The Real Gas Effect on the Stagnation Properties for Supercritical Carbon Dioxide Flows

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ABSTRACT
This paper presents a comprehensive study on the stagnation properties namely the total pressure and total temperature for supercritical CO₂ flows including the methodology, applications and detailed analysis. Due to the high nonlinear real gas effect, it is practically impossible to have explicit expressions between static and its corresponding stagnation properties. The equations of obtaining the real gas stagnation properties as well as their physical meanings related to fluid dynamics need to be reconsidered. In this paper, the stagnation pressure and temperature for sCO₂ flows are accurately calculated in a way that implicitly iterated from stagnation enthalpy and entropy without any addendum assumptions. Accordingly, this approach is applied to typical applications that essentially exert stagnation properties. The total pressure and total temperature of typical sCO₂ flows in which contain significant real gas characteristics are numerically studied by using our in-house CFD code coupled with real gas models. It is found that the real gas tends to preserve more internal energy than the ideal gas during irreversible flow process especially with the presence of shockwaves. Finally, as a regular indicator of viscous flow loss, the total pressure loss for a sCO₂ compressor cascade is evaluated.

NOMENCLATURE

| Symbol | Meaning |
|--------|---------|
| U      | Velocity in x-direction m/s |
| V      | Velocity in y-direction m/s |
| W      | Velocity in z-direction m/s |
| T      | Static temperate K |
| P      | Static pressure Pa |
| h      | Static enthalpy J kg⁻¹ K⁻¹ |
| s      | Static entropy J kg⁻¹ K⁻¹ |
| u      | Magnitude of flow velocity m/s |
| ρ      | Density Kg/m³ |
| T_e    | Critical temperature 304.13K |
| P_e    | Critical pressure 7.3773MPa |
| Z      | Compression factor |
| n_s    | Isentropic exponent[6] |
| m_s    | Isentropic exponent[6] |

Symbols

1 Stagnation condition
s Static condition
I Inflow measurement station
O Outflow measurement station

INTRODUCTION
The merit of using supercritical CO₂ (sCO₂) as the working fluid of closed Brayton Cycle gas turbine is now widely recognized as it offers alternatives for solar, geo-thermal, and nuclear energy conversion. This technique relies on the reduced compression work of the working fluid performing close to the critical point while maintains a compact configuration compared with conventional cycles [1] which results in a strong real gas effect difficulties to be analyzed.

The stagnation quantities (i.e. total properties) are the sum of the static and dynamic properties of flow, which are essential throughout the whole design, testing and simulating processes. They maintain important physical meanings in terms of fluid dynamics, namely an effective measure of total head of the flow. The first example could be the sCO₂ compressor aerodynamic performance, in which the compression ratio is characterized by the total pressure ratio. The deviation on corrected mass flow or total pressure ratio will possibly degrade the whole design. The second example is the Pitot probe, which provides flow velocity from the measured total and static pressures. The third example appears in CFD solvers. Imposing the total temperature and total pressure as the inlet boundary conditions is a common practice in most turbomachinery simulation, yet it becomes non-trivial in real gas simulation as opposed to ideal gas cases because the static pressure and temperature cannot be specified explicitly. The fourth typical example could be the flow loss evaluation by total pressure during the turbomachinery aerodynamic design or analysis. Design methods or loss models need to be modified on a basis of real gas concept in case of misleading in design. Thus, there has been significant interest in understanding the real gas stagnation properties.

However, the total-to-static relationships acquired for ideal gas cannot be directly applied to sCO₂ flows due to the presence of real gas effect. The flow thermal parameters rapidly change when it...
investigated including shockwave, sub-critical condition and trans-critical condition. Finally, the total pressure loss for a \( \text{scCO}_2 \) compressor cascade under gaseous and liquidous operating conditions are studied. In doing this, discussions is placed on elucidation of the physical concepts associated with the real gas features seen in loss coefficient distributions.

