Evaluation of the Performance of the Equations of State Available in CFTurbo for Air

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Abstract: - In this publication, we evaluate the performance of equations of state Perfect Gas, Redlich-Kwong, Aungier/ Redlich-Kwong, Soave/ Redlich-Kwong, Peng-Robinson, and Cool Prop in calculating the properties of air at temperatures between 250 K to 800 K and pressure between 1 bar to 250 bar. Firstly, we research the available literature to find the real density (or molar volume or specific volume) at each point. Then we create these equations and use the temperature and density (or molar volume or specific volume) to calculate the pressure, which is then compared to the pressure of the real values. This comparison evaluates the performance of each equation. Finally, we compare our calculations with online calculators to verify our results and comment on the performance of each equation.

Key-Words: - Thermodynamics, Air properties, Equation of State, Perfect Gas, Redlich-Kwong, Aungier/ Redlich-Kwong, Soave/ Redlich-Kwong, Peng-Robinson, Cool Prop.

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1 Introduction

During the lifetime of a fluid dynamics analyst, they would face many times the challenge of choosing a gas equation of state for their analysis. There are indeed a lot of equations of state and new ones are developed. Each one has its one advantages and disadvantages.

We also found ourselves in the same position. Specifically, we were designing a high-pressure air compressor using the turbomachinery designing software CFTurbo. CFTurbo gives the option of using the following six equations of state to calculate air properties: Perfect Gas, Redlich-Kwong, Aungier/ Redlich-Kwong, Soave/ Redlich-Kwong, Peng-Robinson, and Cool Prop (we must note that Cool Prop is a library with several equations). The question is which of the above equations of state is more suitable to our case as each equation may perform better under different conditions.

Unfortunately, we searched the available literature, and we did not find any publication that would cover our needs. What we need is studies showing the performance of the above models for air from low to high temperature and pressure. What we found is studies using the above equations to evaluate unrelated to our interest phenomena and properties, such as vapor-liquid equilibrium, [1], throttle reduction efficiency, [2], efficiency of air-conditioning, [3], evaluation using different acentric factors, [4], combustion gases properties, [5]. Even academic and specialized literature has limited information about these equations. We found contemporary literature just mentioning some of those equations, [6], and literature presenting only theoretical background and focusing on more advanced topics, [7], [8]. So, we concluded that there is no available literature, at least in public, that provides this information. This is strange as there are high-pressure systems using air and such studies should have been performed. For these reasons, we decided to perform the analysis presented in this article and give public information about the performance of these equations in predicting air properties.

In this publication, we study which of the above equations calculates better air properties (78.08% N_2, 20.95% O_2, 0.93% Ar, and 0.04% CO_2) in the range of temperature values between 250 K to 800 K and the range of pressure values between 1 bar to 250 bar.

2 Problem Formulation

To determine which is the best equation of state to calculate air properties in the above range we searched to find the real properties of air in these conditions. This was achieved by finding the compressibility factor, Z, of air in the ranges. As you will see in the following paragraphs, most of the equations of state are solved to pressure and are complex to be solved to other variables. So, to avoid round-up and iteration errors we calculate the pressure in the specified ranges using the corresponding density (or molar volume or specific volume) and temperature, and we compare the calculated pressure value with the real pressure value corresponding to the used density (or molar volume or specific volume) and temperature.

2.1 Compressibility Factor of Air

The process of finding the compressibility factor of air was challenging as the required range goes far beyond the needs of conventional applications. Also, we must note that after extensive research we did not find contemporary literature providing the compressibility factor of air in the requested ranges. So, our only option is to base our analysis on older literature that provides the wanted data.

We found in total four sources that agree and one with a small deviation from the other four. Specifically, we found a maximum deviation of 1 % between the values in, [9], (approximately 300 pressure-temperature points in the required region) and the values found in [10] and in [11], which provide fewer points (approximately 90). This deviation is considered significant as we aim to achieve the highest accuracy possible for our analysis. The deviation found in the literature is normal to occur as the compressibility factor is calculated using both experimental and computational methods. By carrying out further literature search we found, [12], and, [13], which agree with [10] and [11]. Having found four sources proposing the same values we will use them for our analysis.

