

FURTHER DEVELOPMENT OF A THROUGH-FLOW PROGRAM BY CONSIDERING REAL GAS EQUATION OF STATE

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ABSTRACT

Numerical methods are significant in the turbomachine design process and off-design analysis. One of these methods is the through-flow method in the meridional plane, which is utilised in an early design phase. It provides robust and quick numerical analysis of turbomachinery by only giving a few characteristic geometric parameters.

This work further develops the through-flow program *tFlow* by incorporating real gas equation of state (EOS), in order to verify the application of real gas EOS with the through-flow method. This allows the program to support a more reliable calculation regarding, for instance, carbon dioxide (CO₂) in a high-pressure region, where the gas does not behave like an ideal gas. The program is verified against one-dimensional (1D) solutions for the flow through a converging-diverging nozzle at different flow conditions. Furthermore, the calculation results verify the application of the Jameson-Schmidt-Turkel (JST) scheme in terms of real gas EOS. Consequently, this development brings the possibility to employ *tFlow* in a broader range, for example, for supercritical CO₂ (sCO₂) compressors or turbines.

INTRODUCTION

The modern design process of turbomachinery requires numerical analysis in an early design phase, where only few information is specified. To obtain a relatively robust analysis, the through-flow method [1] is widely applied, since it only solves the flow conditions at the meridional plane and, therefore, does not need numerous parameters especially regarding the geometry in contrast to fully three-dimensional (3D) computational fluid dynamics (CFD) methods. This feature also allows a faster computation. In recent years, researchers such as Baralon et al. [2], Sutrmayr and Hirsch [3], and Pacciani [4] focused on the through-flow method based on the Euler equations with finite-volume method due to its benefit from radial mass transport and capability of using the Euler equations in conjunction with a time-marching approach. Under this background, an Euler-based through-flow computer program

named *tFlow* has been developed by Föllner et al. [5] and extended by Jenzen et al. [6] to solve the flow conditions in axial turbomachines and radial compressors. Caused by the increased interest in real gas properties in recent years, especially in the field sCO₂ applications, it seems sensible to extend through-flow methods to gases like CO₂, which do not behave like an ideal or perfect gas in the considered pressure and temperature range. This development will provide a quick and robust preliminary design phase for e.g. sCO₂ turbomachines.

Thus, aiming this gap, the present work contributes to the through-flow calculation with real gas EOS. Since several assumptions such as some constant parameters are invalid within real gas EOS as mentioned before, special attention has been taken during the calculation of the fluid properties in this work.

In this work, the EOS of Span and Wagner [7] incorporated in Refprop is employed to solve the fluid properties. Furthermore, lookup tables (LUTs) are established to reduce the computation consumption. As a test case, the flow conditions in a converging-diverging verification (CDV) nozzle is calculated and compared with the results of a 1D quasi-analytical analysis as well as results of literature.

GOVERNING EQUATIONS

The through-flow method applied in the presented program is based on Wu's work [1], where the flow field is only solved at the meridional plane $S_{2,m}$, as shown in Figure 1. Therefore, the requirement on geometry and meshing mainly focuses on $S_{2,m}$. Then, the program solves the channel flow by considering a 3D axisymmetric system. The program neglects the calculation of wall boundary layer, namely at the shroud and hub, so that the inviscid Euler equations can be employed as the governing equations. This allows both simpler construction of the equation system (without wall functions and turbulence models) and lower cost of the calculation (lower requirement of cell number) in contrast to the viscous Navier-Stokes equations. This selection keeps the benefit of the through-flow method in computing speed while the robustness of the calculation remains. Finally, the applied Euler equations can be written as [5]

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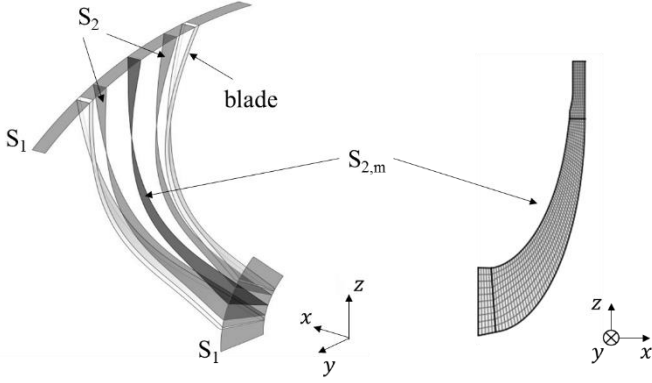


