Real Gas Vs. Ideal Gas

Predicting discharge temperature of a Centrifugal Compressor in a realistic way based on ASME PTC 10

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Thermodynamic equations are greatly simplified if derived based on perfect gas or ideal gas assumptions. Notwithstanding, these equations are the most common basis on which the real gas equations are formulated. For gas compression, it is always easier and quicker to use ideal gas equations for quick estimation of thermodynamic properties. However, these rudimentary estimations may be inaccurate and sometimes lead to unexpected deviation from actual values.

In this article, the concept of predicting discharge temperature for a centrifugal compressor by using Schultz's approach will be discussed. This approach has been adopted by ASME PTC 10 since 1965 [1]. This real gas method of predicting discharge temperature is very useful during conceptual study or the FEED stage of a project which requires a centrifugal compressor, as it assists to identify with higher confidence the sizing and additional requirements (e.g., intercooler or aftercooler) at an early stage. Also, this method can be used to gauge an existing compressor's performance via measurement of the gas thermo properties.

Introduction

The work input of a centrifugal compressor is always benchmarked against ideal compression work, which is commonly either of isentropic or polytropic. Efficiency is the typical indicator for comparison purpose with other compressors for same duty, or as an indicator for compressor design improvement. Polytropic compression will be ideal compression used in this article. As a concise introduction, this compression is actually a summation of infinitesimal isentropic compressions, Yi separated by their constant proportion of irreversibly generated heat (friction, etc.),Δh_f, along the real compression path (Figure 1). That constant proportion is represented by polytropic efficiency, η_p. Therefore, polytropic compression is effectively defined by compression with constant efficiency, rather than by the Equation 1, as the polytropic exponent is not always a constant.

Equation 1

$$P_1 v_1^n = P_2 v_2^n$$

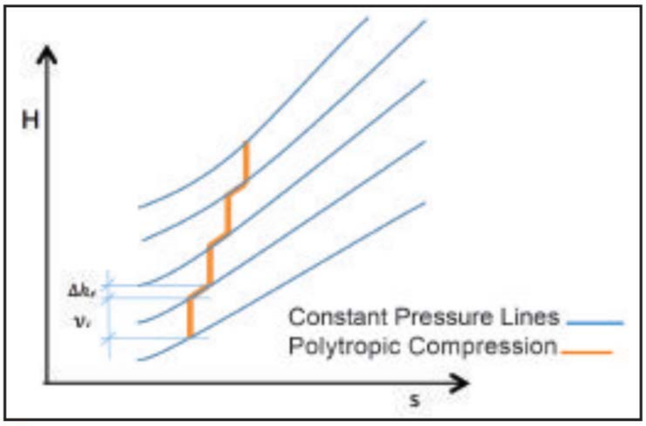

Figure 1. H-S diagram showing polytropic compression.

Since polytropic compression consists of infinite isentropic compressions, its exponent, *n,* for an ideal gas, is related to the isentropic exponent, n_s, *by* Equation 2. Its derivation can be found in Reference 2 [2].

Equation 2

$$\frac{n-1}{n} = \frac{n_S-1}{n_S\,\eta_P}$$

Isentropic compression is further explored since this is the skeleton of polytropic compression. Isentropic compression is reversible and adiabatic, and thus initial entropy, s, is maintained throughout the compression path. For ideal gas, its compression path is generally obtained by Equation 3. Its isentropic exponent, n_s, is exactly the ratio of specific heat at constant pressure (*Cp*) to specific heat at constant volume (*Cv*). Strictly, specific heats of ideal gas varies according to temperature, and thus n, is actually changing slightly along the compression path since temperature changes. Hence, Equation 3 is mathematically correct for perfect gas since its specific heats are constant, whereas for ideal gas, this equation is just a close approximation. In the ideal gas method section later, temperature effect on specific heats will be taken into account.