The values for the compressibility factor Z in the required range are presented in Table 1. Z values are used to calculate the density (or molar volume or specific volume) of air and together with the related temperature are used in the equations of state to calculate the pressure, which then is compared with the pressure of the corresponding point of Z value.

Table 1. Compressibility factor Z of air.

	Compressibility factor Z										
	Pressure (bar) ↴										
Temperature ← (K)	1	5	10	20	40	60	80	100	150	200	250
250	0.9992	0.9957	0.9911	0.9822	0.9671	0.9549	0.9463	0.9411	0.945	0.9713	1.0152
300	0.9999	0.9987	0.9974	0.995	0.9917	0.9901	0.9903	0.993	1.0074	1.0326	1.0669
350	1.0000	1.0002	1.0004	1.0014	1.0038	1.0075	1.0121	1.0183	1.0377	1.0635	1.0947
400	1.0002	1.0012	1.0025	1.0046	1.01	1.0159	1.0229	1.0312	1.0533	1.0795	1.1087
450	1.0003	1.0016	1.0034	1.0063	1.0133	1.021	1.0287	1.0374	1.0614	1.0913	1.1183
500	1.0003	1.002	1.0034	1.0074	1.0151	1.0234	1.0323	1.041	1.065	1.0913	1.1183
600	1.0004	1.0022	1.0039	1.0081	1.0164	1.0253	1.034	1.0434	1.0678	1.092	1.1172
800	1.0004	1.002	1.0038	1.0077	1.0157	1.024	1.0321	1.0408	1.0621	1.0844	1.1061

2.2 Equations of State

We recreated every available equation of state in CFTurbo in Excel software, except Cool Prop, to calculate the pressure of air at each point of Table 1 as described above. The equations are described below.

2.2.1 Perfect Gas

Perfect Gas equation of state is the simplest of all and was used in the following form:

$$P = \rho \cdot R \cdot T \tag{1}$$

Where P – pressure [Pa], ρ – density [kg/m^3], R – air gas constant = 287 $\frac{J}{kg \cdot K}$, and T – temperature [K].

2.2.2 Redlich-Kwong

The Redlich-Kwong equation was taken from a practice engineering book, [14]:

$$P = \frac{R \cdot T}{V_m - b} - \frac{a}{\sqrt{T} \cdot V_m \cdot (V_m + b)} \tag{2}$$

Where P – pressure [Pa], R – air gas constant = 287 $\frac{J}{kg \cdot K}$, T – temperature [K], V$_m$ – molar volume [m^3/mol], b - is a constant that corrects for volume and, α - is a constant that corrects for the attractive potential of molecules.

V$_m$ is calculated with the following equation:

$$V_m = \frac{1}{\rho}\cdot M_w \tag{3}$$

Where M_w – the molar mass of air = 0.029 kg/mol. M_w was calculated using the formula calculating gas mixture properties:

$$M_w = \sum x_i \cdot M_{wi} \tag{4}$$

Where M_{wi} is the molar mass of each component of the air mixture, and x_i is the percentage of each component, which are provided in Table 2.

Table 2. Essential properties of the components of air for the used equations. x – the percentage of each component of air, M_w – molar mass, T_c – the temperature at the critical point, P_c – the pressure at the critical point, V_c - the volume at the critical point, ω – acentric factor.

	N_2	O_2	Ar	CO_2
x (%)	78.08%	20.95%	0.93%	0.04%
M_w (kg/mol)	0.02802	0.03200	0.03995	0.04401
T_c (K)	126.2	154.6	150.8	304.13
P_c (bar)	33.90	50.50	48.65	73.97
V_c (m^3/kg)	0.00318	0.00250	0.00186	0.00214
ω	0.040	0.022	0.001	0.228

α is calculated using Eq. 4 by replacing M_{wi} with α_i values. α_i of each component of air is calculated by the following equation:

$$a_i = \frac{1}{9\cdot(\sqrt[3]{2}-1)}\cdot\frac{R^2\cdot T_{ci}^{2.5}}{P_{ci}} \tag{5}$$

Where T_{ci} and P_{ci} of each component of air are given in Table 2.

b is calculated using Eq. 4 by replacing M_{wi} with b_i values. b_i of each component of air is calculated by the following equation:

$$b_i = \frac{\sqrt[3]{2}-1}{3}\cdot\frac{R\ \cdot T_{ci}}{P_{ci}} \tag{6}$$

Where T_{ci} and P_{ci} of each component of air are given in Table 2.

