Simple, stable and reliable modeling of gas properties of organic working fluids in aerodynamic designs of turbomachinery for ORC and VCC

T Kawakubo
Manager, Turbomachinery and Engine Technology Department,
IHI Corporation, 1, Shin-nakahara-cho, Isogo-ku, Yokohama 235-8501, Japan
E-mail: tomoki_kawakubo@ihi.co.jp

Abstract. A simple, stable and reliable modeling of the real gas nature of the working fluid is required for the aerodesigns of the turbine in the Organic Rankine Cycle and of the compressor in the Vapor Compression Cycle. Although many modern Computational Fluid Dynamics tools are capable of incorporating real gas models, simulations with such a gas model tend to be more time-consuming than those with a perfect gas model and even can be unstable due to the simulation near the saturation boundary. Thus a perfect gas approximation is still an attractive option to stably and swiftly conduct a design simulation. In this paper, an effective method of the CFD simulation with a perfect gas approximation is discussed. A method of representing the performance of the centrifugal compressor or the radial-inflow turbine by means of each set of non-dimensional performance parameters and translating the fictitious perfect gas result to the actual real gas performance is presented.

1. Introduction
The Vapor Compression Cycle (VCC) or the Organic Rankine Cycle (ORC) makes use of the phase transition of the working fluid, thus the compressor or the turbine in the cycle inevitably operates near the vapor saturation boundary. Due to the high non-ideality (typically expressed by the deviation of the compressibility-factor from unity) of the working fluids near the saturation boundary, the designers of VCC compressors or ORC turbines must take the real gas effects into consideration appropriately for the reliable performance prediction in their designs. Although many current meanline performance prediction tools and commercially available Computational Fluid Dynamics (CFD) tools are capable of incorporating real gas models, simulations with such a gas model tend to be awkward and more time-consuming than those with a perfect gas model.

Figure 1 shows an example of the relative comparisons of accuracy and required computational time of CFD simulations with various degrees of fidelity in the gas modeling [1]. The simulation was conducted on an inviscid convergent-divergent nozzle operating with vapour R245fa which has a supersonic region downstream of the throat terminating with a shock wave. The applied equations of state include a perfect gas (PG) model, van der Waals (VDW) model, Peng-Robinson-Stryjek-Vera (PRSV) model and a real gas (RG) model provided by NIST REFPROP. The Mach number deviation was evaluated at an immediate vicinity of the shock wave on the downstream side. PG is the most attractive in terms of computational time. Its level of Mach number deviation is the highest among all
but still acceptably small (less than 2%). VDW is a good compromise between the perfect gas approximation and more sophisticated modeling. PRSV gives highly accurate solution with the half computational time of RG. From this example, it can be stated that by employing RG model we can get a last small improvement in accuracy at the cost of additional high computational burden.

Moreover the CFD simulation with a real gas model can be unstable because it is possible that a part of the internal flow may encounter a mixed-phase condition, especially in off-design conditions, or in the early stage of the CFD simulations when the thermodynamic states can be still far away from the final convergence and may go beyond the saturation boundary erroneously. From these observations, simulations with a perfect gas approximation are still a highly attractive option in order to swiftly and stably conduct design simulations.

The perfect gas model (more rigorously, the calorically perfect gas model for which both the thermal and the caloric equations of state are “perfect”) has only two independent modeling parameters, the gas constant $R$ and the isentropic exponent $\gamma$. The isentropic exponent of a general real gas is defined by

$$\gamma = \frac{\rho}{p} \left( \frac{\partial p}{\partial \rho} \right)_s = \frac{\rho a^2}{p}$$

and equal to the specific heat ratio $C_p/C_v$ under the perfect gas assumption.

What we want to do here is to select a set of the gas constant and the isentropic exponent which can best approximate the specific real gas behavior in terms of non-dimensional parameters. According to the similarity theory, the value of the gas constant does not substantially affect the non-dimensional performance and the isentropic exponent is the only gas property which enters into the problem of expressing the non-dimensional performance characteristic of the compressor or the turbine with a perfect gas as its working medium [2].

$$\psi_{is}, \eta_{is} = f(\phi, Re, M_{tip}, \gamma)$$

Thus, we can select any value as the gas constant. Here we simply define the gas constant by using the actual inlet condition as $R = p_1/\rho_1 T_1$ or in the original form $R = R_i/M_w$.