**METHODOLOGY**

Numerical scheme and real gas model

An in-house code was used to perform the numerical studies, which was designed to solve the compressible three dimensional Reynolds-averaged Navier-Stokes equations. It was discretized in the computational domain by a cell-centered finite volume formulation. Time integration was accomplished by the Euler implicit method with the lower-upper symmetric Gauss-Seidel scheme (LU-SGS), and no inner iterations were introduced. The inviscid fluxes were evaluated by a simple high-resolution upwind scheme (SHUS), which was extended to third-order accuracy by the MUSCL interpolation via implementing a modified form of Venkatakrishnan’s slope limited. The equations system solves for the primitive variables by the vector \( \mathbf{q} = [U, V, W, T, P, k, e] \), in which \( k \) and \( e \) are turbulence transportations. Especially, the inviscid flux is estimated as:

\[
E = \frac{1}{j} \begin{pmatrix}
\rho u_1 & \rho u_2 & \rho \epsilon \\

\rho u_1^2 + p & \rho u_1 u_2 & \rho \epsilon \\

h & \rho u_2 & \rho \epsilon
\end{pmatrix}
\]

Where \( h \) is the total enthalpy while \( j \) is the Jacobian matrix. The cell surface pressure is determined by the split Mach numbers \( M_s \).

\[
p_s = \beta_\parallel p_s + \beta_\perp p_p.
\]

\[
\beta_\parallel = \frac{1}{4} (2 \mp M_s) (M_s \pm 1)^2 \quad \text{if} \ -1 < M_s < 1
\]

\[
\beta_\perp = 1, \quad \beta_\parallel = 0 \quad \text{if} \ M_s > 1
\]

\[
\beta_\perp = 0, \quad \beta_\parallel = 1 \quad \text{if} \ M_s < -1
\]

The mass flux shown in Eq. (1) is calculated with Roe scheme form in Eq. (4), where \( \Delta \) represents the differential between the surface two sides:

\[
m = \frac{1}{2} \left( \rho \nu^*, + (\rho \nu^*) \cdot \nabla \right) \cdot \nabla p - \frac{\nu^*}{2} \left[ \frac{\nu^* | \nu^* - 1 | ^2 p - \nu^* | \nu^* - 1 | ^2 \frac{2p}{\nu^*} \right]
\]

\[
\overline{M} = \frac{\rho}{\Sigma}, \quad \overline{V} = \frac{\rho}{\rho^*}, \quad \overline{P} = \frac{\rho}{\rho^*}, \quad \overline{\nu^*} = \frac{\nu^*}{\Sigma}
\]

For real gas solver, the averaged sound speed is directly estimated by:

\[
\overline{\nu^*} = \sqrt{\frac{c_\parallel^2 + c_\perp^2}{2}}
\]

The real gas properties are calculated with a tabulate method (LUT), which is an alternative analytical equation of Span & Wagner’s EOS, the one that specified used for \( \text{CO}_2 \). All the needed variables including four necessary derivatives \( \rho_1, \rho_2, h_1, h_2 \) are decided by the tabulated variables \( T \) and \( \rho \) by using bilinear interpolations ranging from 230K~400K and 2MPa to 20MPa with cluster at the near critical point. Two schemes of discretization nodes that are 128*128 points and 256*256 points are set and examined. In which, the bisection method are exerted to accelerate
the interpolation time. The accuracy of the interest thermal properties under different real gas conditions are compared in Figure1. It shows a remarkable improvement on the average interpolation error than that of Peng-Robinson EOS, especially for the near critical point. To achieve a better accuracy, the 256*256 points table are utilized. In this paper, the mono-phase flow is considered. For the turbulence calculation respected to sCO2 flow, the standard two-equation $k$-$\omega$ turbulence model was adopted to evaluate the eddy viscosity.

![Figure 1](image1.png)

(a) the critical point  
(b) very close to critical point  
(c) liquid-like  
(d) super critical

**Fig.1 Accuracy of different real gas models compared with NIST data**

**Real gas stagnation properties**

We designed an approach to solve real gas total pressure and total temperature in a way that purely relies on numerical iterations. For a real fluid flow, the total pressure and total temperature are determined by arbitrary pair of static properties plus one property that describes flow speed. Here, we use $T$, $P$, $u$ to define a flow as they are the solving vector in our CFD code.

$$P_t = f_1(T, P, u)$$

$$T_t = f_2(T, P, u)$$

Figure 2 illustrates a real gas flow at an arbitrary local point ($T$, $P$) with a certain velocity and its corresponding stagnation point ($T_t$, $P_t$) in temperature-entropy coordinate. For a general condition, the total enthalpy of a dynamic flow is calculated with Eq. (8).