2.2.3 Aungier/ Redlich-Kwong

The Aungier/ Redlich-Kwong equation was taken from the ANSYS documentation, [15]:

$$P = \frac{R\cdot T}{V-b+c} - \frac{a_0\cdot T_r^{-n}}{V\cdot(V+b)} \tag{7}$$

Where P – pressure [Pa], R – air gas constant = 287 $\frac{J}{kg\cdot K}$, T – temperature [K], V – specific volume [m^3/kg], b and c - are constants that correct for volume and α_0 - is a constant that corrects for the attractive potential of molecules. T_r and n are presented below.

V is calculated using the values of Table 1 and the following equation:

$$V = \frac{P(Table\ 1)}{R\cdot T\cdot Z} \tag{8}$$

α_0 is calculated using Eq. 4 by replacing M_{wi} with α_{0i} values. α_{0i} of each component of air is calculated by the following equation:

$$a_{0i} = 0.42747\cdot\frac{R^2\cdot T_{ci}^{2.5}}{P_{ci}} \tag{9}$$

Where T_{ci} and P_{ci} of each component of air are given in Table 2.

b is calculated using Eq. 4 by replacing M_{wi} with b_i values. b_i of each component of air is calculated by the following equation:

$$b_i = 0.08664\cdot\frac{R\ \cdot T_{ci}}{P_{ci}} \tag{10}$$

Where T_{ci} and P_{ci} of each component of air are given in Table 2.

c is calculated using Eq. 4 by replacing M_{wi} with c_i values. c_i of each component of air is calculated by the following equation:

$$c_i = \frac{R\cdot T_{ci}}{P_{ci}+\frac{a_{0i}}{V_{ci}\cdot(V_{ci}+b)}} + b - V_{ci} \tag{11}$$

Where T_{ci}, P_{ci}, and V_{ci} of each component of air are given in Table 2.

T_r is calculated using the following equation:

$$T_r = \frac{T}{T_c} \tag{12}$$

Where T_c is the temperature at the critical point of air and is calculated using Eq. 4 by replacing M_{wi} with T_{ci} values provided in Table 2.

n is calculated using the following equation:

$$n = 0.4986 + 1.1735\cdot\omega + 0.4754\cdot\omega^2 \tag{13}$$

Where ω – the acentric factor = 0.0360 which is calculated using Eq. 4 by replacing M_{wi} with ω_i values of each component of air. ω_i are provided in Table 2.

2.2.4 Soave/ Redlich-Kwong

The Soave/ Redlich-Kwong equation was taken from the publication of the author himself for this equation, [16]:

$$P = \frac{R \cdot T}{V_m - b} - \frac{a \cdot A}{\sqrt{T} \cdot V_m \cdot (V_m + b)} \tag{14}$$

Where P – pressure [Pa], R – air gas constant = 287 $\frac{J}{kg \cdot K}$, T – temperature [K], V_m – molar volume [m^3/mol], b - is a constant that corrects for volume, α - is a constant that corrects for the attractive potential of molecules and A – is a modification to the attractive term.

V_m is calculated using Eq. 3.

α is calculated using Eq. 4 by replacing M_{wi} with α_i values. α_i of each component of air is calculated by the following equation:

$$a_i = \frac{1}{9 \cdot (\sqrt[3]{2} - 1)} \cdot \frac{R^2 \cdot T_{ci}^2}{P_{ci}} \tag{15}$$

Where T_{ci} and P_{ci} of each component of air are given in Table 2.

A is calculated following equation:

$$A = (1 + (0.480 + 1.574 \cdot \omega - 0.176 \cdot \omega^2) \cdot (1 - \sqrt{T_r}))^2 \tag{16}$$

Where T_r and ω are calculated the same way as described in Eq. 12 and 13 respectively.

b is calculated using Eq. 4 by replacing M_{wi} with b_i values. b_i of each component of air which are calculated using an equation using Eq. 6.

2.2.5 Peng-Robinson

The Peng-Robinson equation was taken from the publication of the authors themselves for this equation, [17]:

$$P = \frac{R \cdot T}{V_m - b} - \frac{a \cdot A}{V_m \cdot (V_m + b) + b \cdot (V_m - b)} \tag{17}$$

Where P – pressure [Pa], R – air gas constant = 287 $\frac{J}{kg \cdot K}$, T – temperature [K], V_m – molar volume [m^3/mol], b - is a constant that corrects for volume, α - is a constant that corrects for the attractive potential of molecules and A – is a modification to the attractive term.