What to do next is to select an appropriate value of the isentropic exponent. Figure 2 shows a variation of the isentropic exponent of R245fa on the $p$-$T$ space. It varies from place to place in a compressor or a turbine, therefore it is natural to select one value which falls in the range of its variation or which represents an average. The problem is that the discharge condition of compressors or the inlet condition of turbines can be close to the critical point where the value of the isentropic exponent can get
smaller than unity. An isentropic exponent less than unity means a negative isobaric specific heat, thus in such a hypothetical fluid the temperature increases while the enthalpy drops.

Another issue associated with the gas modeling is the way the performance parameters should be converted to the actual intended condition when they are acquired in a simulation with a different working fluid than the intended one. Walsh and Fletcher suggest using a set of non-dimensional parameters to convert the performance, such as the tip Mach number, flow coefficient, isentropic load coefficient and efficiency [3]. Roberts and Sjolander [4] took a similar way for a centrifugal compressor but developed a method to correct the effects of the different specific heat ratios.

ASME PTC-10, on the other hand, requests to use the density ratio, flow coefficient, load coefficient and efficiency [5] for the conversion. Similarly, Macchi and Perdichizzi [6] suggest the use of the density ratio to accurately correlate the performance of the axial-flow turbines. Backström [7] described a translation of the compressor characteristic by means of the density ratio.

In the present study, it is intended to provide a way to approximate the real gas nature of an organic working fluid (in this study, R134a for a VCC compressor and R245fa for an ORC turbine) as a perfect gas. Problems in the approximation in the aerodynamic design of the VCC compressor or the ORC turbine were examined. Also discussed is the way to convert the compressor or the turbine performance obtained under a perfect gas approximation to the actual real gas working conditions.

2. Perfect gas approximation

2.1. Isentropic exponent

As mentioned in the introduction, the isentropic exponent is the only parameter to characterize the perfect gas in the non-dimensional term. In this study, the isentropic exponent will take a value close to that given by the perfect gas in the non-dimensional term. In this study, the isentropic exponent will take a value close to either the stage inlet value or the stage outlet one in an expectation that such a value can most closely approximate the actual real gas behavior.

2.2. Conversion rule of the performance characteristic between the real gas and the perfect gas

It is common to use a set of non-dimensional parameters to convert the performance data between different operating conditions or between different working fluids [3]. One may use the tip Mach number, flow coefficient, isentropic load coefficient and efficiency (hereafter designated as Type1), or the density ratio in place of the tip Mach number (designated as Type2).

\[
\begin{align*}
|F_1, p_1, M_{tip}, \psi_{1s}, \Phi, \eta_{is}| & \text{ are given} \\
p_2, \alpha_2, h_2, s_2 & \text{ are calculated from } F_1, p_1 \\
M_{tip} & = M_{tip,p_1} \\
\bar{\alpha} & = \Phi \beta_1, \alpha_{1s} M_{tip} \\
h_{2s} & = h_1 + \psi_{1s} u_{1s} \alpha_{1s} \\
F_2 & = h_2 + \eta_{is} (h_{2s} - h_1) \\
p_2 & = F_2 s_2 \\
p_2 & = \text{ calculated from } h_2, p_2
\end{align*}
\]

(a) Type1 conversion rule

\[
\begin{align*}
|F_1, \bar{p}_1, r_e, \psi_{1s}, \Phi, \eta_{is}| & \text{ are given} \\
p_1, \alpha_1, h_1, s_1 & \text{ are calculated from } F_1, \bar{p}_1 \\
\bar{p}_2 & = \Phi \beta_1 r_e F_1 \\
\bar{\alpha}_1 & = \text{ estimated} \\
\bar{p}_2 & = \text{ calculated from } \bar{p}_2, s_1 \\
\bar{p}_2 & = h_1 + \eta_{is} (h_{2s} - h_1) \\
p_2 & = \text{ calculated from } h_2, p_2
\end{align*}
\]

(b) Type2 conversion rule

**Figure 3.** Conversion rules from PG to RG (upper signs for compressors, lower signs for turbines).

Figure 3 shows how to transform the perfect gas (PG) results into the real gas (RG) condition using these two methods. In both rules, the non-dimensionalization is based on the stage inlet total condition
as usual. When Type2 is applied, an iterative procedure is required to get the stage exit thermodynamic condition. Moreover the rotor speed and the mass flow rate in the PG condition which will correspond to the intended values in the RG condition are unknown at the beginning of the simulation. In the design simulations, they are often used as inputs rather than outputs. Therefore Type2 conversion method cannot be readily incorporated into the conventional design procedure.

