Thermophysical Properties of Ethane from Cubic Equations of State

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Vapour - liquid equilibrium and thermophysical properties of ethane were predicted, along the saturation curve and in the single-phase region. Five cubic equations of state were used: Soave-Redlich-Kwong (SRK), Peng-Robinson (PR), Schmidt-Wenzel (SW), Treble-Bishnoi-Salim and GEOS3C. A wide comparison with NIST recommended data was made. This study shows that the cubic EOSs lead to reasonable predictions of thermophysical properties of ethane, resting simple enough for applications.

Keywords: equation of state, vapour - liquid equilibrium, thermophysical properties, ethane.

Because ethane is both an industrially important fluid and the second member of the interesting alkane series, we have considered that it is necessary to examine the possibility to reproduce its PV

The GEOS3C equation of state

The GEOS3C equation of state is a general form [1, 14] for the cubic equations of state with two, three and four parameters:

\[ P = \frac{RT}{V - b} - \frac{a(T)}{(V - d)^2 + c} \]  

The four parameters \(a, b, c, d\) for a pure component are expressed by:

\[ a = a_e \beta(T_e); \quad a_e = \Omega \frac{T_e^2}{P_e}; \quad b = \Omega \frac{RT_e}{P_e}; \quad c = \Omega \frac{T_e^2}{P_e}; \quad d = \Omega \frac{RT_e}{P_e}. \]

The GEOS3C equation is based on the GEOS equation [11] and uses a new temperature function [11]:

\[ \beta(T_e) = 1 + C_1 y + \frac{C_2 y^2}{2} + \frac{C_3 y^3}{3} \quad \text{for } T_e \leq 1 \]  

\[ \beta(T_e) = 1 + C_1 y \quad \text{for } T_e > 1 \]

The expressions of the parameters \(\Omega, \Omega, \Omega, \Omega\) are:

\[ \Omega = (1 - B)^3; \quad \Omega = Z_e - B; \]  

\[ \Omega_e = (1 - B)^2 (B - 0.25); \quad \Omega_e = Z_e - 0.5(1 - B) \]  

\[ B = \frac{1 + C_1}{\alpha_e + C_1} \quad \alpha_e = \text{Riedel's criterion} \]  

Riedel's criterion, \(\alpha_e\), is calculated using the acentric factor from the equation:

This study shows that the cubic EOSs lead to reasonable predictions of thermophysical properties of ethane, resting simple enough for applications.
\[ \alpha_c = 5.808 + 4.93w \]  

(10)

In our previous papers the \( C_1, C_2 \) and \( C_3 \) parameters were estimated by constraining the equation of state to reproduce the experimental vapour pressure and liquid volume on the saturation curve. In this work we used the values of \( C_1, C_2 \) and \( C_3 \) parameters from a correlation of optimized parameters with acentric factor for the series of n-alkanes from methane to dodecane:

\[ C_1 = -0.4326 \alpha^2 + 0.9843 \alpha + 0.1229 \]  

(11)

\[ C_2 = 0.1054 \alpha^2 + 1.3876 \alpha + 0.1986 \]  

(12)

\[ C_3 = 0.1986 \alpha^2 - 1.4557 \alpha + 0.0854 \]  

(13)

As pointed out previously, the relations (7-9) are general forms for all the cubic equations of state with two, three and four parameters [4, 5, 15]. Our software used in calculations is based on these equations for the reduction of GEOS to different cubic EOS from the literature. This is the meaning of the statement “general cubic equation of state” used for GEOS.

To obtain the parameters of the SRK EOS from the equations (7-9) we set the following restrictions: \( \Omega_c = -(\Omega_d/2)^2 \) and \( \Omega_d = -\Omega_c/2 \). It follows:

\[ \Omega_c = (1-B)^2(B-0.25) = -(Z_c - B)^2/4; \]  

(14)

\[ \Omega_d = Z_c - 0.5(1-B) = -(Z_c - B)/2. \]  

(15)

It results \( Z_c \) (SRK) = 1/3, and the relation for \( B \) (SRK):

\[ B = 0.25 - \frac{1}{36} \left( \frac{1-3B}{1-B} \right)^2; \]  

(16)

Solving iteratively this equation gives \( B \) (SRK) = 0.2467, and correspondingly: \( \Omega_c \) (SRK) = \((1-B)^2 = 0.42748 \) and \( \Omega_d \) (SRK) = \( Z_c - B = 0.08664 \).