V_m is calculated using Eq. 3.

α is calculated using Eq. 4 by replacing M_{wi} with α_i values. α_i of each component of air is calculated by the following equation:

$$a_i = 0.457235 \cdot \frac{R^2 \cdot T_{ci}^2}{P_{ci}} \tag{18}$$

Where T_{ci} and P_{ci} of each component of air are given in Table 2.

A is calculated following equation:

$$A = (1 + (0.37464 + 1.5226 \cdot \omega - 0.26992 \cdot \omega^2) \cdot (1 - \sqrt{T_r}))^2 \tag{19}$$

Where T_r and ω are calculated the same way as described in Eq. 12 and 13 respectively.

b is calculated in Eq. 4 by replacing M_{wi} with α_i values. b_i of each component of air which is calculated by the following equation:

$$b_i = 0.077796 \cdot \frac{R \cdot T_{ci}}{P_{ci}} \tag{20}$$

Where T_{ci} and P_{ci} of each component of air are given in Table 2.

2.2.6 Cool Prop

CoolProp is a C++ library that implements several equations for the calculation of properties of substances and mixtures, as described by the Cool Prop creators on their website *coolprop*. Its construction would require a lot of effort. For this reason, we used the online calculator created by Cool Prop creators themselves, available on their website, which also ensures correct calculations.

3 Problem Solution

In this section, we present the calculations performed to figure in which area the performance of each equation of state of Section 2 is optimized.

As we described in Section 2, we use pressure values to evaluate the performance of each equation of state to avoid computational errors as all the equations are solved to pressure. The error of each point P_i and T_j of the range of the analysis, Table 1, is calculated using the following equation:

$$Error_{ij} = \frac{\left|(Calculated\ Pressure)_{ij} - (Pressure\ of\ Table\ 1)_i\right|}{(Pressure\ of\ Table\ 1)_i} \tag{21}$$

This calculation is used to evaluate the performance of each equation of state. To calculate the pressure of each point in Table 1 we apply the following process. For each point P_i and T_j of Table 1 we calculate their density ρ_{ij} (or molar volume V_{mij} or specific volume V_{ij}) by using the corresponding compressibility factor Z_{ij} of Table 1. Then both T_j and ρ_{ij} (or V_{mij} or V_{ij}) are inserted in the equations to calculate the pressure $(Calculated\ Pressure)_{ij}$, which is used together with the $(Pressure\ of\ Table\ 1)_i$ in equation (21) to calculate the $Error_{ij}$.

For example, we want to calculate the error of the equations at the point 100 bar and 500 K. At this point the compressibility factor is Z = 1.041. This Z corresponds to density $\rho = 66.94$ kg/m^3, specific molar $V_m = 4.33 \cdot 10^{-4}$ m^3/mol, and specific volume $V = 1.493 \cdot 10^{-2}$ m^3/kg. The calculated pressure at this point using the Soave/ Redlich-Kwong equation is 100.43 bar. By using equation (21) we find that the error is 0.43%

The results are presented in the following Tables. The tables present the error of each equation on predicting the properties of air in different combinations of temperature and pressure in the ranges 250 K to 800 K and 1 bar to 250 bar. To facilitate the evaluation, error values equal to or smaller than 0.1 % are colored with blue, error values between 0.1 % and 1 % and equal to 1 % are colored with green, error values between 1 % and 2 % and equal to 2 % are colored with orange, and error values bigger than 2 % are colored with red.