3. Validation of perfect gas approximation in CFD simulations

3.1. VCC centrifugal compressor stage
First of all, a CFD validation of PG was conducted against a refrigerant centrifugal compressor stage. It comprises a splitted impeller, a vaneless diffuser and a volute, but the volute was not modeled for simplicity. In this study and in all later studies, ANSYS Fluent was used. The convection terms were discretized with a second-order upwind scheme. The fluid was assumed to be viscous and the turbulence closure was modeled by the standard \( k-\varepsilon \) model with a near-wall treatment. Only one pitch of the impeller passages was modeled with a periodic boundary condition. Approximately 0.5 million hexahedral cells were used. The total pressure, the total temperature and the flow angle were specified at the impeller inlet while the back pressure was specified at the diffuser exit.

The real gas behaviour of the working fluid (R134a) was modeled by a virial equation provided in [8]. In the PG modeling, the physical gas constant and the inlet isobaric specific heat were used. The isentropic exponent was derived from these two values and slightly larger than the inlet value which is greater than unity. As an intermediate modeling, van der Waals model was also examined. As a conversion rule, the Type1 rule was adopted. The non-dimensional parameters were defined based on the blade tip speed and the density and the speed of sound evaluated at the inlet total condition.

![Normalized isentropic enthalpy rise](image1)

(a) Isentropic enthalpy rise

![Normalized isentropic efficiency](image2)

(b) Isentropic efficiency

**Figure 4.** Overall compressor performance.

Figure 4 shows the comparisons of the overall performance characteristics acquired by three gas models, the perfect gas (PG), van der Waals gas (VG) and the real gas (RG). For PG and VG cases, all these performance parameters were once non-dimensionalized and converted to RG condition by Type1 rule. All the three models predict exactly the same characteristics not only for the mid-range points but also for the highly off-design points. Figure 5 compares the deviation of the blade surface Mach number obtained by PG or VG from the one given by RG. The deviation is the highest at the leading and trailing edges but the level of the deviation is not so high, less than 2% in PG, which is generally acceptable in the usual design simulations. By using VG, the accuracy can be improved over PG considerably and the deviation can be suppressed to the half of PG level.
Thus far, no modeling difficulty has been encountered in the perfect gas approximation, even though the isentropic exponent was selected relatively arbitrarily.

(a) Impeller blade surface Mach number (PG)
(b) Impeller blade surface Mach number (VG)

Figure 5. Deviations in blade surface isentropic Mach numbers.

3.2. ORC radial-inflow turbine stage

Another CFD validation study about PG was conducted against an ORC radial-inflow turbine stage. In order to select an isentropic exponent and a conversion rule, one-dimensional meanline turbine simulations were first carried out. The meanline solver is based on the conservation laws supplemented with some loss models [9]. It can incorporate either RG or PG. At first the turbine was simulated under a specified design condition with a real gas model of R245fa provided by NIST REFPROP. Then several PG simulations were conducted with an isentropic exponent varying from the actual turbine inlet value $\gamma_1 < 1$ to the actual exit value $\gamma_2 > 1$ with a conversion rule either Type1 or Type2. Hereafter we call the perfect gas model with the inlet value PG1, while with exit value PG2. The non-dimensionalization was based on the stage inlet total condition.

Table 1 summarizes the meanline results in terms of Mach numbers and flow angles. As far as PG1 is used, two conversion rules do not make any substantial difference and the deviations from the RG results are satisfactorily small. When PG2 is used with Type2, the deviations are still on acceptable level, but when used with Type1, the deviations are much higher than other cases.

| PG type | PG1 | PG2 |
|---------|-----|-----|
| Conversion rule | Type1 | Type2 | Type1 | Type2 |
| (a) Impeller inlet parameters |
| Absolute Mach number | 0.02 | 0.01 | 0.02 | 0.00 |
| Relative Mach number | 0.01 | 0.01 | 0.02 | 0.00 |
| Relative flow angle (deg) | -0.9 | -0.7 | -3.7 | -1.2 |
| (b) Impeller exit parameters |
| Absolute Mach number | 0.01 | 0.01 | 0.04 | 0.02 |
| Relative Mach number | 0.02 | 0.01 | 0.08 | 0.03 |
| Absolute flow angle (deg) | -0.6 | -0.3 | -5.5 | -1.6 |