For PR EOS we set the restrictions: \( \Omega_c = -2(\Omega_d)^2 \) and \( \Omega_d = -\Omega_c \). It results:

\[ B = 0.25 - \frac{1}{8} \frac{1-3B}{1-B}; \]  

(17)

\[ Z_c = \frac{1 + B}{4} \]

giving \( B \) (PR) = 0.2296, \( Z_c \) (PR) = 0.3074, \( \Omega_c \) (PR) = 0.45724, \( \Omega_d \) (PR) = 0.0778.

The SW equation general form results from the conditions:

\[ u = -2 \Omega_c/\Omega_d; \quad w = \Omega_d/\Omega_d; \]  

(18)

The equations for \( B \) (SW) and \( Z_c \) (SW) are:

\[ B = 0.25 + \frac{u+w+1}{1-4} \frac{1-3B}{1-B}^2; \]  

(19)

\[ Z_c = \frac{B + 1 - 3B}{u+2} \]

The eq. (19) is a general form and the SW EOS is obtained from the conditions \( u+w = 1, \; w = -3\alpha \).

The TBS EOS results from the following conditions:

\[ \Omega_c = (1-B)^2(B-0.25) = -(B_c - B + C_3)^2/2 - D_c^2 \]  

(20)

\[ \Omega_d = Z_c - (1-B)/2 = -(B_c - C_3)/2 \]  

(21)

giving, for optimized \( Z \) (TBS) and \( D_c \) (TBS) parameters, the equation of the \( B \) (TBS):

\[ B = 0.25 + \frac{1}{(1-B)^2} \left( Z_c - B(3Z_c - 1) - (Z_c - (1-B)/2)^2 - D_c^2 \right) \]  

(22)

with the corresponding value for \( \Omega_d \), \( \Omega_c \), \( \Omega_c \), \( \Omega_d \) from equations (7-9).

All equations for \( B \) have been solved iteratively, starting with a zero value of \( B \) in the right hand term. The calculated values \( \Omega_d \), \( \Omega_c \), \( \Omega_d \), \( \Omega_c \) from equations (7-9) for all cubic EOSs are plotted in figure 1. The highest absolute values for all coefficients are those of GEOS. All coefficients, excepting \( \Omega_d \), show a minimum absolute value for SRK equation. The higher value of \( \Omega_d \) for SRK equation is determined by the highest value of the compressibility factor (\( Z_c \)). It must be mentioned that the parameters \( \Omega_d \), \( \Omega_c \), \( \Omega_c \), \( \Omega_d \) for SRK and PR equations have unique values for all substances.

The expressions of the residual departure functions based on GEOS equation may be also used for other cubic equations, which can be converted to the GEOS form.

The following equations for the departure (residual) functions from ideal gas state at the same temperature and pressure were used with the GEOS equation (or GEOS3C) [1,2]:

\[ \Delta U = \left( a - T \frac{\partial a}{\partial T} \right) E \]  

(23)

\[ \Delta H = \left( a - T \frac{\partial a}{\partial T} \right) E + RT(Z - 1) \]  

(24)

\[ \Delta S = -R \ln \left( \frac{V}{V - b} + R \ln Z + \frac{\partial a}{\partial T} \right) E \]  

(25)

\[ \Delta F = RT \ln \left( \frac{V}{V - b} - RT \ln Z - aE \right) \]  

(26)

with
The values of the thermodynamic functions are calculated from:

\[ \Delta G^\circ = RT \ln \frac{V}{V-b} + RT(Z-1) - RT \ln Z - aE \]  

\[ \ln \varphi = \ln \frac{V}{V-b} + Z - 1 - \ln Z - \frac{a}{RT} E \]  

\[ \Delta C_T^\circ = \left[ \frac{\partial (\Delta U^\circ)}{\partial T} \right]_T = T \frac{\partial^2 a}{\partial T^2} E \]  

\[ \Delta C_v^\circ = \Delta C_v^\circ - T \left[ \frac{\partial (\Delta P)}{\partial T} \right]_T \]  