Table 3. The error of Perfect Gas equation calculations from real values

	Error										
	Pressure (bar) ↴										
Temperature ← (K)	1	5	10	20	40	60	80	100	150	200	250
250	0.08%	0.43%	0.90%	1.81%	3.40%	4.72%	5.67%	6.26%	5.82%	2.95%	1.50%
300	0.01%	0.13%	0.26%	0.50%	0.84%	1.00%	0.98%	0.70%	0.73%	3.16%	6.27%
350	0.00%	0.02%	0.04%	0.14%	0.38%	0.74%	1.20%	1.80%	3.63%	5.97%	8.65%
400	0.02%	0.12%	0.25%	0.46%	0.99%	1.57%	2.24%	3.03%	5.06%	7.36%	9.80%
450	0.03%	0.16%	0.34%	0.63%	1.31%	2.06%	2.79%	3.61%	5.78%	8.37%	10.58%
500	0.03%	0.20%	0.34%	0.73%	1.49%	2.29%	3.13%	3.94%	6.10%	8.37%	10.58%
600	0.04%	0.22%	0.39%	0.80%	1.61%	2.47%	3.29%	4.16%	6.35%	8.42%	10.49%
800	0.04%	0.20%	0.38%	0.76%	1.55%	2.34%	3.11%	3.92%	5.85%	7.78%	9.59%

From Table 3 we observe that the Perfect Gas equation provides excellent calculations (error equal to or less than 0.1 %) only near the atmospheric pressure of 1 bar while its calculations worsen as the pressure increases. However, for applications that require less than 1 % error this model can be used up to 10 bar and some points between 20 bar and 150 bar and temperatures between 300 K and 400 K. All the other areas have more than 1 % error with more than 2 % error to appear mainly after 60 bar and 400 K.

Table 4. The error of Redlich–Kwong equation calculations from real values

	Error										
	Pressure (bar) ↴										
Temperature ← (K)	1	5	10	20	40	60	80	100	150	200	250
250	0.03%	0.11%	0.18%	0.29%	0.54%	0.73%	0.89%	0.99%	1.12%	1.30%	1.72%
300	0.03%	0.09%	0.17%	0.30%	0.58%	0.81%	1.00%	1.24%	1.71%	2.13%	2.58%
350	0.01%	0.08%	0.15%	0.32%	0.61%	0.89%	1.13%	1.40%	1.96%	2.49%	3.01%
400	0.01%	0.09%	0.19%	0.31%	0.61%	0.86%	1.15%	1.47%	2.09%	2.69%	3.23%
450	0.01%	0.08%	0.18%	0.30%	0.60%	0.91%	1.15%	1.44%	2.16%	3.16%	3.63%
500	0.01%	0.10%	0.13%	0.30%	0.59%	0.89%	1.21%	1.46%	2.16%	2.86%	3.46%
600	0.01%	0.09%	0.13%	0.29%	0.57%	0.88%	1.15%	1.46%	2.24%	2.87%	3.50%
800	0.01%	0.07%	0.12%	0.24%	0.51%	0.79%	1.04%	1.34%	2.01%	2.71%	3.32%

From Table 4 we observe that the Redlich–Kwong equation provides excellent calculations almost up to 5 bar while again its calculations worsen as the pressure increases. Generally, it performs better than the Perfect Gas equation and provides less than 1 % error up to and around 60 bar. The area with errors of more than 2% is limited between 150 bar and 250 bar, and between 300 K and 800 K.

Aungier/ Redlich-Kwong, Table 5, is an even better equation as it provides excellent calculations up to 5 bar, almost in the same area as Redlich–Kwong while again its calculations worsen as the pressure increases. Generally, it performs better than the Redlich–Kwong as it provides less and 1 % error up to 80 bar, including a triangular area between 100 bar and 250 bar and between 250 K and 350 K. The area with errors of more than 2% is even smaller in this case between 200 bar and 250 bar, and between 400 K and 800 K. So, regarding high-pressure analyses, Aungier/ Redlich-Kwong equation performs well at low temperatures between 250K and 350 K.

Table 5. The error of Aungier/ Redlich-Kwong equation calculations from real values