Equation 3

$$P_1 v_1^{n_s} = P_2 v_2^{n_s}$$

By definition, ideal gas is a hypothetical gas of which

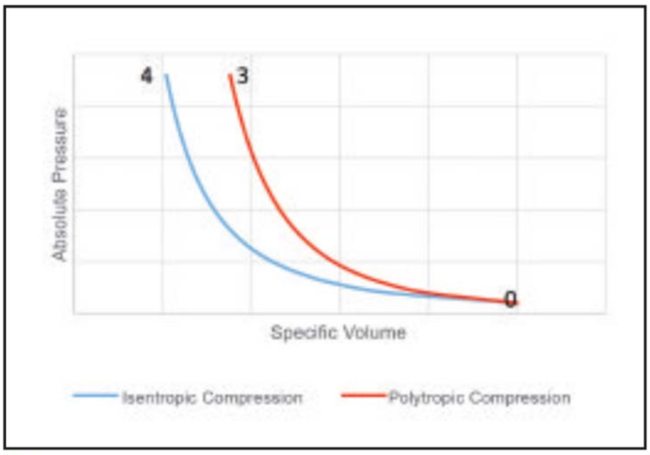

Figure 2. Isentropic and polytropic compression paths.

the gas molecules occupy negligible space and have no interaction forces between each other. This ideal gas model can only be approximated if the compressed gas is at much lower pressure and/or higher temperature relative to their critical point. When the compressed gas path is approaching its critical point, its thermodynamic behavior deviates more and more from that of ideal gas. Hence, Equations 1 to 3 no longer provide convincing results. In such circumstances, thermodynamic equations that are derived based on real gas approach will produce reliable results. This approach basically means compressibility factor, Z, is treated as variable strictly from the beginning of any thermodynamic equation derivation till the resultant equations. Schultz's method, which is used by ASME PTC 10 for real gas calculation, fulfils this requirement, though correction factor, *f*, is proposed to account for the variation effect of polytropic exponent.

Two examples in the following section are presented to demonstrate this deviation of using ideal gas model. Before that, the discharge temperature-estimating method as earlier-mentioned is elaborated as follows:

Real gas method

Based on ASME PTC 10, after a performance test, polytropic exponent is derived by using Equation 4, of which subscript *0* and *3* denote initial and final measured states (Figure 2). From Equation 4, P_0, P_3 and v_0 are known values since they are specified, whereas v_3 has to be derived from actual discharge temperature via equation of state. Also, isentropic exponent is required since it is part of the correction factor, *f*, and it is derived as per Equation 5. It can be seen clearly that n_s, is already a known value even before the performance test is conducted, as v_4 at P_3 is simply the specific volume at the same entropy of initial state. v_4 can be obtained by solving equation of states, which can be of Benedict-Webb-Rubin-Starling (BWRS), Redlich-Kwong-Soave (RKS), Lee-Kesler-Plecker (LKP), etc., depending on the gas composition and pressure range used [3].

Equation 4

$$n = \frac{log_{10}(^{P_3}/_{P_o})}{log_{10}(^{v_o}/_{v_3})}$$

Equation 5

$$n_s = \frac{log_{10}(^{P_3}/_{P_o})}{log_{10}(^{v_o}/_{v_4})}$$

Moving on to the correction factor, *f*, as proposed by Schultz for making correction onto polytropic head due to variation of n along the real compression.

Equation 6

$$f = \frac{h_4 - h_o}{(\frac{n_s}{n_s - 1})(P_3 v_4 - P_o v_o)}$$

Equation 7

$$\eta_p = \frac{f \times (\frac{n}{n-1})(P_3 v_3 - P_o v_o)}{h_3 - h_o}$$

From Equation 6, it is apparent that this correction is assumed to resemble the correction used for isentropic head (with final state at point 4, Figure 1), since n_s, also varies. Likewise as with v_4, h_4 is already a known value and can be obtained from equation of state. Equation 7 shows how polytropic efficiency is calculated from ASME PTC 10, its numerator is polytropic head and its denominator is actual head.