\[ \gamma = \frac{C_v}{C_p} \]  

\[ W_s = -\frac{C_v - V^2}{M} \left[ \frac{\partial P}{\partial V} \right] \gamma^{0.5} \]  

\[ \mu_{IR} = \frac{1}{C_1} \left[ f \left( \frac{\partial V}{\partial T} \right) - V \right] \]  

with

\[ E = \frac{1}{2\sqrt{c}} \ln \frac{V-d+\sqrt{c}}{V-d-\sqrt{c}} \]  

\[ E = \frac{1}{\sqrt{c}} \operatorname{arctg} \frac{\sqrt{c}}{V-d} \]  

\[ E = \frac{1}{V-d} \]  

where \( Y^* \) is the ideal gas contribution, and \( \Delta Y^\circ \) is the residual (departure) function at the same temperature and pressure calculated from the equation of state.

**Results and discussions**

Five equations of state have been used in this work, to calculate the phase equilibrium and the thermophysical properties for ethane: Soave-Redlich-Kwong (SRK), Peng-Robinson (PR), Schmidt-Wenzel (SW), Treble-Bishnoi-Salim (TBS) and GEOS3C. The investigated PVT range covers single-phase (liquid or gas) and two-phase (liquid-vapor) regions, using recommended NIST data as pseudo experimental values. The calculations were made with the software package PHEQ (Phase Equilibria) developed in our laboratory [16].

The values of the parameters \( C_1, C_2, C_3 \) of the GEOS3C equation, the critical data and acentric factor for ethane are presented in table 1.

The following thermophysical properties have been predicted: compressibility factor \( (Z) \), enthalpy \( (H) \), enthalpy of vaporization \( (\Delta_vH) \), entropy \( (S) \), heat capacity at constant pressure \( (C_p) \), heat capacity at constant volume \( (C_v) \), heat capacity ratio \( (C_p/C_v) \), speed of sound \( (W_s) \), fugacity coefficient \( (\varphi) \), Joule-Thomson coefficient \( (JT) \). No data on these thermophysical properties were regressed in this work. The ideal gas contribution to the thermophysical properties was calculated using the heat capacity functions recommended in [17].

The following observations can be made on the basis of the results of the tables 2-4.

The vapour pressures and saturated volumes are better reproduced by TBS and GEOS3C, compared to the results obtained using other equations. The saturated liquid volumes calculated with the SRK, and PR equations have higher deviations relative to NIST recommended data.

The advantage of the GEOS3C equation is that the liquid volume is improved by the parameter \( C_1 \), without translation [2].

The GEOS3C equation predicts better results for the enthalpies and the entropies in the both saturated liquid and vapour phase. The enthalpy of vaporization is well represented by all EOSs.

The difference in performance between the EOSs is less noticeable for other thermophysical properties on the saturation curve and in the single phase region: heat capacities, adiabatic coefficient, speed of sound and Joule Thomson \( (JT) \) coefficient. The GEOS3C equation predict better the isobaric heat capacity and the \( JT \) coefficient in

<table>
<thead>
<tr>
<th>Component</th>
<th>( C_1 )</th>
<th>( C_2 )</th>
<th>( C_3 )</th>
<th>( T_C ) (K)</th>
<th>( P_C ) (bar)</th>
<th>( Z_c )</th>
<th>( \omega )</th>
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<td>Ethane</td>
<td>0.2163</td>
<td>0.3374</td>
<td>-0.0572</td>
<td>305.3</td>
<td>48.7</td>
<td>0.2793</td>
<td>0.0993</td>
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</table>

**Table 1** VALUES OF \( C_1, C_2, C_3 \) PARAMETERS FOR ETHANE OBTAINED FROM Eqs (11-13). CRITICAL DATA AND ACENTRIC FACTOR FROM NIST DATABASE [12]

