Numerical Study on Subsonic-Supersonic Laval Nozzle Using MacCormack Scheme

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Abstract. Due to the wide application of the Delaware nozzle in many fields, the flow characteristics of the subsonic-supersonic isentropic flow in the De-Laval nozzle are analyzed numerically. The flow in the nozzle can be simplified to a quasi-one-dimensional flow problem. First, the MacCormack format is employed to discretize the control equations in conservative form. Then, the results with and without artificial viscosity are compared. Grid independence is also discussed. The results show that the numerical solution and the theoretical solution agree very well, indicating that the numerical simulation results are very reliable. In addition, a higher pressure will reduce the peak and valley values of Mach number, pressure, density, temperature and velocity in the nozzle, and these extreme values of subsonic supersonic isentropic nozzle appear earlier. Additionally, the shock wave is accurately captured, and the shock wave is behind the throat. This research is of great significance to understand the flow characteristics in the nozzle.

1. Introduction
The nozzle is a model designed to control the motion of the fluid and it can accelerate the fluid by converting the pressure and heat to kinetic energy. The De-Laval nozzle is invented by Gustaf de Laval, a Swedish inventor and it is a converging-diverging type of nozzle whose front end gradually narrowed and finally converged into a throat. The back of it grows from small to large and expend outwards [1]. The image of the De-Laval nozzle is shown in Figure 1 below.
Furthermore, the De-Laval nozzle is used to accelerate the hot, pressurized gas to supersonic speed along the axial direction. Through this process, the heat energy of the flow is converting to kinetic energy [2]. The process is that the subsonic gas continues to accelerate before reaching the throat and eventually exceeds the speed of sound. The supersonic gas will be further accelerated after passing through the throat because, for the supersonic fluids, the flow velocity is proportional to the cross-sectional area [3]. Due to these properties, the De-Laval nozzle is widely applied in many science fields. In aeronautics, the nozzle is used as rocket exhausts and it can optimize the engine thrust during the takeoff phase. Besides, it is applied in the wind tunnels experiment as well in order to study the aerodynamics of miniaturized static shuttles or plans facing the gas at high speed. What’s more, it is even used in powder metallurgy [4]. Due to the wide application of the De-Laval nozzle in the science fields, it is important and necessary to keep studying it.

There are various researches on the De-Laval nozzle. According to the research of Li, J, et al [5], the transonic shock problem of ‘Full compressible Euler system’ in two-dimensional De-Laval nozzle is studied and it is solved in a nozzle whose divergence is small and arbitrary perturbations in the divergence. Besides, the compressible Euler system of ‘steady isentropic’ and ‘irrotational smooth transonic’ flows in two-dimensional De-Laval nozzle are studied by Wang, C and Xin, Z [6]. According to [7], Matz, M and Aumiller, M compare the cylindrical nozzle and de Laval nozzle in wire arc spraying are compared. Base on the measurement, they draw that the gas velocity closely correlates with the atomization of the droplets. According to [8], Cheng, J, et al studies the well-posedness theory of the incompressible flow in the De-Laval nozzle with a certain outlet pressure. Base on the results, they find that there is an interval of Bernoulli’s constant in a flow with certain mass flux in the upstream and certain pressure in the outlet. There exists a smooth incompressible jet flow from the nozzle if Bernoulli’s constant is in that interval. Besides, in the De-Laval nozzle, Dykas, S, et al compared the results of studies on the wet steam flow with spontaneous condensation obtained by ‘in-house Computational Fluid Dynamics (CFD) code’ and the ‘Ansys CFX commercial package’ [9]. According to [10], Xu, L, et al use the commercial CFD software to study the atomizer with a De-Laval nozzle. The simulation results indicate that as a result of gas interaction, the mass loading effect is significant. According to [11], Hatta, N, et al describe the analytical procedure of gas-particle mixtures in the supersonic nozzle flow for a prescribed nozzle configuration. In addition, N. D. Deshpande, et al applied equations for one-dimensional nozzle flow to analyze the De-Laval nozzle and use the CFD software ANSYS Fluent to simulate the flow [1]. Base on the results, they draw several conclusions that: (1) The flow velocity increases from the inlet to the outlet and the speed at the throat and outlet are approximately Mach 1 and Mach 3.03. (2) The temperature keeps decreases from the inlet to the outlet and that of the outlet is 1760.89K. 3. The pressure keeps decreases from the inlet to the outlet and that of the outlet is 0.729 bar. Furthermore, the shock waves cause a sudden decrease in pressure after the throat.
The above research is of great significance for understanding the flow mechanism of the nozzle. The study of the flow state inside the nozzle is of great significance for the application of the nozzle. Therefore, the flow in the nozzle is also studied and the shock wave is captured. The McCormack scheme is used to discretize the governing equations of the flow in the nozzle.