This is how polytropic efficiency is obtained for compressor tested based on ASME PTC 10 - by using real gas method. Most of the compressors are tested using ASME PTC 10. It then follows logically that the polytropic efficiency database from which compressor vendors use for new compressor performance prediction is obtained based on ASME PTC 10 method. As such, if we would like to estimate or predict discharge temperature of a compressor during design stage, based on estimated polytropic efficiency in that range of flow coefficient, the same approach as per ASME PTC 10 should be utilized for consistency. This approach is analogous to reverse engineering.

Equation 8

$$\eta_p = \frac{\frac{h_4 - h_o}{(\frac{n_s}{n_s - 1})(P_3 v_4 - P_o v_o)} \times \left[\frac{\frac{log_{10}(^{P_3}/_{P_o})}{log_{10}(^{v_o}/_{v_3})}}{\frac{log_{10}(^{P_3}/_{P_o})}{log_{10}(^{v_o}/_{v_3})} - 1}\right](P_3 v_3 - P_o v_o)}{h_3 - h_o}$$

The Equation 7 is expanded to Equation 8 by substituting Equations 4 and 6. With a known n_p, it can be deducted that v3 is the only unknown as h3 is implicitly linked to v_3. Since P_3 is a known value, by obtaining a second thermodynamic property (e.g., v_3) the other properties can be obtained (e.g., h_3, T_3, s_3). The problem is therefore reduced into solving an equation with only one unknown. This can be done by rearranging the equations in a convenient way to solve for v_3 and h_3 to obtain T_3. A real gas equation which links these properties is needed in the solving steps. Due to the complexity of solving the roots of equation of states directly, it is more convenient to obtain them via root-finding algorithms (e.g., Newton-Raphson method -two variables). The initial value of T_3 that is estimated was calculated via the $[T_3 = T_o(\frac{P_3}{P_o})^{(n-1)}/_n\ ]$ ideal gas equation. However, for simultaneous solving of multiple variables and equations, Newton- Raphson is a more appropriate method. While it may appear to be an inconvenient approach to calculate T_3, once this algorithm is automated, it is just a matter of seconds to check for every new case. The methods of resolving equation of states are beyond the scope of this paper and therefore only the basic concept is described. Now we can proceed for similar approach for ideal gas method before the comparison.

Equation 9

$$\eta_p = \frac{\frac{n_S-1}{n_S}}{\frac{n-1}{n}} = \frac{\left(\frac{\frac{c_{p0}avg}{c_{p0}avg-R}-1}{\frac{c_{p0}avg}{c_{p0}avg-R}}\right)}{\left[\frac{\frac{log_{10}\left(P_3/P_o\right)}{log_{10}\left(P_3T_o/P_oT_3\right)}-1}{\frac{log_{10}\left(P_3/P_o\right)}{log_{10}\left(P_3T_o/P_oT_3\right)}}\right]}$$

Equation 10

$$\frac{c_{p0}}{R} = a_o + a_1T + a_2T^2 + a_3T^3 + a_4T^4$$

Gas composition, in mol%	20% Methane 25% Ethane 50% Propane 5% N-butane
Suction pressure, P_o, bara	13.79
Suction temperature, T_o	46.11
Discharge pressure, P_3, bara	44.82
Polytropic efficiency, %	78.1

Table 1. Input data for real gas and ideal gas method calculation.