Figure 1: Stream surfaces in a blade row [1, 6]

$$\frac{\partial \mathbb{U}}{\partial t} + \frac{\partial \mathbb{F}}{\partial x} + \frac{\partial \mathbb{G}}{\partial y} + \frac{\partial \mathbb{H}}{\partial z} = \mathbb{S}, \quad (1)$$

where

$$\mathbb{U} = \begin{pmatrix} \rho \\ \rho w_x \\ \rho w_y \\ \rho w_z \\ \rho e_t \end{pmatrix}, \quad \mathbb{F} = \begin{pmatrix} \rho w_x \\ \rho w_x^2 + p \\ \rho w_x w_y \\ \rho w_x w_z \\ \rho w_x h_t \end{pmatrix},$$

$$\mathbb{G} = \begin{pmatrix} \rho w_y \\ \rho w_y w_x \\ \rho w_y^2 + p \\ \rho w_y w_z \\ \rho w_y h_t \end{pmatrix}, \quad \mathbb{H} = \begin{pmatrix} \rho w_z \\ \rho w_z w_x \\ \rho w_z w_y \\ \rho w_z^2 + p \\ \rho w_z h_t \end{pmatrix}.$$

The parameters $t, x, y, z, \rho, w, p, e_t$ and h_t represent time, x -, y -, z -coordinate, density, relative velocity, pressure, specific total internal energy and specific total enthalpy respectively. \mathbb{U} denotes the vector of conservative variables, while \mathbb{F} , \mathbb{G} and \mathbb{H} are the inviscid flux vectors. The Euler equations are combined with an additional source term \mathbb{S} expressed by

$$\mathbb{S} = \rho \mathbf{f}_{blockage} + \rho \mathbf{f}_b + \rho \mathbf{f}_f + \rho \mathbf{f}_{cor} + \rho \mathbf{f}_c. \quad (2)$$

The first term $\rho \mathbf{f}_{blockage}$ represents volume forces caused by tangential blockage due to blade number and thickness. $\rho \mathbf{f}_b$ and $\rho \mathbf{f}_f$ introduce the blade force and losses respectively. The last two terms denote Coriolis and centrifugal forces in a moving frame such as rotor block and, therefore, can be neglected for computation of a non-moving frame like stator.

The blockage model considers the tangential blockage factor given by Hirsch and Warzee [8], which is introduced to the Euler-equations as an integration factor according to Yao and Hirsch [9]. To enable this model, blockage in conjunction with the coordinates in meridional plane must be specified as input data for the through-flow program. The blade force model introduces the blade force \mathbf{f}_b , which describes the flow deviation due to blade profile without generating losses. The time-marching approach of Sturmayer [10] is employed here to describe the blade

force, where a target flow angle at the trailing edge must be specified to define the flow deviation.

In eq.(1), seven variables to be solved are identified from five equations: $\rho, w_x, w_y, w_z, p, e_t$ and h_t , where

$$e_t = e + \frac{1}{2}(w_x^2 + w_y^2 + w_z^2), \quad (3)$$

$$h_t = h + \frac{1}{2}(w_x^2 + w_y^2 + w_z^2). \quad (4)$$

Since the specific enthalpy h relates to the specific internal energy e , the pressure p and the specific volume $v = 1/\rho$, namely $h \equiv e + p/\rho$, one of the variables can be solved with this correlation. Therefore, an equation is still required to solve the entire equation system. To fill this gap, the equation of state is applied which can be expressed by

$$p = p(\rho, e). \quad (5)$$

It describes that the pressure is calculated from the density and the internal energy, which are the reference states in the presented program. Since this work focuses on CO_2 flow, the EOS of Span and Wagner [7] is applied to solve eq.(5). However, the direct incorporation of the EOS of Span and Wagner does not exhibit benefit in computing speed, because

- 1) the EOS is in form of the Helmholtz energy based on density and temperature and requires additional iterations once the reference states differ to them (e.g. density and internal energy used in the presented program) and
- 2) the EOS is a polynomial consists of the ideal-gas part and the residual part of the Helmholtz energy that include 8 and 42 terms respectively [7] and, thus, contains much more calculation process in contrast to an ideal gas EOS.