Even though the present meanline method accepts the negative isobaric specific heat as in PG1 with no difficulty, it would turn out later that the CFD simulation can be unstable with such a fictitious specific heat value. So we had to give up PG1. Also we gave up Type2 conversion rule due to the troublesome iterative procedure which would hardly be implemented in the usual CFD design simulations. Though the flow angle deviations are relatively high under the combination of PG2 and Type1, the impeller inlet relative flow is low subsonic so the incidence mismatch may not yield a severe difference in the incidence loss, and the exit absolute flow angle does not strongly affect the impeller component efficiency, therefore we decided to use PG2 with Type1 conversion rule. Any $\gamma$ value greater
than unity but smaller than \( \gamma_2 \) would give better result but not used because the closer the \( \gamma \) value to unity the more unstable the CFD simulation may become.

A comparison of CFD with RG/PG models was conducted next. The turbine stage has a volute, a vaned nozzle and an impeller, but again the volute was not included in the model for simplicity. The rotor-stator interface was connected by a mixing-plane. The realizable \( k-\varepsilon \) model with the enhanced near-wall treatment was used. The other conditions were similar to those used in the compressor case.

Figure 6 compares the overall turbine performance. For PG case, all these performance parameters were once non-dimensionalized and converted to the RG condition by means of Type1 conversion rule. In these performance comparisons, there can be observed little substantial difference between solutions. Figure 7 shows the deviation of the isentropic Mach number on the impeller blade surface or on the nozzle vane surface. No substantial difference can be observed in the nozzle passage. On the other hand, the deviation in the impeller is as high as 0.1. The level of this deviation is compatible with the one predicted by the meanline analysis and considered non-negligible.

If we simplify the turbine expansion process as isentropic and the working fluid as PG, then the density ratio can be expressed as

\[
\frac{\rho_{04}}{\rho_{01}} = \left\{1 - (\gamma - 1)\psi_{\Omega}M_{\text{tip}}^2\right\}^{1/(\gamma-1)}
\]

This expression suggests that the higher the \( \gamma \), the lower the exit density. The adopted value of \( \gamma \) in PG2 is the highest one in the actual turbine passage therefore PG2 should predict an excessively low exit density. The deviation in Mach number is mainly caused by this excessive decrease of the density, which results in the higher through-flow velocity.

**Figure 6.** Overall turbine performance (total-total).

**Figure 7.** Deviations in blade/vane surface isentropic Mach numbers (PG2).

3.3. Improvement of perfect gas approximation for ORC turbine
In an attempt to improve the PG modeling, Type1 conversion rule was modified. Now, as in the compressor case, the non-dimensionalization will be conducted based on the lowest pressure condition (Type3), the isentropic exit condition which is defined by the stage inlet total temperature and total pressure and the stage exit static pressure. These three quantities are the CFD input, so no iterative procedure will be required. The tip Mach number and the flow coefficient are defined as \( M_{\text{tip}} = \frac{u_{\text{tip}}}{a_{2S}} \) and \( \Phi = \frac{G}{(\rho_{2S}D_{\text{tip}}^2u_{\text{tip}})} \), respectively. The gas constant and the isentropic exponent of the revised perfect gas model (PG2S) are defined \( R = \frac{p_{2S}(\rho_{2S}T_{2S})}{\gamma} \) and \( \gamma = \frac{\rho_{2S}a_{2S}^2}{p_{2S}} \), respectively. By defining gas properties and non-dimensional parameters as above, we do not have to translate the rotor speed and the mass flow rate. The inlet condition of PG is defined so that the isentropic loading coefficient and the back pressure will be same as RG. A meanline simulation was again carried out and the maximum Mach number deviations and the flow angle deviations in the nozzle/impeller were 0.02/0.01 and +0.7(deg)/+1.3(deg), respectively. Therefore the expected accuracy of the revised method is better than Type1 and comparable to Type2.