According to fundamental thermodynamics, stagnation point is the state that flow isentropically decelerates into zero velocity. During this process, the flow yields:

$$h_t = h + 0.5u^2$$

$$s_t = s$$

![Figure 2](image2.png)

**Fig.2 A sketch to illustrate the relation between a pair of total quantities and static quantities in T-s diagram**

Thus, it turns to be finding the point ($P_t$, $T_t$) that exactly satisfy the correct entropy and total enthalpy ($h_t$, $s_t$) values at the same time. Since the relevant variables are also determined by temperature and pressure, it is difficult to reach the correct solution at one time. A nest-loop procedure is configured. The inner iteration is applied to obtain a series of points that yield the true entropy value. The outer iteration is applied to pick up the correct one that yields target total enthalpy value. To accelerate the iteration, the Secant method is employed. The whole procedure are illustrated as Figure 3 shows.

![Figure 3](image3.png)

**Fig.3 Flowchart of the proposed approach**

**Inner loop:**

The iterative procedure is started with an input of arbitrary initial guess of total temperature, labeled as $T_t^0$ in Figure 3. Here, the upper subscript records the number of iterations. By setting two different total pressure values $P_t^0$ and $P_t^1$, the inner iterative process can be initialized. After a few iterations, the $P_t^0$ that corresponds to $T_t^0$ (i.e. yields the correct entropy value) can be resolved. Although this point ($T_t^0$, $P_t^0$) fulfills target entropy value, it is certainly not the desired one for the target total enthalpy $h_t$ since the total temperature $T_t^0$ is arbitrarily chosen at current stage.

**Outer loop:**

Set another total temperature $T_t^1$ and repeat the previous step, now we obtain two pairs of ($T_t^1$, $P_t^0$) and ($T_t^1$, $P_t^1$) locating on the
constant entropy curve. Similarly, the target $T_t$ and $P_t$ can be achieved within a few iterations with Secant method. It should be noticed that each outer iteration embeds an execution of inner iterative procedure.

This current approach relies solely on mathematical iterations, avoiding to derive the complex real gas entropic relations. Theoretically, it provides accurate predictions of real gas stagnation properties. Furthermore, this proposed approach are not restricted to any procedure on modeling the real fluid. For example, in authors’ previous study [9], we showed the detailed algorithm when applied with Peng-Robinson EOS.

APPLICATIONS WITH REAL GAS STAGNATION PROPERTIES

Real gas Pitot probe

The Pitot tube is simple yet indispensable tool to obtain the flow total pressure and incoming velocity. For ideal gas, there are explicit expressions between total to static properties (Eq. (10-11)), where $\gamma$ is the specific heat ratio with constant value. The flow total pressure and static pressure are directly measured while the flow velocity can be calculated by using Eq. (10).

$$\frac{P_t}{P} = \left(1 + \frac{\gamma - 1}{2} M_t^2\right)^{\frac{\gamma}{\gamma - 1}} \quad (10)$$

$$\frac{T_t}{T} = \left(1 + \frac{\gamma - 1}{2} M_t^2\right)^{\frac{\gamma - 1}{\gamma}} \quad (11)$$

For real fluids, however, those relations become invalid. How to measure the real gas flow velocity by Pitot tube is of significant importance. Assume that the total temperature is known by certain means and the Pitot tube is pointing directly to the inflow. The real gas velocity can be obtained by using the current approach. Figure 4 describes the general idea of the data post-processing procedure. Having the measured total pressure and total temperature, the total enthalpy and entropy can be directly known. The static temperature can thus be searched implicitly by entropy and measured static pressure. Accordingly, the flow velocity can be derived with Eq. (8). The presented approach is possible to be extended into three-hole probes or other sophisticated probes to cover a wide range of real fluid measurements.

