b_9 \rho^9}{\exp[-c_21(A T)^2]} + \frac{b_{10} \rho^{10}}{\exp[-c_21(A T)^2]} \]

where the reduced temperature and density are

\[ T' = \frac{T}{T_c}, \quad \rho' = \frac{\rho}{\rho_c}, \quad A T = 1 - T' \quad \text{and} \quad \Delta \rho = 1 - 1/\rho'. \]

The parameters \( b_2, b_3, \ldots, b_8 \) are functions of temperature (see Table 2). The last three terms are the “nonanalytical” terms used to reproduce the critical isotherm. We note that the term “nonanalyticity” is used to denote the critical fluctuations exhibited by the scaled variables \( \Delta \rho \) and \( A T \) in the...
Table 1. Selected data used to evaluate the constants in the equation of state

<table>
<thead>
<tr>
<th>Data source</th>
<th>Property</th>
<th>Temp. range [K]</th>
<th>Pres. range [MPa]</th>
<th>No. of points</th>
</tr>
</thead>
<tbody>
<tr>
<td>Michels et al.17) (1937)</td>
<td>Vap. pres.</td>
<td>276-304.2</td>
<td>3.75-7.38</td>
<td>10</td>
</tr>
<tr>
<td>Michels et al.16) (1950)</td>
<td>Vap. pres.</td>
<td>217-276.2</td>
<td>0.53-3.77</td>
<td>19</td>
</tr>
<tr>
<td>Michels and Michels14) (1934a)</td>
<td>P-V-T</td>
<td>276.3-423.3</td>
<td>1.68-24.57</td>
<td>190</td>
</tr>
<tr>
<td>Michels et al.15) (1935b)</td>
<td>P-V-T</td>
<td>276.2-423.3</td>
<td>7.57-315.9</td>
<td>140</td>
</tr>
<tr>
<td>Michels et al.17) (1937)</td>
<td>P-V-T (Critical)</td>
<td>276.0-313.2</td>
<td>3.68-9.98</td>
<td>156</td>
</tr>
<tr>
<td>Vargaftik18) (1975)</td>
<td>P-V-T (Liquid)</td>
<td>220.0-320.0</td>
<td>2.0-60.0</td>
<td>89</td>
</tr>
<tr>
<td>Din3) (1956)</td>
<td>P-V-T (Gas)</td>
<td>193.2-263.2</td>
<td>0.05-2.53</td>
<td>57</td>
</tr>
<tr>
<td>Din3) (1956)</td>
<td>Enthalpy departure</td>
<td>263.2-413.2</td>
<td>2.83-50.67</td>
<td>39</td>
</tr>
</tbody>
</table>

Table 2. Constants Ci and reduction parameters* to be used in Eq. (1)

<table>
<thead>
<tr>
<th>i</th>
<th>Cl</th>
<th>i</th>
<th>Ci</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.376194</td>
<td>15</td>
<td>-2.79489</td>
</tr>
<tr>
<td>2</td>
<td>0.118836</td>
<td>16</td>
<td>5.62393</td>
</tr>
<tr>
<td>3</td>
<td>-3.04379</td>
<td>17</td>
<td>-2.93831</td>
</tr>
<tr>
<td>4</td>
<td>2.727453</td>
<td>18</td>
<td>0.988759</td>
</tr>
<tr>
<td>5</td>
<td>-1.23863</td>
<td>19</td>
<td>-3.04711</td>
</tr>
<tr>
<td>6</td>
<td>0.250442</td>
<td>20</td>
<td>2.32316</td>
</tr>
<tr>
<td>7</td>
<td>-0.115350</td>
<td>21</td>
<td>1.07379</td>
</tr>
<tr>
<td>8</td>
<td>0.675104</td>
<td>22</td>
<td>-0.599724E-4</td>
</tr>
<tr>
<td>9</td>
<td>0.198861</td>
<td>23</td>
<td>0.85339E-4</td>
</tr>
<tr>
<td>10</td>
<td>0.216124</td>
<td>24</td>
<td>0.316418E-2</td>
</tr>
<tr>
<td>11</td>
<td>-0.583148</td>
<td>25</td>
<td>10.</td>
</tr>
<tr>
<td>12</td>
<td>0.119747E-1</td>
<td>26</td>
<td>50.</td>
</tr>
<tr>
<td>13</td>
<td>0.537278E-1</td>
<td>27</td>
<td>80,000.</td>
</tr>
<tr>
<td>14</td>
<td>0.265216E-1</td>
<td>28</td>
<td>304.19K; ( \rho_c = 10.6340 \text{ g mol/liter} )</td>
</tr>
</tbody>
</table>