Next the CFD simulation based on the revised method was carried out. Figure 8 compares the performance characteristics. In the previous Figure 6, the pressure ratio and the efficiency were defined by total-total basis, but in order to emphasize the influence of the density on the performance they are now defined by total-static basis. The efficiency discrepancy between RG and PG2 is about 1%, rather a big difference, and is caused by the difference in the discharge velocity and density. By applying PG2S and Type3, the efficiency is predicted quite closely to RG. The output power is not affected whether define in total-total or total-static, and PG2S predicts it as accurately as PG2. Figure 9 displays the Mach number difference between PG2S and RG. The deviation in the nozzle increased only slightly compared with PG2 but still negligible. On the other hand, the deviation in the impeller is greatly suppressed. No deviation can be observed in the leading edge part, implying that the new method can correctly predict the inlet flow vector. The gradual increase of the deviation toward the trailing edge observed in PG2 is also suppressed. From these results, it can be concluded that the modified perfect gas model can effectively substitute the RG simulation for the design purpose.

![Figure 8](image-url)  
Figure 8. Overall turbine performance (total-static).
4. Conclusion
A method to approximate the real gas nature of organic compounds by a perfect gas and the way to convert the CFD results obtained with a perfect gas approximation into the real gas condition were proposed. The validity was examined by comparative CFD simulations. The method proved to be quite reliable in the prediction of the overall performance and very helpful to accelerate and stabilize the design CFD simulations of VCC compressors and ORC turbines.

5. Nomenclature

- \( a \) Speed of sound (m/s)
- \( r_v \) Density ratio
- \( C_p, C_v \) Isobaric/Isochoric specific heat (J/kg/K)
- \( D_{\text{tip}} \) Impeller tip diameter (m)
- \( G \) Mass flow rate (kg/s)
- \( h \) Enthalpy (J/kg)
- \( s \) Entropy (J/kg·K)
- \( T \) Temperature (K)
- \( u_{\text{tip}} \) Blade tip speed (m/s)
- \( \gamma \) Isentropic exponent
- \( M, M' \) Absolute/Relative Mach number
- \( M_{\text{tip}} \) Tip Mach number = \( u_{\text{tip}} / a \)
- \( M_W \) Molar mass (kg/kmol)
- \( p \) Pressure (Pa)
- \( \rho \) Density (kg/m\(^3\))
- \( R \) Gas constant (J/kg·K)
- \( R_u \) Universal gas constant (J/kmol·K)
- \( \eta_{\text{is}} \) Isentropic efficiency
- \( \pi \) Pressure ratio
- \( \Phi \) Flow coefficient = \( G / (\rho D_{\text{tip}}^2 u_{\text{tip}}) \)
- \( \psi_{\text{is}} \) Isentropic load coefficient = \( \Delta h_{\text{is}} / u_{\text{tip}}^2 \)

6. References

[1] Kaneko, Y., et.al, 2015, Design method of a radial-inflow turbine for an organic rankine cycle generator using CFD with perfect gas assumption, Proc. of the 13\textsuperscript{th} Asian Int. Conf. on Fluid Machinery (Tokyo, Japan) Paper No. AICFM13-198.
[2] Dixon, S. L., 1998, Fluid mechanics, thermodynamics of turbomachinery
[3] Walsh, P. and Fletcher, P., 2004, Gas turbine performance,(Blackwell-Publishing).
[4] Roberts, S. K. and Sjolander, S. A., 2005, Effect of the specific heat ratio on the aerodynamic performance of turbomachinery, ASME J. of Engg. for Gas Turbines and Power, vol.127, pp.773-780.
[5] ASME, 1997, Performance test code on compressors and exhausters, ASME.
[6] Macchi, E. and Perdichizzi, A., 1981, Efficiency prediction for axial-flow turbines operating with nonconventional fluids, ASME J. of Engg. for Power, vol.103, pp.718-724.
[7] Von Backström, T. W., 2008, The Effect of specific heat ratio on the performance of compressible flow turbo-machines, Proc. of ASME Turbo Expo 2008, (Berlin, Germany), Paper No. GT2008-50183.
[8] JAR and JFGA, 1991, Thermophysical properties of environmentally acceptable fluorocarbons – HFC-134a and HCFC-123, JAR and JFGA
[9] Rodgers, C., 1987, Mainline performance prediction for radial inflow turbines, VKI Lecture Series 1987-07.