Total quantity implementation in CFD code

It is a common practice to specify the total $T_t$ and $P_t$ combined with inflow direction at the inlet boundary for internal flow simulations such as turbo machines or duct flows. This implementation, however, requires special treatment for real gas flows due to the lack of total-to-static entropic relations.

An available way to impose total quantities for real fluid CFD solver is suggested by using the proposed method. The primitive variables $\Omega$ is stored at the cell center as shown in Figure 5. It is thus required to find the first cell center’s static pressure and temperature with the given total quantities. Having the known total temperature and pressure, the total enthalpy and entropy can be calculated with NIST Refrop or EOS. The velocity is extrapolated from the interior computational domain, and the static enthalpy and entropy can be calculated explicitly. Similarly, the desired static pressure and temperature are resolved by aforementioned nest-loop iterative approach. It follows the same logic when it is applied with total enthalpy and entropy as the inlet boundary conditions.

**Fig. 4 Data process of Pitot tube measurement for real gas flows**

**Fig. 5 Inlet boundary and the first cell center for CFD code**

**Fig. 6 The P-T variations along nozzle centerline for the three investigated cases**
Figure 7 presents the validation for the numerical method with Case A. Here, the black dots labeled with SHUS present the results calculated by Arina [11], in which the real gas were modeled with Carbahian-Starling-De Santis EOS. It is clearly seen that the results agree well with each other.

**Supercritical condition with shockwave (Case A)**

The real gas effect on sCO2 flows with the presence of shockwave is discussed in this section. The shallow blue curve represents flow Mach number at nozzle center line. For comparison purpose, the distributions for ideal gas are also presented, which is calculated by Rankine-Hugoniot relation. The sCO2 flow predicted by this current approach is shown with red lines in Figure 8 and 9. We also calculated those two quantities with Baltadjiev’s method [6], which is the explicit theoretical equations derived by real gas isentropic relation shown in Eq. (13-14). It is clearly seen those equations present in quite a similar form with their ideal gas counterparts (Eq. (10-11)). Note that the isentropic exponents \( n_s \) and \( m_n \) are assumed to be constant during the stagnation process which are actually vary with states. This approximation is of somewhat higher order than the assumption of constant specific constant heat ratio of ideal gas [8], while it significantly helped us to obtain the explicit formulas on a basis of thermodynamics.

\[
\frac{P}{P_i} = \left[ 1 + \frac{n_s - 1}{2} M^2 \right]^{\frac{n_s}{n_s - 1}} 
\]

(13)

\[
\frac{T}{T_i} = \left[ 1 + \frac{n_s - 1}{2} M^2 \right]^{\frac{n_s}{n_s - 1}} 
\]

(14)

It is found that the real gas effect have an appreciable influence on flow energy conversion when across the shock. There is no difference for the two total properties at shock upstream between real fluids and ideal fluids. However, lower total pressure and total temperature are found at shockwave downstream. For the total pressure distribution, shock downstream values are specified as 21.48MPa for real gas and 21.417MPa for ideal gas, with a 0.3% deviation. The total temperature, on the other hand, is expected to remain constant in this adiabatic workless change of state. However, this principle is no longer true for non-ideal flows. As demonstrated in Figure 9, the total temperature is decreased by 3.54K at the shock downstream, accounting for 0.9% of the inlet total temperature. It is considered as the real gas behavior that certain of the flow kinetic energy is converted to molecular thermal vibrational energy. It is deemed that the energy conversion between flow mechanical energy and internal energy is enhanced compared with ideal gas flows. The real gas effect tend to reserve more internal energy during the suddenly compressible process.

For the total properties calculated with Baltadjiev’s method [6], negligible difference predicted by the two approaches is shown with low-speed region. However, visible deviation is seen as Mach number exceeds 0.4. Accuracy diminishes as Mach number increasing, reaching maximum at the shockwave position. Larger discrepancy with wider Mach number is seen in total temperature prediction. This theoretical method shows a maximum discrepancy of 6.5% in total pressure and 7.3% in total temperature.