\[ T_c = 304.19 \text{ K}, \quad \rho_c = 10634 \text{ kg mol/m}^3 \]

\* \[ b_2 = \left( \frac{C_1}{T} + \frac{C_3}{T^2} + \frac{C_5}{T^3} + \frac{C_7}{T^4} + \frac{C_9}{T^5} \right) \]

Equation (1) is particularly accurate in the critical region. Figure 4 shows the agreement with the data of Michels17) (○) and Wentorf19) (×) on the critical isotherm. Three other equations of state, i.e. Bender,3) Benedict-Webb-Rubin4) (BWR), and Martin-Hou,12) are included for comparison. While Bender’s and exponents. This is to be distinguished from the exponentials in the original Bender equation in terms of ordinary variables (\( \rho' \) and \( T' \)). All 27 coefficients were determined through the use of a nonlinear regression subroutine by fitting the formula to the \( P-V-T \), vapor pressure and thermal data. (We have also derived the fugacity and enthalpy expression from (1). The results are given in Appendix. Detailed information is available elsewhere [Huang7]). In addition, Eq. (1) is constrained to satisfy the critical conditions: \( \frac{\partial P}{\partial \rho} \bigg|_{T_c, \rho_c} = 0 \), and \( \frac{\partial^2 P}{\partial \rho^2} \bigg|_{T_c, \rho_c} = 0 \) at the critical point of carbon dioxide (\( T_c = 304.19 \text{ K}, \quad \rho_c = 10.6340 \text{ g mol/liter} \)). The range of pressures tested reaches 400 MPa.9) The temperatures span the gamut from 216.57 K (triple point) to 1280 K.10) Figure 1 depicts the range of \( P-T \) states used to develop the equation. We divide the fluid range of \( CO_2 \) according to Bender into three regions as I, II, and III (Fig. 2): region I is the dilute (gas) region, region II the critical region and region III the dense fluid (or liquid) region. The accuracy of prediction is summarized in Table 3 for all three regions. In region I the accuracy of pressure calculation is within 0.1% (in average absolute deviations, or AAD), in region II, 0.1%, and in region III, 1%. For density calculations, the accuracy is 0.16% in region I, 0.9% in region II and 0.1% in region III. The predictive capabilities of Eq. (1) are noted in the remarkable agreement of calculated densities in the critical region (II), where physically a small change in pressure can cause vast changes in density. Without the Wagner functions, the best the remainder analytic equation can do is 2% in AAD (for 113 data points) together with a maximum deviation of 21%. With the Wagner corrections, the deviation is cut in half, with a maximum error of only 5.3%. Also note that in the liquid region small changes in density can give rise to large pressure variations. Thus the density predictions (0.1% in error) are far superior to the pressure predictions (1% in this region). Figure 3 gives the \( P-\rho \) diagram for nine isotherms. The lines are obtained from our equation while the points represent experimental data. Again we observe the close agreement with data over wide ranges of pressures and temperatures.
Martin-Hou's equations are fairly reliable, the present equation is more accurate. Our equation is able to follow the "flatness" of the $P_\rho$ curve near the critical point. This is attributed to the Wagner terms. Equation (1) is extremely accurate in vapor pressure predictions, with 0.066% AAD based on the data of Michels, from near the triple point (216.58 K) to the critical point (304.19 K). (See Table 4). The vapor pressure calculations were based on matching the pressure, temperature and fugacities of both vapor and liquid phases. In practice, this procedure is time-consuming. We have thus fitted the vapor pressure