Therefore, lookup tables (LUTs) are applied to overcome this issue. It is achieved by extracting fluid states from Refprop based on reference states (ρ and e) and sorting out them in different tables. Gradient of states regarding reference states is also calculated to enable the linear Taylor series interpolation of the states, for example

$$p = p_{i,j} + \Delta \rho \left(\frac{\partial p}{\partial \rho} \right)_{e,(i,j)} + \Delta e \left(\frac{\partial p}{\partial e} \right)_{\rho,(i,j)}, \quad (6)$$

where i and j are the index of the density and internal energy vector. Since the differences $\Delta \rho$ and Δe between adjoining elements in the vectors are constant, it is simple to interpolate index i and j by following for instance $i = \text{ceil}((\rho - \rho_{i=1}) / \Delta \rho)$. This avoids the dependence of computation speed on the size of LUT. Finally, LUTs with a size of 1300 x 1300 are established covering pressure from 1 to 1300 bar and temperature from 0 to 1000 °C. In the current work, the application of LUTs reduces the computation time by a factor of about 20, in contrast to calculation with the EOS of Span and Wagner.

NUMERICAL SCHEME

Since a real gas EOS is applied in the present work, special care shall be taken when a numerical scheme for the flux discretization is being selected. Numerical schemes using central differencing and applying artificial viscosity like the Jameson-Schmidt-Turkel (JST) scheme [11] are well suited since assumptions regarding the EOS are not a necessary condition during the derivation. Therefore, this work applies the JST scheme. In contrast, other schemes like the flux difference scheme of Roe [12] are derived assuming a perfect gas when eq.(1) is linearized by finding the Jacobian matrix of the flux vectors. These schemes required modification before applied to real gas EOS [13].

VALIDATION AND DISCUSSION

The extension of the through-flow program with real gas EOS has been validated by comparing the calculation results to those obtained by a 1D quasi-analytical analysis¹ and Tegethoff et al. [13], where calculations of CO₂ flow in the NASA CDV nozzle are conducted. The correlation between the cross-sectional area A and the axis coordinate x is written as

$$A(x) = \begin{cases} 1.75 - 0.75 \cos((0.2x - 1) \cdot \pi), & x < 5 \\ 1.25 - 0.25 \cos((0.2x - 1) \cdot \pi), & x \geq 5 \end{cases} \quad (7)$$

Note that the unit of length is given in inch. To reduce the influence of mesh on the results, a mesh independence analysis is implemented. The reference mesh resolution has 20 cells in x -direction and 2 in z -direction (20 x 2), whose outlet Mach number Ma_{out} is regarded as the reference one $Ma_{out,ref}$. The definition of refinement factor is introduced to normalise the refinement of the mesh resolution in both directions. Finally, a mesh refinement factor of 10 (resolution of 200 x 20) is applied according to Figure 2, not only considering a balance between computation speed and accuracy but also keeping the resolution at the shock location as same as that in the reference.

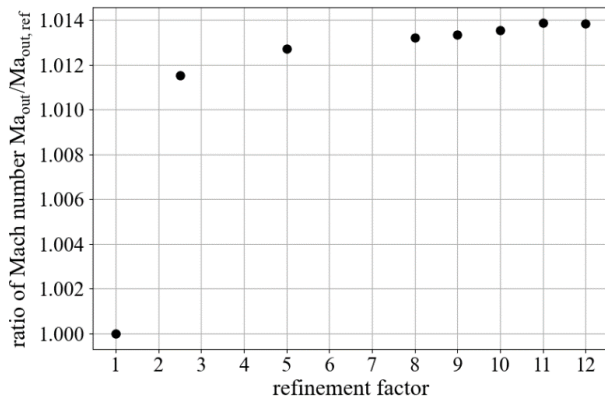


Figure 2: Mesh independence analysis based on reference condition ($p_{out}/p_{t,in} = 0.08$) regarding outlet Mach number

¹ The 1D quasi-analytical analysis program calculates the fluid properties at each selected section by considering real gas EOS. Concrete description is given in Appendix A.