![Fig. 7 Dimensionless density distribution along nozzle centerline for Case A](image1)

![Fig. 8 The Pt distribution along nozzle centerline for Case A (supercritical condition with shockwave)](image2)

![Fig. 9 The Tt distribution along nozzle centerline for Case A (supercritical condition with shockwave)](image3)

### Table 1 Boundary conditions for three investigated cases

| Case     | \( P_i \) [MPa] | \( T_{t1} \) [K] | \( P_2 \) [MPa] | Z-factor |
|----------|-----------------|------------------|----------------|-----------|
| Case A   | 23              | 410              | 18             | 0.54-0.70 |
| Case B   | 12              | 300              | 9.5            | 0.17-0.24 |
| Case C   | 12              | 330              | 10.5           | 0.35-0.42 |

The deviation in shockwave downstream total pressure and total temperature from ideal gas theory is further investigated. Keeping the inlet condition unchanged, by adjusting the nozzle back pressure, Figure 10 presents shockwave downstream total quantities versus shock intensity. It is clearly seen that real gas flows maintain a lower total quantities compared with their ideal gas counterparts. As upstream Mach number exceeds 1.26 for total pressure while 1.1 for total temperature, visible deviation from ideal flows are observed. The stronger the shock is, the lower the downstream total quantities.

![Fig. 10 Shockwave downstream total quantities versus shock intensity](image4)
Total temperature is seen more sensitive to real gas effect than total pressure.

**Sub-critical condition (Case B)**

The sub-critical sCO2 flows is concerned in this section, which is provided with inlet density as high as 800kg/m³, like liquid. This flow performs highly real gas behavior, sustaining Z-factor around 0.2. The inlet of sCO₂ compressor usually situates under this condition for the sake of compression work reduction. This also benefits the compactness of whole cycle layout. The nozzle is provided with total pressure of 11Mpa and total temperature of 300K. The back pressure was set as 9.5MPa, making the pressure at throat was exactly the critical pressure value.

Figure 11 and 12 present the total pressure and total temperature distributions along nozzle centerline. For a better illustration, the Mach number is also plotted in the same figure. Slight oscillation of total pressure appears at the nozzle throat for both two methods, with a maximum relative error of 0.046%. It is considered to be caused by entropy calculation. The current approach shows an accurate prediction on total temperature while slightly under-estimation is found through the whole nozzle by means of Baltadjiev’s method, in particular, 0.4K difference at throat while 0.1K at downstream. This suggests that the isentropic exponents do departure from constant assumption when close to the critical point.

**Trans-critical condition (Case C)**

There is a maximum in the specific heat \( C_p \) as the temperature or pressure changes across an extension line of the saturation curve, referred as the ‘Pseudo curve’. This curve is viewed as the transition line between gas-like and liquid-like behavior in supercritical fluids. The sharp increase in \( C_p \) tend to easily trigger numerical instability in that area. The characteristic of total properties for trans-critical flows is studied in Case C. In this case, the flow at nozzle centerline goes along pseudo-critical curve and approaches to the critical point at throat.

The total pressure and total temperature distributions are presented in Figure 13 and 14. Both total quantities keep the same as their ideal gas counterparts, means that total temperature keeps constant for irreversible process even for real gas flows. It again shows an accurate prediction in total temperature. Oscillation in total pressure is observed as flow close to throat, with a maximum relative error of 0.04% for current approach while 0.07% for Baltadjiev’s method, the later holds a wider range with a larger amplitude. Additionally, over-estimation is found in total temperature calculation, up to a value of 0.5K.
REAL GAS TOTAL PRESSURE LOSS ANALYSIS