	Error										
	Pressure (bar) ↴										
Temperature ← (K)	1	5	10	20	40	60	80	100	150	200	250
250	0.02 %	0.08 %	0.12 %	0.16 %	0.27 %	0.31 %	0.31 %	0.23 %	0.08 %	0.33 %	0.30 %
300	0.03 %	0.06 %	0.11 %	0.19 %	0.35 %	0.46 %	0.54 %	0.66 %	0.82 %	0.96 %	1.14 %
350	0.01 %	0.05 %	0.10 %	0.23 %	0.42 %	0.60 %	0.75 %	0.93 %	1.26 %	1.57 %	1.89 %
400	0.01 %	0.07 %	0.15 %	0.23 %	0.45 %	0.63 %	0.83 %	1.08 %	1.51 %	1.94 %	2.31 %
450	0.01 %	0.07 %	0.15 %	0.23 %	0.46 %	0.70 %	0.88 %	1.11 %	1.67 %	2.53 %	2.87 %
500	0.01 %	0.08 %	0.10 %	0.24 %	0.47 %	0.71 %	0.97 %	1.17 %	1.73 %	2.32 %	2.80 %
600	0.01 %	0.08 %	0.11 %	0.24 %	0.47 %	0.74 %	0.97 %	1.24 %	1.91 %	2.45 %	2.99 %
800	0.01 %	0.06 %	0.10 %	0.21 %	0.45 %	0.70 %	0.92 %	1.19 %	1.79 %	2.43 %	2.97 %

Table 6. The error of Soave/ Redlich-Kwong equation calculations from real values

	Error										
	Pressure (bar) ↴										
Temperature ← (K)	1	5	10	20	40	60	80	100	150	200	250
250	0.00 %	0.03 %	0.11 %	0.29 %	0.62 %	1.01 %	1.41 %	1.85 %	2.87 %	3.50 %	3.57 %
300	0.01 %	0.06 %	0.13 %	0.28 %	0.58 %	0.90 %	1.23 %	1.48 %	2.09 %	2.50 %	2.66 %
350	0.02 %	0.06 %	0.13 %	0.24 %	0.49 %	0.71 %	0.95 %	1.12 %	1.56 %	1.83 %	1.93 %
400	0.01 %	0.04 %	0.07 %	0.21 %	0.40 %	0.60 %	0.76 %	0.84 %	1.13 %	1.28 %	1.35 %
450	0.01 %	0.04 %	0.06 %	0.17 %	0.32 %	0.43 %	0.57 %	0.65 %	0.76 %	0.43 %	0.54 %
500	0.01 %	0.01 %	0.09 %	0.12 %	0.23 %	0.31 %	0.35 %	0.43 %	0.49 %	0.42 %	0.36 %
600	0.00 %	0.00 %	0.04 %	0.05 %	0.10 %	0.09 %	0.11 %	0.07 %	0.09 %	0.19 %	0.35 %
800	0.00 %	0.01 %	0.01 %	0.02 %	0.08 %	0.16 %	0.22 %	0.34 %	0.58 %	0.92 %	1.19 %

Table 7. The error of Peng–Robinson calculations from real values

	Error										
	Pressure (bar) ↴										
Temperature ← (K)	1	5	10	20	40	60	80	100	150	200	250
250	0.05 %	0.21 %	0.37 %	0.64 %	1.13 %	1.47 %	1.72 %	1.89 %	2.28 %	3.00 %	4.23 %
300	0.04 %	0.13 %	0.25 %	0.44 %	0.80 %	1.07 %	1.29 %	1.54 %	2.06 %	2.66 %	3.44 %
350	0.01 %	0.09 %	0.16 %	0.34 %	0.63 %	0.89 %	1.11 %	1.35 %	1.87 %	2.44 %	3.11 %
400	0.01 %	0.08 %	0.17 %	0.27 %	0.52 %	0.72 %	0.95 %	1.23 %	1.75 %	2.33 %	2.91 %
450	0.01 %	0.06 %	0.14 %	0.22 %	0.45 %	0.68 %	0.86 %	1.09 %	1.69 %	2.63 %	3.10 %
500	0.00 %	0.07 %	0.08 %	0.21 %	0.41 %	0.63 %	0.87 %	1.06 %	1.61 %	2.24 %	2.80 %
600	0.01 %	0.07 %	0.08 %	0.19 %	0.38 %	0.60 %	0.80 %	1.04 %	1.67 %	2.21 %	2.78 %
800	0.01 %	0.05 %	0.08 %	0.17 %	0.35 %	0.57 %	0.76 %	1.00 %	1.55 %	2.17 %	2.71 %

According to Table 6, the Soave/ Redlich-Kwong equation has almost similar performance to the Aungier/ Redlich-Kwong equation with the difference that it performs better at high temperatures. Soave/ Redlich-Kwong equation has a bigger area of low error (less than 0.1 %) between 1 bar and 10 bar which extends also mainly up to 40 bar but only for high temperatures between 600 K and 800 K. Its area with less than 1 % is also bigger and covers all the area of analysis excluding a triangular area between 60 bar and 250 bar, and between 250 K and 400 K.