\begin{table}[h]
\centering
\caption{Prediction of $P-V-T$ property using Eq. (1)}
\begin{tabular}{lcc}
\hline
\multicolumn{1}{c}{Property} & \multicolumn{2}{c}{Abs. deviation* [\%]} \\
\hline
& \multicolumn{1}{c}{Eq. (1)} & \multicolumn{1}{c}{Eq. (1) without correction terms} \\
\hline
\text{Region I} & & \\
\text{(Gas)} & & \\
\text{No. of points} & & 284 \\
\text{Pressure:} & & \\
\text{Average} & 0.11 & 0.11 \\
\text{Maximum} & 0.90 & 0.90 \\
\text{Density:} & & \\
\text{Average} & 0.16 & 0.16 \\
\text{Maximum} & 0.98 & 0.98 \\
\hline
\text{Region II} & & \\
\text{(Critical)} & & \\
\text{No. of points} & & 113 \\
\text{Pressure:} & & \\
\text{Average} & 0.10 & 0.11 \\
\text{Maximum} & 1.19 & 1.19 \\
\text{Density:} & & \\
\text{Average} & 0.91 & 2.06 \\
\text{Maximum} & 5.30 & 21.48 \\
\hline
\text{Region III} & & \\
\text{(Liquid)} & & \\
\text{No. of points} & & 228 \\
\text{Pressure:} & & \\
\text{Average} & 1.01 & 1.01 \\
\text{Maximum} & 14.26 & 14.26 \\
\text{Density:} & & \\
\text{Average} & 0.10 & 0.10 \\
\text{Maximum} & 0.43 & 0.43 \\
\hline
\end{tabular}
\end{table}

* Deviation [\%] = 100 * (Calc. - Exp.) / Exp.
Table 4. Prediction of saturated properties using Eq. (1)

<table>
<thead>
<tr>
<th>Property</th>
<th>Data source</th>
<th>Temp. range [K]</th>
<th>Pres. range [MPa]</th>
<th>No. of points</th>
<th>Abs. dev. [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Avg.</td>
</tr>
<tr>
<td>Vapor pressure</td>
<td>Michels(^{16,17}) (1937, 1950)</td>
<td>217.1-304.2</td>
<td>0.53-7.37</td>
<td>29</td>
<td>0.066</td>
</tr>
<tr>
<td></td>
<td>Meyers(^{13}) (1933)</td>
<td>216.6-304.2</td>
<td>0.52-7.37</td>
<td>17</td>
<td>0.040</td>
</tr>
<tr>
<td></td>
<td>Vargaftik(^{18}) (1975)</td>
<td>216.6-304.2</td>
<td>0.52-7.37</td>
<td>44</td>
<td>0.048</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>90</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.35</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>56.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2.07</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1.27</td>
</tr>
<tr>
<td>Saturated liquid density</td>
<td>Michels(^{13}) (1937)</td>
<td>276-304.2</td>
<td>3.75-7.37</td>
<td>9</td>
<td>1.36</td>
</tr>
<tr>
<td></td>
<td>Din(^{5}) (1956)</td>
<td>216.6-304.2</td>
<td>0.52-7.21</td>
<td>19</td>
<td>0.27</td>
</tr>
<tr>
<td></td>
<td>Vargaftik(^{18}) (1975)</td>
<td>216.6-303</td>
<td>0.52-7.18</td>
<td>43</td>
<td>0.36</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
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<td>71</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>5.62</td>
</tr>
<tr>
<td>Saturated vapor density</td>
<td>Michels(^{13}) (1937)</td>
<td>276-304.2</td>
<td>3.75-7.37</td>
<td>9</td>
<td>0.82</td>
</tr>
<tr>
<td></td>
<td>Din(^{5}) (1956)</td>
<td>216.6-304.2</td>
<td>0.52-7.21</td>
<td>19</td>
<td>0.59</td>
</tr>
<tr>
<td></td>
<td>Vargaftik(^{18}) (1975)</td>
<td>216.6-303</td>
<td>0.52-7.18</td>
<td>43</td>
<td>0.36</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>71</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>5.22</td>
</tr>
</tbody>
</table>

Equation (1) was used to calculate the enthalpy of carbon dioxide. Figure 6 gives the pressure-enthalpy diagram. Agreement with Vargaftik's\(^{18}\) compiled data is good. We have also made comparison with the data of Koppel and Smith\(^{11}\) and Din.\(^{5}\) Similar results are obtained. The average error is between 2–5J/g over wide ranges of pressures (to 60 MPa) and temperatures (243 K–413 K).