<table>
<thead>
<tr>
<th>EOS</th>
<th>( P^0 )</th>
<th>( V^0 )</th>
<th>( T^0 )</th>
<th>( \Delta_{molar}H )</th>
<th>( H^f ) (kJ/kg)</th>
<th>( H^f ) (kJ/kg)</th>
<th>( S^f ) (kJ/kg/K)</th>
<th>( S^f ) (kJ/kg/K)</th>
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<tbody>
<tr>
<td>SRK</td>
<td>4.73</td>
<td>10.9</td>
<td>19.2</td>
<td>7.36</td>
<td>10.07</td>
<td>13.13</td>
<td>0.06</td>
<td>0.08</td>
</tr>
<tr>
<td>PR</td>
<td>5.55</td>
<td>10.5</td>
<td>19.2</td>
<td>7.36</td>
<td>11.91</td>
<td>6.03</td>
<td>0.07</td>
<td>0.03</td>
</tr>
<tr>
<td>SW</td>
<td>1.46</td>
<td>3.4</td>
<td>3.35</td>
<td>1.7</td>
<td>8.93</td>
<td>7.72</td>
<td>0.06</td>
<td>0.06</td>
</tr>
<tr>
<td>TBS</td>
<td>1.69</td>
<td>0.89</td>
<td>1.13</td>
<td>1.61</td>
<td>9.81</td>
<td>6.47</td>
<td>0.06</td>
<td>0.04</td>
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<tr>
<td>GEOS3C</td>
<td>1.89</td>
<td>2.07</td>
<td>2.14</td>
<td>4.48</td>
<td>6.89</td>
<td>5.76</td>
<td>0.04</td>
<td>0.04</td>
</tr>
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**Table 2** PVT AND THERMODYNAMIC FUNCTION DEVIATIONS ON THE SATURATION CURVE FOR ETHANE. TEMPERATURE RANGE (K): 90.3–305.3. PRESSURE RANGE (BAR): 1.13×10^4–48.7. NUMBER OF DATA POINTS: 201

<table>
<thead>
<tr>
<th>EOS</th>
<th>( C_1 )</th>
<th>( C_2 )</th>
<th>( C_p/C_v )</th>
<th>( C_p/C_v )</th>
<th>( W_s )</th>
<th>( W_s )</th>
<th>( JT )</th>
<th>( JT )</th>
</tr>
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<tbody>
<tr>
<td>SRK</td>
<td>13.62</td>
<td>17.19</td>
<td>9.63</td>
<td>5.86</td>
<td>14.3</td>
<td>3.53</td>
<td>117.42</td>
<td>89.67</td>
</tr>
<tr>
<td>PR</td>
<td>15.56</td>
<td>17.65</td>
<td>8.7</td>
<td>5.99</td>
<td>14.49</td>
<td>2.88</td>
<td>104.35</td>
<td>89.13</td>
</tr>
<tr>
<td>SW</td>
<td>14.92</td>
<td>17.29</td>
<td>9.58</td>
<td>5.98</td>
<td>14.2</td>
<td>3.5</td>
<td>110.2</td>
<td>89.1</td>
</tr>
<tr>
<td>TBS</td>
<td>13.04</td>
<td>17.72</td>
<td>8.99</td>
<td>6.08</td>
<td>15.08</td>
<td>2.91</td>
<td>72.81</td>
<td>89.55</td>
</tr>
<tr>
<td>GEOS3C</td>
<td>8.16</td>
<td>18.44</td>
<td>9.73</td>
<td>6.98</td>
<td>43.99</td>
<td>3.84</td>
<td>41.34</td>
<td>89.89</td>
</tr>
</tbody>
</table>

**Table 3** THERMODYNAMIC FUNCTION DEVIATIONS AT SATURATION FOR ETHANE. TEMPERATURE RANGE (K): 90.3–305.3. PRESSURE RANGE (BAR): 1.13×10^4–48.7. NUMBER OF DATA POINTS: 201
the liquid phase, but it predict with large deviations the speed of sound values in the liquid phase.

The AAD\% given in tables 3 and 4 for the JT coefficient in the saturated liquid are relatively high, determined by very small values of the JT coefficients.

The speeds of sound values in liquid phase and in single-phase region, predicted by GEOS3C, have large deviations in comparison with NIST recommended data. The value of $W_s$ (speed of sound) is dependent of both heat capacity ratio and the derivative $\left(\frac{\partial P}{\partial V}\right)$, eq. (32). The GEOS3C equation predicts reasonable the heat capacity ratio, but the derivative $\left(\frac{\partial P}{\partial V}\right)$ has higher deviations relative to NIST equation of state.