Peng–Robinson, Table 7, has almost similar performance to Redlich–Kwong with the difference that it performs better at high temperatures. Its tendency to perform better in high temperatures is clear even in the low error area (error less than 0.1 %) covering a wide triangular area between 1 bar and 10 bar. Its area with less than 1 % extends almost up to 80 bar, excluding a small triangular area between 250 K and 350 K. Its area with almost and more than 2 % error is between 150 bar and 250 bar.

Table 8. The error of Cool Prop calculations from real values

	Error										
	Pressure (bar) →										
Temperature ↓ (K)	1	5	10	20	40	60	80	100	150	200	250
250	0.00 %	0.02 %	0.01 %	0.04 %	0.06 %	0.07 %	0.04 %	0.03 %	0.01 %	0.01 %	0.05 %
300	0.00 %	0.00 %	0.00 %	0.00 %	0.02 %	0.04 %	0.07 %	0.03 %	0.02 %	0.03 %	0.01 %
350	0.02 %	0.01 %	0.01 %	0.02 %	0.03 %	0.04 %	0.03 %	0.06 %	0.08 %	0.10 %	0.10 %
400	0.02 %	0.01 %	0.03 %	0.02 %	0.05 %	0.04 %	0.06 %	0.13 %	0.16 %	0.21 %	0.21 %
450	0.02 %	0.00 %	0.04 %	0.02 %	0.06 %	0.10 %	0.10 %	0.14 %	0.25 %	0.67 %	0.60 %
500	0.02 %	0.02 %	0.01 %	0.04 %	0.07 %	0.12 %	0.19 %	0.20 %	0.30 %	0.44 %	0.50 %
600	0.02 %	0.02 %	0.00 %	0.05 %	0.10 %	0.18 %	0.22 %	0.31 %	0.53 %	0.63 %	0.73 %
800	0.01 %	0.01 %	0.01 %	0.04 %	0.12 %	0.22 %	0.28 %	0.39 %	0.59 %	0.84 %	1.00 %

Finally, the most accurate calculations were achieved by Cool Prop, Table 8, which is a library with several equations. The maximum error is 1 % at the point 250 bar and 800 K. Its low error area (less than 0.1 %) covers almost all the range of the analysis, excluding a triangular area between 60 bar and 250 bar and between 350 K and 800 K. And this triangular area has a maximum error of 1 %. And thus Cool Prop is the best model for predicting air properties in the range of 1 bar to 250 bar and 250 K to 800 K.

The fact that many of our calculations are close to the real values is a good sign that our calculations are correct. However, we must check if this is the case or if we have underestimated an equation. So, we will compare our equations with existing calculators from other sources. The Ideal Gas was not verified as it is simple enough to not require validation. Also, Cool Prop does not require validation as we used the original calculator of Cool Prop creators.

A comparison with equations is presented in Table 9. To compare them we calculated the properties of air in fewer points which cover the ranges of analysis, focusing on the points where our equations presented the highest errors because our equations and the equations from other sources presented the same error pattern. So, we compared the maximum errors found.

For the Redlich-Kwong equation, we used the online calculator found on the website of vCalc which is an open calculator, equation, and dataset library. Its calculations are slightly better than ours. At their worst point, our equation has a 3.634 % error while the online calculator has a 3.628 % error. Their difference is 0.006 % which is very small.

For the Soave/ Redlich-Kwong equation, we used the vCalc website. Its calculations are a lot worse than ours. At their worst point, our equation has a 3.57 % error while the online calculator has a 27.38 % error. Their difference is 23.81 % which is significant. This may be the result of the different ways these equations can be used for mixtures, such as air. One way is that the constants of the equations, α, α_0, b, c, can be calculated by considering air as a mixture and using equation (4), as we described. Another way is that these constants can be calculated by considering air as a pure substance and using equations (5), (6), (9), (10), (11), (15), (18), (19), and (20), ignoring the i index and calculating them by using the critical temperature and critical pressure of air instead of each component. Both methods can be applied, and this may be the reason for the high difference that appeared.

For the Peng-Robinson equation, we used the vCalc website. Its calculations are worse than ours. At their worst point, our equation has a 4.23 % error while the online calculator has a 7.64 % error. Their difference is 3.41 %.