Other properties such as heat of vaporization, saturated vapor and liquid densities, entropy, and second virial coefficient are also calculated\(^{7}\) and compared with experimental data. All comparison
Table 5. Comparison of Eq. (1) with other equations of state on $P$-$V$-$T$ property predictions

<table>
<thead>
<tr>
<th>Region</th>
<th>Property</th>
<th>Abs. deviation [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>BWR</td>
<td>IUPAC</td>
</tr>
<tr>
<td></td>
<td>No. of points</td>
<td></td>
</tr>
<tr>
<td>I (Gas)</td>
<td>Pressure:</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Average 0.21 0.05 0.14 0.11 0.11 0.11</td>
<td>284</td>
</tr>
<tr>
<td></td>
<td>Maximum 0.87 0.54 0.51 0.65 0.90 0.90</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Density:</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Average 0.37 — 0.22 0.18 0.16</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Maximum 2.30 — 1.08 1.26 0.98</td>
<td></td>
</tr>
<tr>
<td>II (Critical)</td>
<td>Pressure:</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Average 0.50 0.24 0.20 0.22 0.10</td>
<td>113</td>
</tr>
<tr>
<td></td>
<td>Maximum 1.86 1.19 1.10 1.83 1.19</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Density:</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Average 3.90 — 2.15 2.98 0.91</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Maximum 18.77 — 20.79 27.97 5.30</td>
<td></td>
</tr>
<tr>
<td>III (Liquid)</td>
<td>Pressure:</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Average — 1.00 — 1.28 1.28 1.01</td>
<td>228</td>
</tr>
<tr>
<td></td>
<td>Maximum — 12.36 — 30.32 30.32 14.26</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Density:</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Average 3.85 — — 0.12 0.10</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Maximum 7.56 — — 0.78 0.43</td>
<td></td>
</tr>
</tbody>
</table>

Fig. 5. Experimental and calculated supercritical isotherms for CO$_2$. Solid lines, this work; dotted lines, Bender equation; points, experimental data.

Fig. 6. Pressure-enthalpy diagram for CO$_2$. Curves, this work; O, experimental data (Vargaftik, 1975).

The enthalpy departure is related to the equation of state by the following equation:

$$\frac{H - H^0}{RT} = (Z - 1) - \int_0^{\rho'} T \left( \frac{\partial^2 \rho}{\partial T^2} \right) \frac{d\rho}{\rho'} \quad (A-1)$$

When Eq. (1) is applied to the above equation, the expression for the enthalpy departure has the following form:

have shown the superiority of the present equation.

Appendix

Expressions for the enthalpy, entropy, fugacity and other properties can be derived from the usual thermodynamic relationships.
\[
\frac{H - H^0}{RT} = (Z - 1) + \left( \frac{C_2}{T} + \frac{C_3}{T^2} + \frac{C_4}{T^3} + \frac{C_5}{T^4} + \frac{C_6}{T^5} \right) \rho^0 \\
+ \frac{1}{2} \left( \frac{C_8}{T^2} + \frac{C_9}{T^3} \right) \rho^2 + \frac{1}{3} \left( \frac{C_{10}}{T} \right) \rho^3 \\
+ \frac{1}{4} \left( \frac{C_{13}}{T^4} \right) \rho^4 + \frac{1}{5} \left( \frac{C_{14}}{T} \right) \rho^5 \\
+ \frac{1}{2C_2^3} \left( \frac{C_{18} + 4C_{19} + 5C_{20}}{T^4} \right) \rho^6
\]