The total pressure loss for a real gas compressor cascade is investigated with the purpose of understanding the real gas effect on total pressure loss analysis. Due to the lack of sCO2 cascade test data, we herein choose an axial compressor cascade C4 as an interpretive example. This is more a fundamental study than an attempt to find the aerodynamic design principle. Table 2 lists the original geometry of the studied cascade. The flow field of inlet Reynolds number of $4 \times 10^5$ with inlet Mach number of 0.15 is concerned. Simulation are performed by single passage with periodic boundary in pitch direction. In order to estimate the real gas total pressure loss, two distinct sCO2 inflow conditions are provided. A gaseous inflow condition with inlet total pressure of 1.06$P_i$, and total temperature of 1.027, while a liquid-like inflow condition with the same inlet total temperature but inlet total pressure of 1.4$P_i$ are investigated. For all cases, the inlet Reynolds number and Mach number are fixed by adjusting the chord dimension and back pressure. The performance of a compressor cascade is traditionally reported in the form of a total pressure loss coefficient $\omega$, where $P_{t1}$ and $P_{t2}$ are the averaged stagnation pressure at inlet and outlet of the cascade while $P_{t1} - P_{t2}$ is the dynamic pressure of inflow:

$$\omega = \frac{P_{t1} - P_{t2}}{P_{t1} - P_{i1}}$$  \hspace{1cm} (15)

Table 2 Specifics for C4 cascade [12]

| chord    | 152.4mm |
|----------|----------|
| stagger angle | 34.6° |
| camber angle  | 20° |
| Solidity   | 1 |

Six different inlet incidence angles changing from $-9^\circ$ to $11^\circ$ are examined. Figure 15 presents the variation of total pressure loss coefficient with incidence angle. Sharply increased total pressure loss is observed as the incidence angle is as large as $11^\circ$. It is suggested from the test data that blade stall occurs under this inflow condition. The gray curve and black dots compare the data between simulation and tests for ideal air flow. The simulations agree well with the experiments for most incidence angles. However, RANS failed to capture the significant increase in total pressure loss at large incidence angle which is characterized by severe flow separations. Although numerical simulation cannot repeat the measured loss coefficient for incidence angle of $11^\circ$, generally the tendency that flow loss reaches maximum under this inflow condition is well reproduced.

The real gas effect on total pressure loss for compressor cascade is clearly seen. Since the inlet Reynolds number and Mach number are kept the same, it is recognized that the total loss coefficient for air and CO$_2$ under ideal gas state should be same. Herein we take the results for ideal air equivalent to that for ideal CO$_2$. The total pressure loss coefficient generally behaves a same tendency as that for perfect gas while the s CO$_2$ cascades maintain a slightly lower shockwaves. It is found that the total pressure and total temperature sustain a lower value at shockwave downstream than ideal gas.

![Fig.15 The total pressure loss coefficient versus incidence angle for gaseous and liquid-like sCO2 compared with perfect air for C4 cascade (inlet Re: $4 \times 10^5$, inlet Ma: 0.15).](https://example.com/fig15)

![Fig.16 The normalized total pressure counter at incidence 11°](https://example.com/fig16)

CONCLUSIONS

In this paper, the real gas stagnation pressure and temperature are comprehensively studied. The method to solve real gas total pressure and total temperature, the associated applications as well as their physical meanings are throughout investigated. The physical meaning of total properties in real gas flows are investigated. Main conclusions are summarized as following:

1. An iterative approach to accurately obtain real gas total pressure and total temperature is developed which is a purely mathematical algorithm without inducing any assumptions and functionally interchangeable with arbitrary pair of thermal properties. Additionally, it is not restricted with equation of state or look-up table method.

2. This approach is extended into two applications that exert total properties as a must: the real gas Pitot tube measurement and inlet boundary implement for CFD code. The data process procedure of real gas Pitot tube is presented. We also provide a possible solution to impose total properties as the inlet boundary conditions for CFD codes.

3. Typical sCO2 flows are numerically studied. The total properties behave distinct from ideal gas flows when there exist shockwaves. It is found that the total pressure and total temperature sustain a lower value at shockwave downstream than ideal gas.

![Image](https://example.com/image)
flows. Especially, the total temperature no longer keep constant when across shockwaves. The stronger the shockwave, the lower the downstream total properties.

4. The physical meaning of total pressure and total temperature are discussed. It was found that the total temperature no longer represents total enthalpy for real gas flows when there is irreversible process. The total pressure, however, still evaluates the flow dynamic loss. It shows the lower loss generated when working fluid is sCO2 than perfect air. The operating range seems potentially wider for liquid-like than their air counterpart.

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