The rest of the paper is organized as follows: The second section introduces the method for numerical simulation. The third section presents the results and discussion. Then the last section is the conclusion.

2. Method

2.1. Governing Equations

For the flow problem in the convergent-divergent nozzle in Figure 2, the shape of the Laval nozzle is a hyperbola, which satisfies $A(x) = 1 + 2.0(x - 1.5)^2$. The flow in the nozzle can be considered as subsonic supersonic isentropic flow. It can be regarded as a quasi-one-dimensional flow problem due to the symmetry, and the conservation form of the governing equations are

\[
\frac{\partial (\rho A)}{\partial t} + \frac{\partial (\rho AV)}{\partial x} = 0
\]

\[
\frac{\partial (\rho AV)}{\partial t} + \frac{\partial (\rho AV^2 + pA)}{\partial x} = p \frac{\partial A}{\partial x}
\]

\[
\frac{\partial [\rho(e + V^2/2)A]}{\partial t} + \frac{\partial [\rho(e + V^2/2)AV]}{\partial x} = - \frac{\partial (pAV)}{\partial x}
\]

Where $A$ is the cross-sectional area of nozzle, $\rho$ the density, $p$ the pressure, $V$ the velocity and $e$ the internal energy.
Non-dimensional variables are commonly used to express the flow field in the nozzle flow. Furthermore, use the nondimensional variables correctly can avoid the large disparity in the calculation and avoid increasing the error. The definition of nondimensional variables is shown below. The flow at the inlet to the nozzle comes from a reservoir where the pressure $\rho_0$ and temperature $T_0$ are constants. Denoting the length of the nozzle as $L$, the speed of sound in the reservoir as $a_0$, the sonic throat area as $A_0$. Then the nondimensional variables can be defined as:

$$
T' = \frac{T}{T_0}, \rho' = \frac{\rho}{\rho_0}, x' = \frac{x}{L}, V' = \frac{v}{A_0}, t' = \frac{t}{L/a_0}, A' = \frac{A}{A_0}
$$

(4)

Where $a_0 = \sqrt{\gamma RT_0}$. By introducing the nondimensional variables, the conservation form of the governing equations become:

$$
\frac{\partial (\rho' A')}{\partial t'} + \frac{\partial (\rho' A'V')}{\partial x'} = 0
$$

(5)

$$
\frac{\partial (\rho' A'V')}{\partial t'} + \frac{\partial (\rho' A'V'^2 + \frac{1}{\gamma} p'A')}{\partial x'} = \frac{1}{\gamma} p' \frac{\partial A'}{\partial x'}
$$

(6)

$$
\frac{\partial [\rho' (\frac{e'}{\gamma - 1} + \frac{\gamma}{2} V'^2) A']}{\partial t'} + \frac{\partial [\rho' (\frac{e'}{\gamma - 1} + \frac{\gamma}{2} V'^2)V' A' + p'A'V']}{\partial x'} = 0
$$

(7)

Where $\gamma$ is the specific heat ratio. It can be expressed in the following first-order hyperbolic partial differential equation,

$$
\frac{\partial U}{\partial t} = -\frac{\partial F}{\partial x} + J
$$

(8)