For the Aungier/ Redlich-Kwong equation, we did not find an online calculator, so we used CFTurbo for the calculations. Its calculations are slightly worse than ours. At their worst point, our equation has a 2.99 % error while the CFTurbo has a 3.32 % error. Their difference is 0.33 % which is very small.

With the above comparison, we showed that the performance of our equations is close to the performance of available calculators, excluding the Soave/ Redlich-Kwong equation which was outperformed by our approach. So, we can trust that our calculations and the results of this analysis do not underestimate the performance of any equation.

Table 9. Comparison of our equations with equations from other sources (*calculated using CFTurbo)

	Maximum Error (%)		Difference (Ours-Online)	Best results (Ours/ Online)
Equation	Our Equations	Online Calculators		
Perfect Gas	10.58 %	-	-	-
Redlich –Kwong	3.634 %	3.628 %	0.006 %	Other
Aungier/ Redlich-Kwong	2.99 %	*3.32 %	- 0.33 %	Ours
Soave/ Redlich-Kwong	3.57 %	27.38 %	- 23.81 %	Ours
Peng–Robinson	4.23 %	7.64 %	- 3.41 %	Ours
Cool Prop	-	1.00 %	-	-

4 Conclusion

After the above calculations, we have studied the available models in a wide range of conditions. The percentages presented in Table 3, Table 4, Table 5, Table 6, Table 7 and Table 8 describes the error of each model at the specific temperature and pressure condition.

It is very interesting to observe how the performance of each model varies. Specifically, we notice that as the complexity of a model increases so does its accuracy.

Table 3, Table 4, Table 5, Table 6, Table 7 and Table 8 provide valuable data for an analyst to choose, based on their intentions, the best model for their analysis to achieve the desired accuracy and save computational cost.

Also, if they need the same analysis for a different substance, they can follow the steps described in this article to realize it.

According to the results of Section 3, we come to the following conclusions about each equation of state.

According to Table 3, the calculations of the Perfect Gas equation have a maximum of 1 % error mainly at low pressures between 1 bar and 20 bar.

According to Table 4, the calculations of Redlich–Kwong have a maximum of 1 % error from 1 bar to 60 bar of pressure.

According to Table 5, the calculations of the Aungier/ Redlich-Kwong equation are even better by having a maximum 1 % error from 1 bar to 80 bar including a small triangular area between 100 bar to 250 bar and 250 K to 350 K.

According to Table 6, the calculations of the Soave/ Redlich-Kwong equation have a maximum of 1 % error inside all the ranges of the analysis excluding a triangular area between 60 bar to 250 bar and 250 K to 400 K and the point of 250 bar and 800 K.

According to Table 7, the calculations of Peng–Robinson have a maximum of 1 % error from 1 bar to 80 bar excluding a small triangular area between 40 bar to 80 bar and 250 K to 350 K.

Finally, according to Table 8, the calculations of Cool Prop have a maximum of 1 % error inside all the ranges of the analysis.

So, if someone needs to calculate the properties of air and has available all the above equations the best option is Cool Prop. However, there is no available Cool Prop setup for all the substances in every conventional software, especially for custom mixtures.

The next best options for air are the Aungier/ Redlich-Kwong equation and Soave/ Redlich-Kwong equation as they cover a larger area than the other equations. Also, they perform well in different areas which means that combined cover almost all the areas of analysis. Both have calculations with a maximum 1% error from pressures greater than 100 bar. Above this pressure, Aungier/ Redlich-Kwong equation has a maximum 1% error in a triangular area between 250 K and 350 K, while Soave/ Redlich-Kwong equation in the area between 450 K and 800 K, excluding point 250 bar and 800 K. We notice that the other part of the triangular area between 250 K and 350 K and the point 250 bar and 800 K have more than 1% errors. However, we notice that if we use each model where it performs better, calculations with a maximum of 2% error can be achieved. This is an exceptionally good performance considering the relative simplicity of these two equations.

An interesting and useful future study would be to evaluate the performance of these equations using other substances in the same area and to observe if each equation performs better for different substances.

Even more interesting and useful future studies would be to collect analyses of different substances and search for a relationship between the performance of the equations and key properties of the substances, e.g. the performance of the equations to P_r and T_r.

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