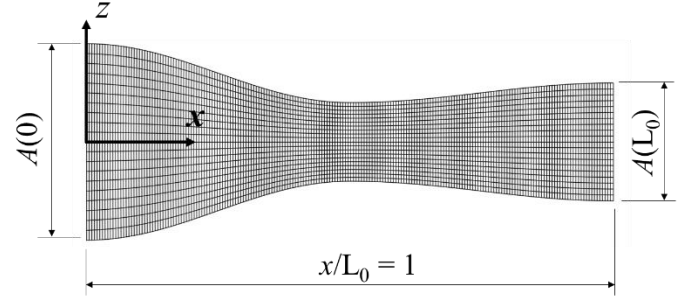


Figure 3: Mesh of the NASA CDV nozzle [5]

Considered L_0 as the maximum of x (where $x = 10$), the mesh is shown in Figure 3. Since the nozzle is considered as a 2D geometry, the value of the area is applied one to one for z -coordinate. In 2D calculation, the gradient of flow properties is sensitive to the gradient of the cross-sectional area A . This could cause 2D effects in the diverging part of the nozzle and, therefore, influence the result at the outlet. Indeed, this anxiety is observed from the simulation result.

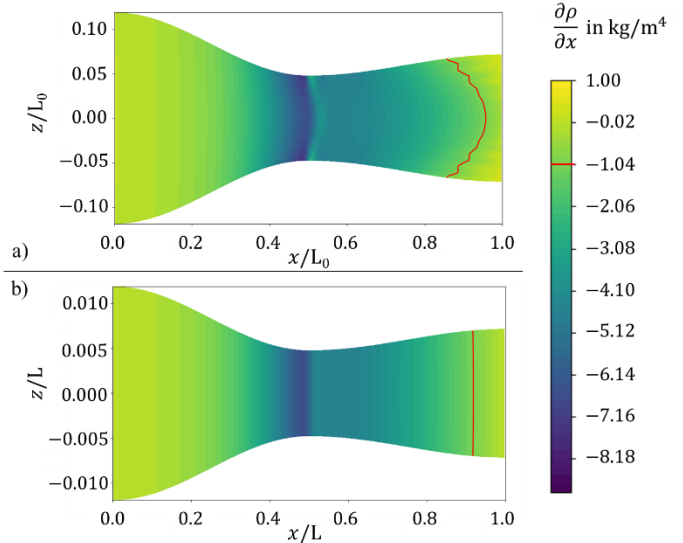


Figure 4: a) 2D effect within original NASA CDV nozzle; b) elimination of 2D effect through extended NASA CDV nozzle with factor 10

As shown in Figure 4 a), the density gradient in x -direction is quasi constant in the converging part, but it becomes higher at the mean line in the diverging part and builds peaks. An example is denoted by the red curve at the gradient of density $\frac{\partial \rho}{\partial x} = -1.04 \text{ kg/m}^4$. Such effect can be explained by phenomena “expansion plane” normally observed in converging-diverging nozzle with a sharp gradient at the throat. Finally, this effect causes a higher calculated Mach number at the outlet. Since both the 1D quasi-analytical analysis and Tegethoff’s calculation do not include

such 2D effect, measure needs to be taken to avoid this. Thus, the original geometry of the NASA CDV nozzle is extended considering a factor of 10 in x -direction, namely $L = 10L_0$, as shown in Figure 5. This extension reduces the gradient of the nozzle's cross-sectional area significantly and, therefore, almost eliminates this effect, as shown in Figure 4 b). Based on this measure, the calculation results from $tFlow$ are comparable with the references.