So, the equations for one-dimensional flow in conservation form can be expressed in a generic form

$$
U = \left( \begin{array}{c}
\rho' A' \\
\rho' A'V' \\
\rho' (\frac{e'}{\gamma - 1} + \frac{\gamma}{2} V'^2) A'
\end{array} \right), F = \left( \begin{array}{c}
\rho' A'V' \\
\rho' A'V'^2 + \frac{1}{\gamma} p'A' \\
\rho' (\frac{e'}{\gamma - 1} + \frac{\gamma}{2} V'^2)V' A' + p'A'V'
\end{array} \right), J = \left( \begin{array}{c}
0 \\
\frac{1}{\gamma} p' \frac{\partial A'}{\partial x'} \\
0
\end{array} \right)
$$

(9)

2.2. MacCormack Scheme and Discrete governing equations.

MacCormack scheme is a numerical two-step method that capable of discretizing non-linear equation and hyperbolic partial differential equation. Essentially, the MacCormack scheme is an advanced variant originated from the Lax-Wendroff technique but with a simpler approach, additional predictor and corrector, no necessity to calculate the intermediate value on mid-point of the function likewise.

To illustrate the scheme, consider the first-order hyperbolic partial differential equation,

$$
\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + J = 0
$$

(10)

Where $U$ is the quantity vector to be solved, and $F$ and $J$ are vector functions of $U$. The application of the MacCormack scheme to Eq. (10) proceeds in two steps.
2.2.1. Predictor step.

On the grid, as shown in Figure 3, \( \overline{U}_{i,j}^{t+\Delta t} \) represents the value of \( U \) at grid \( i \) at time \( t \). Then we have

\[
\overline{U}_{i,j}^{t+\Delta t} = U_i^t - \Delta t \left( \frac{F_i^{t+1} - F_i^{t-1}}{2\Delta x} + J_i^t \right)
\]

(11)

Where \( \overline{U}_{i,j}^{t+\Delta t} \) is the predicted value of \( U \) at grid \( i \) at time \( t + \Delta t \). Then \( F_i^{t+\Delta t} \) and \( J_i^{t+\Delta t} \) can be obtained from \( \overline{U}_{i,j}^{t+\Delta t} \).

2.2.2. Corrector step. In the corrector step, the predicted value \( \overline{U}_{i,j}^{t+\Delta t} \) is corrected according to the following equation

\[
U_i^{t+\Delta t} = U_i^{t+\Delta t/2} - \frac{\Delta t}{2} \left( \frac{F_i^{t+\Delta t} - F_i^{t-\Delta t}}{\Delta x} + J_i^{t+\Delta t} \right)
\]

(12)

Note that the corrector step uses a backward finite difference scheme for spatial derivative. Also, the time-step used in the corrector step is \( \Delta t/2 \) in contrast \( \Delta t \) in the predictor step.

Replacing the \( U_i^{t+\Delta t/2} \) by the temporal average

\[
U_i^{t+\Delta t/2} = \frac{U_{i,j}^{t+\Delta t} + U_i^t}{2}
\]

(13)

Finally, the corrector can be obtained

\[
U_i^{t+\Delta t} = \frac{U_{i,j}^{t+\Delta t} + U_i^t}{2} - \frac{\Delta t}{2} \left( \frac{F_i^{t+\Delta t} - F_i^{t-\Delta t}}{\Delta x} + J_i^{t+\Delta t} \right)
\]

(14)

2.2.3. Artificial viscosity. Besides, to get a smooth and stable solution, artificial viscosity is added in the process of numerical simulation.

\[
S_i^t = C_x \frac{|p_{i+1}^t - 2p_i^t + p_{i-1}^t|}{p_{i+1}^t + 2p_i^t + p_{i-1}^t} (U_{i+1}^t - 2U_i^t + U_{i-1}^t)
\]

(15)

According to Section 2.1, \( p \) can be obtained from \( U \).