\[x \left[ 1 - \left( 1 + C_{21} \rho^2 \right)^3 \exp\left( -C_{21} \rho^2 \right) \right]
- 2C_{22} C_{21} T' A T \exp\left( -C_{27} (z T')^2 \right) \\
+ \frac{C_{23} C_{22}}{C_{25}} T' A T \exp\left( -C_{25} (\Delta \rho)^2 - C_{27} (A T)^2 \right)
+ \frac{1}{2} \left( \frac{C_8 + C_9}{T^2} \right) \rho^2 + \frac{1}{3} \left( \frac{C_{10} + C_{11}}{T} \right) \rho^3 \\
+ \frac{1}{4} \left( \frac{C_{12} + C_{13}}{T} \right) \rho^4 + \frac{1}{5} \left( \frac{C_{14}}{T} \right) \rho^5 \\
+ \frac{1}{2C_{21}} \left( \frac{C_{15} + 4C_{16} + 5C_{17}}{T^4} \right) \left[ 1 - \exp\left( -C_{21} \rho^2 \right) \right]
+ \frac{1}{2C_{21}} \left( \frac{C_{18} + C_{19} + C_{20}}{T^5} \right) \left[ 1 - (1 + C_{21} \rho^2) \exp\left( -C_{21} \rho^2 \right) \right]
+ C_{22} \rho^2 \left[ -C_{27} (A T)^2 \right] \\
- \frac{C_{24}}{2C_{26}} \exp\left[ -C_{26} (\Delta \rho)^2 - C_{27} (A T)^2 \right]
\]

where \( H \) is the enthalpy of the fluid and \( H^0 \) is the ideal gas-state enthalpy of the fluid at the system temperature.

The thermodynamic relation between the entropy departure and the equation of state is:

\[
S - S^0 = -\ln(\rho RT) - \int_0^\rho \left( \frac{\partial Z}{\partial T} - T \right) \frac{dp'}{p'}
\]

Substituting Eq. (1) into the above equation yields the following expression for the entropy departure:

\[
S - S^0 = -\ln(\rho RT) - \int_0^\rho \left( \frac{C_1 + C_3}{T} + \frac{C_4}{T^2} - \frac{3C_5}{T^3} - \frac{4C_6}{T^4} \right) \frac{dp'}{p'}
\]

\[
+ \frac{1}{2} \left( C_7 - C_8 \right) \rho^2 + \frac{1}{3} \left( C_{10} \rho^3 \right) + \frac{1}{4} \left( C_{12} \rho^4 \right)
+ \frac{1}{2C_{21}} \left( C_{15} + 4C_{16} + 5C_{17} \right) \left[ 1 - \exp\left( -C_{21} \rho^2 \right) \right]
+ \frac{1}{2C_{21}} \left( C_{18} + 4C_{19} + 5C_{20} \right) \left[ 1 - (1 + C_{21} \rho^2) \exp\left( -C_{21} \rho^2 \right) \right]
\]

\[
\times \left[ 1 - (1 + C_{21} \rho^2)^3 \exp\left( -C_{21} \rho^2 \right) \right]
- 2C_{22} (1 + 2C_{25} T' A T) \rho^2 \exp\left( -C_{25} (A T)^2 \right)
+ \frac{C_{23}}{2C_{25}} \left( 1 + 2C_{25} T' A T \right) \exp\left[ -C_{25} (\Delta \rho)^2 - C_{27} (A T)^2 \right]
+ \frac{C_{24}}{2C_{26}} \left( 1 + 2C_{25} T' A T \right) \exp\left[ -C_{26} (\Delta \rho)^2 - C_{27} (A T)^2 \right]
\]

where \( S \) is the entropy of the fluid and \( S^0 \) is the ideal gas-state entropy of the fluid at the system temperature and unit pressure.

Equation (A-4) assumes that at unit pressure the gas is ideal.