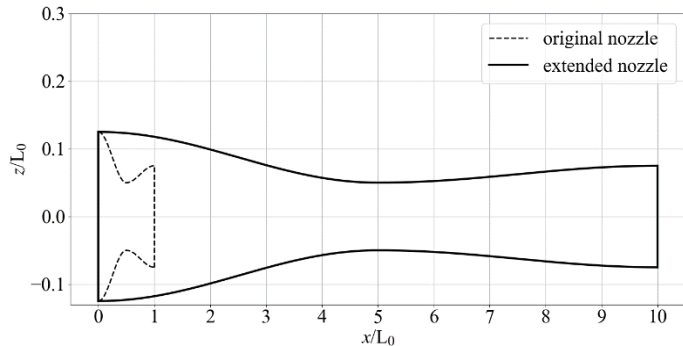


Figure 5: Extension of the original NASA CDV nozzle considering a factor of 10

Since Tegethoff et al. have developed a numerical scheme based on Roe scheme called Generalised Ideal Roe (GIRoe) scheme [13], which is available for solving real gas properties, and employed it in her calculation, it is a good chance to compare the calculation results of $tFlow$ with her work. In her case, the inlet total pressure is set to 1200 bar and the total inlet temperature is 500 K. A ratio of pressures $p_{out}/p_{t,in} = 0.75$ is considered for the shocked flow case, while another one equal to 0.08 is set for the supersonic flow case. The pressure is relatively high because a large deviation of the compressibility factor between ideal and real gas is intended to exhibit the robustness of the calculation with “strong” real gas effect.

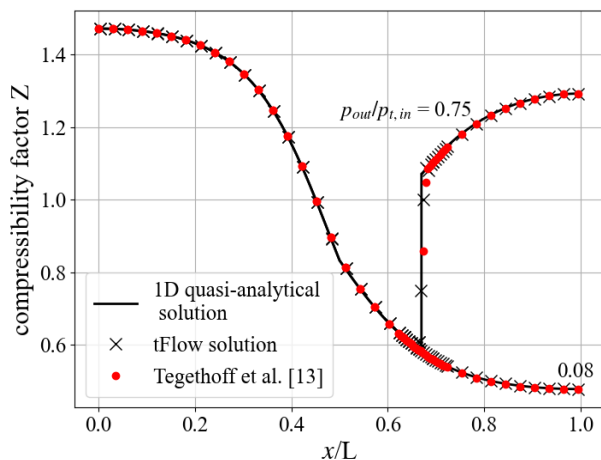


Figure 6: Comparison of compressibility factor

Figure 6 shows the comparison of both pressure ratios with respect to the compressibility factor. In the case of supersonic flow, the compressibility factor varies from about 1.5 to 0.5,

where a relatively large difference to ideal gas ($Z = 1$) is involved in this validation as desired, indicating good robustness and accuracy of this through-flow program for calculating flow properties of real gas. The case of shocked flow validates the shock location as well as the fluid states after the shock. Denser grid points are displayed around this location to show more details of the shock. The skip of the compressibility factor from 0.60 to 1.06 further verifies the robustness of the calculation for a dramatic change of the compressibility factor. Figure 7 shows the comparison by means of Mach number, indicating an excellent agreement between $tFlow$, the 1D quasi-analytical analysis and Tegethoff's calculation as well.

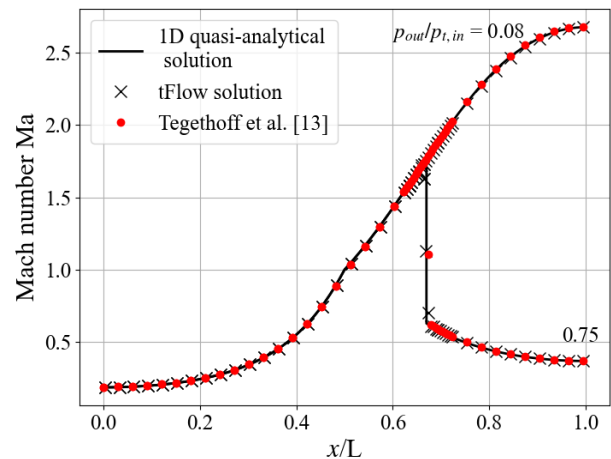


Figure 7: Comparison of Mach number

Besides, the good agreement also means that there is no obvious difference between Roe-based and JST scheme. Therefore, this study verifies the application of JST scheme in the through-flow method by considering real gas EOS.

CONCLUSION

This work develops the through-flow program, $tFlow$, further by considering real gas EOS. The JST scheme is firstly applied since other schemes incorporated in the program are not available for real gas EOS. In addition, a set of LUTs is established to speed up the calculation and, hence, keeps the benefit of the through-flow method.