To sum up, the McCormack scheme with artificial viscosity is as follows
\[ \overline{U}_{i}^{t+\Delta t} = U_{i}^{t} - \Delta t \left( \frac{F_{i+1}^{t} - F_{i}^{t}}{2\Delta x} + J_{i}^{t} \right) + S_{i}^{t} \] (predictor step) (16)

\[ U_{i}^{t+\Delta t} = \frac{U_{i}^{t+\Delta t} + U_{i}^{t}}{2} - \frac{\Delta t}{2} \left( \frac{F_{i+1}^{t+\Delta t} - F_{i-1}^{t+\Delta t}}{\Delta x} + J_{i}^{t+\Delta t} \right) + \frac{S_{i}^{t+\Delta t}}{2} \] (corrector step) (17)

Where,

\[ S_{i}^{t+\Delta t} = C_{i} \left[ p_{i+1}^{t+\Delta t} - 2p_{i}^{t+\Delta t} + p_{i-1}^{t+\Delta t} \right] \left( U_{i+1}^{t+\Delta t} - 2U_{i}^{t+\Delta t} + U_{i-1}^{t+\Delta t} \right) \]

### 2.3. Boundary Conditions

For nozzle problems, whereas other factors including density and temperature remain constants at the boundary of inflow (i.e. will not change with time),

\[ \rho_{1}^{t} = 1, T_{1}^{t} = 1 \] (18)

For the subsonic inflow boundary, the velocity at the boundary is allowed to change. Here we implement John D. Anderson’s method and set the boundary conditions as follows [12],

\[ U_{1,1} = \rho_{1}^{t} A_{1}^{t} = c_{1} \] (19)

\[ \frac{\partial U_{2,1}}{\partial x} = c_{2} \] (20)

\[ U_{3,1} = U_{1,1} \left( \frac{T_{1}^{t}}{\gamma - 1} + \frac{\gamma}{2} V^{2} \right) \] (21)

Where \( U_{i,1} \) are i-th term in the \( U \) of the first node and \( c_{1}, c_{2} \) and \( c_{3} \) are constants. \( \gamma \) is the coefficient of thermalization.

For supersonic outflow boundary, all factors have to be allowed to change. Use extrapolation to obtain their values likewise,

\[ \frac{\partial U_{1,N}}{\partial x} = c_{3} \] (22)

\[ \frac{\partial U_{2,N}}{\partial x} = c_{4} \] (23)

\[ \frac{\partial U_{3,N}}{\partial x} = c_{5} \] (24)

Where \( U_{i,1} \) are i-th term in the \( U \) of the last node. And \( c_{3}, c_{4} \) and \( c_{5} \) are constants.

Initial conditions including density and temperature for outflow in the different region according to the nozzle shape are given by,

\[ \rho^{t}(0) = 1, T^{t}(0) = 1, x \in [0,0.5) \] (25)

\[ \rho^{t}(0) = 1 - 0.37(x - 0.5), T^{t}(0) = 1 - 0.12(x - 0.5)^{2}, x \in [0.5,3] \] (26)
3. Results and Discussion

3.1. Comparison of theoretical and numerical solutions

By comparing the theoretical and numerical solutions in terms of Mach number and pressure in Figure 4, it can be found that they are basically matched. The horizontal coordinate represents the position in the nozzle. Besides, the error between the numerical and theoretical solutions is found to be very small, and the position of the shock wave can be clearly seen by the analysis. This means that the numerical simulation results in this paper are accurate and can be used for subsequent analysis.

3.2. Comparison of different grids
In the following, the study focuses on the variations of Mach number, pressure, density, temperature and velocity for different grids. The control condition is to maintain an outlet pressure of 0.68 and change the grid length $\Delta x$ to be 0.02, 0.05 and 0.1.

In Figure 5(a), when the grid is divided into smaller and finer, such as taking $\Delta x$ for 0.02, the maximum Mach number achievable in the nozzle is about 1.91. By comparison, it is found that as $\Delta x$ gradually decreases, the maximum Mach number in the nozzle increases. As the mesh is divided finer and finer, the maximum Mach number will gradually converge to a definite value rather than an infinite growth. It also finds that the position where the shock wave appears is almost unaffected, all around the horizontal coordinate of 2.1. In Figure 5(e), the variation rule of the velocity is basically the same as the Mach number.