Ideal gas method

Ideal gas model is much simpler as per Equation 2, it can be re-arranged with substitution of n and n_s to generate Equation 9. Please note that c_{p0} avg is the average of c_{p0} at initial and final state. Now, for specific heat at constant pressure of ideal gas, c_{p0}, it only depends on temperature and thus it can be fitted by a polynomial series as per Equation 10, of which the constant a_i is specific for each gas [4]. Also, the effective representative c_{p0} of a specified gas composition is just a summation of product of each c_{p0i} and its mole fraction. We can now substitute Equation 10 into Equation 9, the resultant equation is too extensive to be presented here. Again, T_3 is the only variable at RHS of the resultant equation, and the solution can be done by the Newton Raphson method (with one variable). The same initial T_3 as that of above real gas method can be used. It is noted that the method presented here is an analytic solution, which in fact yields the same result of the usual iterative method, of which c_{p0} of final state and T_3 are iterated till they are matched.

Comparison between real gas and ideal gas method for discharge temperature

	Table C.6.2	Real gas method (with LKP)	Ideal gas method*
Discharge temperature, T_3, deg C	118.22	118.06	108.83
Comparison to Table C.6.2, % **	0	-0.04	-2.40

*Refer to Table A in Appendix 1 for the ideal gas specific heats used for calculation, extracted from Reference 4.
**Comparison based on absolute temperature scale.

Table 2. Comparison of results.

For a general and reliable reference, example from Table C.5.1, Table C.6.1 and Table C.6.2 of ASME PTC 10 is used, as well as LKP as the equation of state [5, 6]; the required input for T_3 estimation are listed in Table 1 .

Additionally, another comparison is done on a high discharge pressure (approximately 550 bara) and high CO2 (approx. 20%) case, of an EPC project (not to be named). (See Tables 3 and 4.)

Table 2 shows the comparison results. It is evident that result from the real gas model deviates negligibly by only -0.04%, while that of the ideal gas model deviates significantly more than 2%.

Gas composition, in mol%	~20% CO_2 ~60% Methane The rest not disclosed.
Suction pressure, P_o, bara	212.8
Suction temperature, T_o	40
Discharge pressure, P_3, bara	550
Polytropic efficiency, %	65.8

Table 3. Input data for real gas and ideal gas method calculation (high discharge pressure case).

	Vendor's data	Real gas method (with LKP)	Ideal gas method
Discharge temperature, T_3, deg C	107.1	110.0	131.7
Comparison to vendor's data, % **	0	0.77	6.47

** Comparison based on absolute temperature scale.

Table 4. Comparison of results.

Table 4 shows the comparison results. It is evident that the result from the real gas model deviates by only -0.77%, while that of the ideal gas model deviates significantly more than 6%.

Conclusion

Table 3.3 of ASME PTC 10 states the limits beyond which the ideal gas method is inadvisable to use; in this case, the example gas used would have exceeded the limits, and therefore the above deviation is expected. The intention for this comparison is that the real gas method shall be the prevailing method - regardless of whether the gas is close to ideal gas - by always checking the limits in Table 3.3. The ideal gas region is a sub-set of the real gas region, and hence, the result of the real gas method is always with the least deviation. Although the real gas method of ASME PTC 10 also has its favourable region (reduced pressure much lower than 1 and reduced temperature higher than 1.6) as reported in Reference [7], it is still the most realistic method to be used until superceded by a new method that becomes the standard or is adopted by ASME PTC 10. The real gas method has been tested across multiple compressor vendors for projects executed under Technip, and the T_3 difference averages 0.5%. In other words, this method, which is strictly consistent with ASME PTC 10, provides reliable results.

See references at: http://ct2.co/references

Appendix 1

Table A. Ideal gas specific heat parameters for selected gases.

			Cp⁰/R (ideal gas)				
Gas name	Mol. Wt.	Temperature range, K	a^0	a^1 ($x10^3$)	a^2 ($x10^5$)	a^3 ($x10^8$)	a^4 ($x10^{11}$)
Methane	16.043	50-1000	4.568	-8.975	3.631	-3.407	1.091
Ethane	30.070	50-1000	4.178	-4.427	5.66	-6.651	2.487
Propane	44.097	50-1000	3.847	5.131	6.011	-7.893	3.079
Butane	58.123	200-1000	5.547	5.536	8.057	-10.571	4.134

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