The validation of this development is conducted by comparing the results of $tFlow$ with those of the 1D quasi-analytical analysis and Tegethoff's calculation with respect to sCO_2 flow in the NASA CDV nozzle, where the fluid states vary within a wide range of compressibility factor involving “strong” real gas effect. Since 2D effect is found by the original nozzle geometry and not included in both 1D quasi-analytical and Tegethoff's calculation, the nozzle is extended by a factor of 10 to eliminate this impact. The comparison shows an excellent agreement between $tFlow$, the 1D quasi-analytical analysis and Tegethoff's calculation, validating the application of real gas EOS in the presented through-flow program. Additionally, the wide range (between 0.5 and 1.5) and the dramatic variation (from 0.6 to 1.06) of the compressibility factor exhibit good

robustness of the calculations by means of using the EOS of Span and Wagner. Moreover, this study also verifies the application of JST-scheme for the through-flow method in terms of real gas EOS.

The incorporation of real gas EOS into *tFlow* not only develops the functionality of the program further but also exhibits good potentials for application of real gas EOS in the through-flow method. As the next step, the program is to be further extended for calculation of compressors using real gas as working fluid, e.g. sCO₂ compressors.

NOMENCLATURE

A	area (inch ² , m ²)
c	absolute flow velocity (m/s)
f_b	blade force vector
$f_{blockage}$	volume force vector due to blockage
f_f	vector of losses
f_{cor}	Coriolis force vector
f_c	centrifugal force vector
\mathbb{F}	inviscid flux vector in x-direction
\mathbb{G}	inviscid flux vector in y-direction
\mathbb{H}	inviscid flux vector in z-direction
h	specific static enthalpy (J/kg)
L	length of nozzle (inch, m)
\dot{m}	mass flow rate (kg/s)
Ma	Mach number (-)
n_s	isentropic volume exponent for real gas
p	static pressure (bar)
R	specific gas constant (J·kg ⁻¹ ·K ⁻¹)
s	specific entropy (J/kg)
$\$$	additional source term
T	temperature (K, °C)
\mathbb{U}	vector of conservative variables
v	specific volume (m ³ /kg)
w	relative flow velocity
x	coordinate in x-direction (inch, m)
y	coordinate in y-direction (inch, m)
z	coordinate in z-direction (inch, m)
Z	compressibility factor (-)
Δ	difference (-)
κ	isentropic exponent (-)
ρ	density (kg/m ³)
π	the ratio of a circle's circumference to its diameter (-)

subscript

crit	parameter at critical state
e	parameter at constant internal energy
i	index of density vector
in	inlet
j	index of internal energy vector
out	outlet
p	parameter at constant pressure
ref	reference parameter
t	total parameter / stagnation state
th	parameter at throat of nozzle

T	parameter at constant temperature
x	parameter in x-direction
y	parameter in y-direction
z	parameter in z-direction
ρ	parameter at constant density

Abbreviations

CDV	Converging-Diverging-Verification
CFD	Computational Fluid Dynamics
CO ₂	Carbon dioxide
EOS	Equations of State
GIRoe	Generalised Ideal Roe
JST	Jameson-Schmidt-Turkel
LUT	Lookup Table
NASA	National Aeronautics and Space Administration
sCO ₂	Carbon dioxide in supercritical state
1D	one-dimensional
2D	two-dimensional
3D	three-dimensional

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ANNEX A

CALCULATION METHOD OF THE 1D QUASI-ANALYTICAL ANALYSIS

GOVERNING EQUATIONS

In this work, a one-dimensional program is developed to predict nozzle flows by using real gas EOS. Although classic correlations exist, such as the correlation between static and total pressure or the correlation between cross-sectional area A and Mach number Ma described in [14], assumptions made for ideal gas must be taken into account. If the compressibility factor Z differs a lot to 1, like 0.3 by CO_2 near the critical point, these assumptions are not valid anymore, and, therefore, the derivation of such correlations for real gas should differ to those mentioned above. Actually, there are some easy ways to incorporate real gas EOS into the existing correlations. One of them is to consider the isentropic volume exponent n_s for real gas instead of κ . This parameter is mentioned by Lüttke [15] and applied by Pham et al. [16] for predicting performance maps of sCO₂ compressors. This provides an efficient method to develop performance prediction of sCO₂ turbomachines, but it does not show the plausibility of the use of this parameter in the mentioned correlations. Thus, efforts are made to derive the governing equations for real gas nozzle flow.