Moreover, the change in pressure, density and temperature are also basically similar. Therefore, the pressure distribution is chosen as an example to be analysed. As $\Delta x$ decreases from 0.1 to 0.02, the minimum value of pressure generated within the nozzle becomes smaller. When $\Delta x$ is divided into finer and finer, the minimum value of pressure does not keep decreasing but converges to an exact value of 0.14. The curve of temperature is a bit special, when the mesh is relatively small such as $\Delta x = 0.02$, the change of temperature starts to fluctuate at the position where the horizontal coordinate is greater than 2.1.

The above results show that the smaller the $\Delta x$ is, the more accurate the variable distributions are. In general, increasing the number of grids can improve the measurement accuracy but also increase the complexity of the calculation. However, as $\Delta x$ decreases to 0.05, the accuracy of the curve hardly changes anymore and it is almost the same as when $\Delta x = 0.02$. So $\Delta x = 0.05$ is chosen in the present work.
3.3. Comparison of numerical results with and without artificial viscosity term

Figure 6 shows the comparison of the Mach number, pressure, density, temperature and velocity profiles with and without the artificial viscosity. It is shown that if the artificial viscosity term is added, the results of the numerical calculations will become more stable, more convergent. Without adding the artificial viscosity term, the numerical results are very oscillating and inaccurate, especially in the
region of supersonic speed before the shock wave. So, adding the artificial viscosity term is chosen in the present work.

3.4. Comparison at different outlet pressures

In order to compare the influences of different outlet pressures on the flow state inside the nozzle, simulations are carried out separately for different outlet pressure $p_e$.

![Figure 7. Comparison at different outlet pressures.](image)
Figure 7(a) shows the Mach number distributions of the nozzle under different outlet pressures. The overall trend is to first increase and then reach a maximum point, followed by a sharp drop in Mach number over a little distance, and finally, the curve flattens out. The cusp of the curve represents the shock wave, which appears behind the throat. As $pe = 0.68$, the shock wave appears at the position where the dimensionless distance equals nearly 2.1. While $pe$ is equaled to 0.5, the shock wave appears near the dimensionless distance of 1.8. As $pe$ equals 0.9, the position of the shock wave appears at about 2.4. In general, as the $pe$ increases, the location where the shock wave appears also moves to the right. The Mach number becomes larger as the outlet pressure increases at the same location after the appearance of the shock wave.

The pressure distributions under different outlet pressures are shown in Figure 7(b). As can be seen, the pressure changes very little near the initial position, and then the pressure starts to gradually decrease as $x$ reach 0.6. After reaching the lowest point, it turns sharply up and finally levelled off near the nozzle outlet. After comparison, it is found that the pressure is the same at the position before the appearance of the shock wave, regardless of the outlet pressure. After the appearance of the shock wave, the pressure gradually becomes larger at the same position with the increase of $pe$. At a $pe$ of 0.5, the dimensionless value of pressure at the point of 2.5 is only 0.44, while this value becomes 0.87 when the $pe$ increases to 0.9.

In addition, the distribution of density and temperature and the distribution of pressure can be found to be consistent. The distributions of velocity and Mach number are consistent. The above analysis provides a clear understanding of the influences of outlet pressure on the flow state in the nozzle.

4. Conclusion

The McCormack scheme is used to discretize the conservation form of the governing equations of the flow in the nozzle. The problem can be reduced to a quasi-one-dimensional flow problem. The results indicate that the numerical solution is in good agreement with the theoretical solution. The artificial viscosity term can make the solution smoother and more accurate. More, larger pressure will cause less peak and trough values of Mach number, the pressure within the nozzle, density, temperature and velocity with the earlier appearance of these extremum values for the subsonic-supersonic isentropic nozzle. Besides, the shock wave was accurately captured and located behind the throat. Finally, the flow state inside the nozzle can be understood in detail through the research results of this paper. Since there are many factors that can influence the basic properties of the fluid within the nozzle and the location of the shock wave, the further and comprehensive study should be taken on integrating all factors that can impact the results, different methods likewise, in order to obtain a solution which can be implemented in real situations.

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