For a pure component existing at equilibrium in two phases at a given temperature and pressure, the thermodynamic variable defining equilibrium is the fugacity, which must be the same for both phases. The fugacity of a pure substrate is related to the equation of state by

\[
\ln f = (Z - 1) + \ln(\rho RT) + \int_0^\rho \left( \frac{Z - 1}{\rho} \right) \frac{dp'}{p'}
\]

The fugacity can also be expressed in terms of enthalpy departure and entropy departure by the following relation:

\[
\ln f = \frac{H - H^0}{RT} - \frac{S - S^0}{R}
\]

When Eq. (1) is used in Eq. (A-5) or both Eqs. (A-2) and (A-4) are substituted in the above equation, the expression for the fugacity has the following form:

\[
\ln f = (Z - 1) + \ln(\rho RT) + \left( \frac{C_1 + C_3}{T} + \frac{C_4}{T^2} + \frac{C_5}{T^3} + \frac{C_6}{T^4} \right) \rho^0
\]

\[
+ \frac{1}{2} \left( \frac{C_8}{T^2} + \frac{C_9}{T^3} \right) \rho^2 + \frac{1}{3} \left( \frac{C_{10} + C_{11}}{T} \right) \rho^3
\]

\[
+ \frac{1}{4} \left( \frac{C_{12} + C_{13}}{T} \right) \rho^4 + \frac{1}{5} \left( \frac{C_{14}}{T} \right) \rho^5
\]

\[
+ \frac{1}{2C_{21}} \left( \frac{C_{15} + 4C_{16} + 5C_{17}}{T^4} \right) \left[ 1 - \exp\left( -C_{21} \rho^2 \right) \right]
+ \frac{1}{2C_{21}} \left( \frac{C_{18} + C_{19} + C_{20}}{T^5} \right) \left[ 1 - (1 + C_{21} \rho^2) \exp\left( -C_{21} \rho^2 \right) \right]
\]

\[
+ C_{22} \rho^2 \left[ -C_{25} (A T)^2 \right] \\
- \frac{C_{24}}{2C_{26}} \exp\left[ -C_{26} (\Delta \rho)^2 - C_{27} (A T)^2 \right]
\]

The above three equations assume that the gas is ideal at unit pressure, so that the reference fugacity \( f^0 = 1.0 \).

Literature Cited

GAS ABSORPTION IN A MULTI-STAGE GAS-LIQUID SPOUTED VESSEL

MASABUMI NISHIKAWA, KAZUHIRO SHIINO, TAKASHI KAYAMA, SHIGERU NISHIOKA AND KENJI HASHIMOTO
Department of Nuclear Engineering, Kyushu University, Fukuoka 812

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Introduction

In the gas-liquid spouted vessel, where power is supplied from a pump to the liquid and the gas is introduced at a nozzle attached to the bottom of the vessel, gas bubbles are finely broken at the nozzle outlet and dispersed into the vessel as reported by Nishikawa et al.8–10) Due to the large liquid energy concentrated at the nozzle and the strong turbulence in the vessel, the liquid-phase spouted vessel is highly effective in fluidizing or dissolving solid particles6,7) and dispersing gas bubbles because of the choking effect at the outlet of a spouting nozzle.8,10) It was also reported by Nishikawa et al. that a large gas holdup and a large capacity coefficient were easily obtained in the gas-liquid or the solid-gas-liquid spouted vessel.10) However, in the calm uniform-flow section of a large-scale gas-liquid spouted vessel some bubbles eventually coalesce, lowering local gas holdup and consequently local capacity coefficient. This effect can be excluded by proper placing of spouting nozzles or multi-stage spouted vessels. This report is about gas holdup, bubble size and gas absorption capacity coefficient in a multi-stage gas-liquid spouted vessel where the calm uniform-flow section of the vessel is divided into several sections by perforated plates, and various performances observed for the multi-stage spouted vessel are compared with those obtained for the ordinary single-stage spouted vessel or the bubbling column.

1. Experimental Apparatus

A sketch of the experimental apparatus used in this study is shown in Fig. 1. The process liquid is circulated through a pump from the overflow section to the spouting nozzle attached to the bottom of the vessel. The process gas is supplied from a cylinder to the upper part of the spouting nozzle. The vessel is made of PVC resin of 5 mm thickness and the vessel diameter is 10 or 15 cm. A three-stage vessel with a 60° cone at the bottom is used as for the multi-stage