Examples of calculated properties are presented in the figures 2-14. Figures 2 and 3 show the pressure – density diagrams for ethane. Points figure NIST data, while the curves are calculated with the GEOS3C and SRK equations, for the saturation region and subcritical and supercritical isotherms. The liquid saturated densities calculated with the GEOS3C equation are in better agreement with the experimental data (NIST), in comparison with the densities calculated with the SW equation.

The calculated enthalpies by GEOS3C and PR equations, on the saturation curve and in the single phase region are shown in figure 4 and figure 5 (points: NIST recommended data). The GEOS3C equation give better predicted values of enthalpies in the entire range of $T$ and $P$.

The pressure – entropy diagrams of ethane calculated by GEOS3C and TBS equations are presented in figure 6. The GEOS3C calculated entropy values are in good agreement with the NIST data. The predictions of TBS equation have higher deviations from the NIST data especially in the liquid region (saturation curve and subcritical isotherms).

The isochoric heat capacity ($C_V$) predictions from GEOS3C, SRK, PR and SW equations, on the saturation curve, are shown in the figure 7. As observed, the NIST isochoric heat capacity shows unusual behaviour, not proved experimentally. The cubic EOSs predict a different form of this curve. As it is known, the cubic EOSs do not predict an infinite value of $C_V$ at critical temperature.

The temperature-isobaric heat capacity diagram (saturation curve) of ethane is presented in figure 8. Points figure NIST data while the curves are calculated with the GEOS3C and SW equations. The values calculated with GEOS3C equation are in better agreement with experimental data in the liquid region. The infinite value of $C_V$ in the critical point is well predicted by GEOS3C.

The figures 9 and 10 show the isotherms for $C_p$ and adiabatic coefficient calculated with GEOS3C equation in comparison with NIST recommended data. The predictions are in good agreement with experimental data especially for the $C_p$ values.

The figures 11 and 12 show the pressure – speed of sound diagram predicted by GEOS and SW equations for ethan, in the entire range of $T$ and $P$. The predicted values are in better agreement with the NIST data for SW equation in the liquid region (table 3).

Figure 13 shows the dependence of derivative $\left(\frac{\partial P}{\partial V}\right)$ of temperature. As can be seen GEOS has the highest value of this derivative in comparison to the other cubic EOSs. This behaviour explains the higher values of predicted speed of sound by GEOS equation in liquid phase (fig. 11). From this analysis, it results that the good correlation of vapour pressure and saturated liquid density does not guarantee accurate values of the derivative $\left(\frac{\partial P}{\partial V}\right)$ in the liquid region.

Joule Thomson coefficient predictions on the saturation curve for ethane by GEOS3C, TBS and SRK equations are plotted in figure 14. The NIST data show an unusual behaviour in the vapour region, which explains the AAD\% (89 \% in table 3) of all cubic EOSs. In the original paper [13], the JT coefficient experimental data were not included in the development of the multiparameter EOS, and the predicted values of this property were not reported.

<table>
<thead>
<tr>
<th>EOS</th>
<th>S</th>
<th>H</th>
<th>Z</th>
<th>$C_p$</th>
<th>$W_s$</th>
<th>$C_p/C_V$</th>
<th>JT</th>
</tr>
</thead>
<tbody>
<tr>
<td>SRK</td>
<td>0.05</td>
<td>7.67</td>
<td>1.77</td>
<td>5.41</td>
<td>4.05</td>
<td>1.85</td>
<td>12.63</td>
</tr>
<tr>
<td>PR</td>
<td>0.08</td>
<td>13.07</td>
<td>2.21</td>
<td>6.74</td>
<td>5.32</td>
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<td>20.07</td>
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<tr>
<td>SW</td>
<td>0.06</td>
<td>15.26</td>
<td>0.71</td>
<td>8.9</td>
<td>4.59</td>
<td>2.47</td>
<td>51.03</td>
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<tr>
<td>TBS</td>
<td>0.05</td>
<td>8.36</td>
<td>1.27</td>
<td>5.61</td>
<td>8.32</td>
<td>1.89</td>
<td>18.03</td>
</tr>
<tr>
<td>GEOS3C</td>
<td>0.05</td>
<td>10.26</td>
<td>2.44</td>
<td>3.86</td>
<td>23.79</td>
<td>2.54</td>
<td>26.11</td>
</tr>
</tbody>
</table>

Table 4

| THERMODYNAMIC FUNCTION DEVIATIONS IN SINGLE-PHASE REGION FOR ETHANE. TEMPERATURE RANGE (K): 100 – 625. PRESSURE RANGE (BAR): 1.0×10⁻³ – 700. NUMBER OF DATA POINTS: 276 |
Fig. 4. Pressure-enthalpy diagram for ethane. Points: NIST data [12]. Lines: prediction with the GEOS3C equation.