The 1D quasi-analytical analysis is based on the mean-line method, where the Span and Wagner EOS [7] is employed to solve the fluid states of CO_2 . Because iterations exist during solving the fluid states, it is regarded as a quasi-analytical method. For this analysis, two assumptions are made: 1) the Mach number in front of the throat is less than one (subsonic inlet condition); 2) the nozzle wall is frictionless and adiabatic (isentropic process if there is no shock, and no heat addition). For flow through a nozzle without shock, following equations are valid:

$$\dot{m}(x) = A(x)c(x)\rho(x) = \dot{m}, \quad (8)$$

$$h_t = h_{t,in} = f(p_{t,in}, T_{t,in}), \quad (9)$$

$$s = s_{in} = f(p_{t,in}, T_{t,in}), \quad (10)$$

where f represents the EOS correlation. Equation (8) considers the mass conservation, eq.(9) considers the energy conservation, and eq.(10) considers the reversible process of a throughflow. However, since both velocity c and density ρ are normally unknown, one of them needs to be guess in the first step and updated iteratively. The iterative solution is achieved by considering eq. (8) and equations as follows:

$$h_t = h + \frac{1}{2}c^2, \quad (11)$$

$$h = f(\rho, s) \text{ or } \rho = f(h, s). \quad (12)$$

Once the density ρ is solved, other thermodynamic parameters can be obtained through the EOS.

Furthermore, equations for solving shock waves are considered. Denoting the fluid properties directly in front of the shock with subscript "1" and directly after the shock with subscript "2", the shock can be described by

$$\rho_1 c_1 = \rho_2 c_2, \quad (13)$$

$$p_1 + \rho_1 c_1^2 = p_2 + \rho_2 c_2^2, \quad (14)$$

$$h_1 + \frac{1}{2}c_1^2 = h_2 + \frac{1}{2}c_2^2. \quad (15)$$

where the conservation of mass, momentum and energy for a normal shock [14] is taken into account. Guessing a parameter after the shock in the first step, e.g. c_2 , the parameters after the shock can be solved with the Newton's method, if the parameters in front of the shock are known. Note that the flow condition before the shock must be supersonic.

CALCULATION PROCESS

Normally, the given parameters are the total pressure and temperature at the nozzle inlet, and the static pressure at the nozzle outlet. The 1D quasi-analytical analysis will firstly distinguish the flow condition by calculating the transition points between subsonic, shocked and supersonic flow. If the case is subsonic, the mass flow rate is calculated based on the given pressure at the outlet. Otherwise, the flow is regarded as choked, and the mass flow rate is then calculated by considering $Ma = 1$ at the throat. The transition point between shocked and supersonic flow is calculated by considering a shock wave directly at the outlet of the nozzle [17]. The determination of the flow condition is necessary, because normally there are two solutions (subsonic and supersonic) for a certain cross-sectional area.

After determining the flow condition, the Mach number distribution can be preliminarily distinguished. For subsonic case, the Mach number is less than one in both converging and diverging part. For supersonic case, the Mach number is less than one in the converging part and greater than one in the diverging part. Subsequently, the Mach number and other fluid properties like pressure, temperature etc. can be calculated based on eq.(8) - (12). Shocked flow is regarded as a special case here since it causes loss (increased entropy) and its location needs to be fixed. However, in this case, properties in the converging part are calculated as same as in the case of supersonic flow, because both the cases have reached the choking condition. In the diverging part, the Mach number is firstly greater than one in front of the shock and thereafter less than one. The shock location is solved with the Newton's method as well, by guessing an x -coordinate at first and solving the pressure at the nozzle outlet iteratively. In each iteration, the properties after the shock are calculated by eq.(13) - (15), considering a supersonic condition before the

shock at the specified location. The calculation process ends, once the calculated outlet pressure fits to the given one.

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