School of Aerospace 宇航学院
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Space Propulsion 空间推进

Equation of State for Nitrous Oxide   中文

Pressure of gaseous nitrous oxide can be calculated by:
Ideal gas law by *Boyle & Gay Lussac* [1-3]:

$$pv = RT$$

where p — gas pressure, Pa
R — universal gas constant, R = 8.314472 J/mol/K
T — gas temperature, K
$$v = \frac{\mu}{\rho}$$ molar volume, m^3/mol
μ — molar mass, kg/mol
ρ — gas density, kg/m^3

The *van der Waals* equation [1-3]:

$$\left(p + \frac{a}{v^2} \right)(v - b) = RT$$

where a, b — gas constants for the equation
a = 0.2060842 Pa m^6 mol^{-2}
b = 3.2458×10^{-5} m^3 mol^{-1}

The *Berthelot* equation [1,3]:

$$p = \frac{RT}{v - b} - \frac{a}{Tv^2}$$

where a, b — gas constants for the equation
a = 87.198 Pa K m^6 mol^{-2}
b = 3.2458×10^{-5} m^3 mol^{-1}

The *Dieterici* equation [1,3]:

$$p = \frac{RTe^{-a/RTv}}{v - b}$$

where a, b — gas constants for the equation
a = 0.500275 Pa m^6 mol^{-2}
b = 4.86×10^{-5} m^3 mol^{-1}

The *Benedict-Webb-Rubin* (BWR) equation of state [2,3] within temperature range from -30 to 150°C, for densities up to 900kg/m^3, and maximum pressure of 200bar:

$$p = \frac{RT}{v} + \left(B_0 RT - A_0 - \frac{C_0}{T^2} \right)\left(\frac{1}{v} \right)^2 + (bRT - a)\left(\frac{1}{v} \right)^3 + a\alpha\left(\frac{1}{v} \right)^6 + \frac{c}{T^2}\left(\frac{1}{v} \right)^3 \left[1 + \gamma\left(\frac{1}{v} \right)^2 \right] \exp\left[-\gamma\left(\frac{1}{v} \right)^2 \right]$$

where $A_0, B_0, C_0, a, b, c, a, \gamma$ — gas constants for the equation
A_0 = 0.313 kg m^5 s^{-2} mol^{-2}
B_0 = 5.1953×10^{-5} m^3 mol^{-1}
C_0 = 1.289×10^4 kg m^5 K^2 s^{-2} mol^{-2}
a = 1.109 ×10^{-5} kg m^8 s^{-2} mol^{-3}
b = 3.775×10^{-9} m^6 mol^{-2}
c = 1.398 kg m^8 K^2 s^{-2} mol^{-3}
a = 9.377×10^{-14} m^9 mol^{-3}
γ = 5.301×10^{-9} m^6 mol^{-2}

The Harmens-Knapp equation [3]:

$$p = \frac{RT}{v - b} - \frac{a}{v^2 + bcv - b^2(c - 1)}$$

where b, c — gas constants for the equation
$$a = 0.415676\left[1 + 0.601011762\left(1 - \sqrt{T/T_c} \right) - 0.010514755(1 - T_c/T) \right]^2$$ Pa m^6 mol^{-2}
b = 2.78292×10^{-5} m^3 mol^{-1}
c = 1.922537
T_c — critical point temperature, K

The *Peng-Robinson* equation of state [4]:

$$p = \frac{RT}{v - b} - \frac{a\alpha(T)}{v(v + b) + b(v - b)}$$

where a, b — gas constants for the equation

a = 0.417602925 Pa m^6 mol^{-2}

b = 2.76046×10^{-5} m^3 mol^{-1}

$$\alpha(T) = \exp\left[0.40154\left(1 - T/T_c\right)\left|1 - T/T_c\right|^{0.09692} + 0.13400\left(T_c/T - 1\right)\right]$$

T_c — critical point temperature, K

Figure 1 shows comparison of pressure-temperature data obtained by the above equations of state to the data by the National Institute of Standards and Technology (NIST).
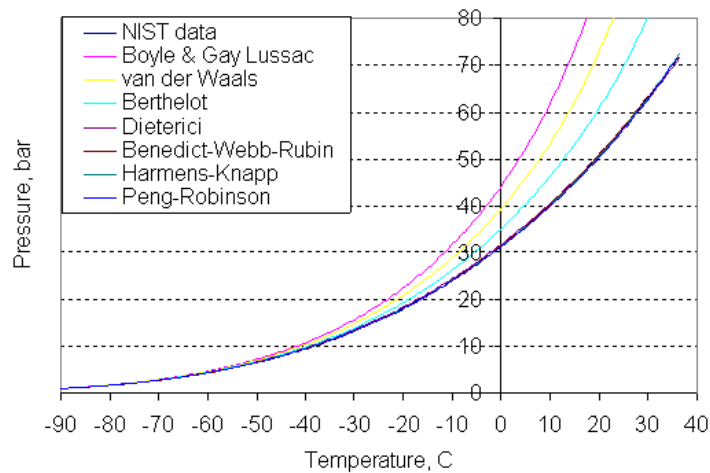

Figure 1. P-T saturation data comparison

Although for low temperatures all data are in good agreement for Boyle & Gay Lussac, van der Waals, and Berthelot equations the discrepancy arises with increasing temperature. Table 1 suggests that Dieterici, Benedict-Webb-Rubin, Harmens-Knapp, and Peng-Robinson equations of state give satisfactory correlation with NIST data for vapor pressure of saturated nitrous oxide.

Table 1. The R-squared value for selected equations

Equation of State	R^2
Boyle & Gay Lussac	0.911566
van der Waals	0.95507
Berthelot	0.993837
Dieterici	0.999837
Benedict-Webb-Rubin	0.999976
Harmens-Knapp	0.9999913
Peng-Robinson	0.9999837

Although Benedict-Webb-Rubin and Harmens-Knapp equations of state give satisfactory correlation with NIST data for vapor pressure of saturated nitrous oxide their prediction of critical point is rather poor (Table 2).

Table 2. Critical point parameters

Parameter	NIST	Benedict-Webb-Rubin	Harmens-Knapp
Pressure, bar	72.54	74.039	72.54
Temperature, K	309.584	310.968	309.576
Density, kg/m^3	452.5	423.9	401.1

References

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