Fig. 5. Pressure-enthalpy diagram for ethane. Points: NIST data [12]. Lines: prediction with the PR equation.

Fig. 6. Pressure-entropy diagram for ethane. Points: NIST data [12]. Lines: prediction with the GEOS3C and TBS equations.

Fig. 7. Temperature-isochoric heat capacity diagram (saturation curve) of ethane. Points: NIST data [12]. Lines: prediction with the GEOS3C, SW, PR and SRK equations.

Fig. 8. Temperature-isobaric heat capacity diagram (saturation curve) of ethane. Points: NIST data [12]. Lines: prediction with the GEOS3C and SW equations.

Fig. 9. Pressure-isobaric heat capacity diagram (isotherms) of ethane. Points: NIST data [12]. Lines: prediction with the GEOS3C equations.
Conclusions

The vapour–liquid equilibrium and the thermophysical properties of ethane were predicted by five equations of state: SRK, PR, SW, TBS and GEOS3C on a wide PVT range, including the entire saturation region. A large comparison with PVT and thermodynamic recommended NIST data was made.

The following thermophysical properties were calculated: compressibility factor, enthalpy, enthalpy of vapourisation, entropy, heat capacity at constant pressure, heat capacity at constant volume, heat capacity ratio, speed of sound, fugacity coefficient, Joule-Thomson coefficient. The comparisons with recommended NIST data for these properties were also presented.

The GEOS3C and TBS equations give better the vapour pressure and saturated liquid and vapour volumes than the other cubic equations of state. Regarding the thermophysical properties, the GEOS3C equation predicts better the enthalpies and the entropies in the entire PVT range. The speed of sound values predicted for liquid on the saturation curve by GEOS3C have large errors relative to NIST recommended data. The isobaric heat capacity and Joule Thompson coefficient for liquid on the saturation curve are better predicted by GEOS3C equation.

The difference in performance between the five EOSs is less noticeable for other thermophysical properties: the isochoric heat capacities in the entire range of $T$ and $P$, the speed of sound and the Joule Thompson coefficient for vapour on the saturation curve.

This study shows that the cubic EOSs lead to reasonable predictions of thermophysical properties of ethane, resting simple enough for applications.
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List of symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>a, b, c, d</td>
<td>parameters in GEOS</td>
</tr>
<tr>
<td>AAD</td>
<td>absolute average deviation</td>
</tr>
<tr>
<td>B</td>
<td>dimensionless parameter in GEOS, defined by eq. (7)</td>
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<tr>
<td>C1, C2 and C3</td>
<td>parameters in GEOS3C temperature function</td>
</tr>
<tr>
<td>CV, CP</td>
<td>isochoric and isobaric heat capacities</td>
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<td>expression based on GEOS, defined by eq. (18)</td>
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<tr>
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Greeks

<table>
<thead>
<tr>
<th>Greek</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>αc</td>
<td>Riedel’s criterium (parameter in GEOS)</td>
</tr>
<tr>
<td>β</td>
<td>reduced temperature function in GEOS</td>
</tr>
<tr>
<td>φ</td>
<td>fugacity coefficient</td>
</tr>
<tr>
<td>Ωa, Ωb, Ωc, Ωd</td>
<td>parameters of GEOS</td>
</tr>
<tr>
<td>ω</td>
<td>acentric factor</td>
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Subscripts

<table>
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<th>Subscript</th>
<th>Description</th>
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<tbody>
<tr>
<td>c</td>
<td>critical property</td>
</tr>
<tr>
<td>r</td>
<td>reduced property</td>
</tr>
</tbody>
</table>

Superscript

exp | experimental (NIST recommended) data |
eos | calculated values |
R | residual (departure) function |

References


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