Numerical simulation of flow field in a Laval nozzle based on one-dimensional Euler equation

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Abstract. Numerical simulation refers to a computer research method which runs calculation based on a specific mathematical model to simulate actual physical processes. It is a powerful tool to analyse complex engineering problems. In this paper, a numerical method for solving the steady one-dimensional Euler equations using a two-step second-order difference scheme is developed. The method is implemented by a Python code. The method is applied to numerical simulation of flows in a Laval nozzle and used to investigate the influence of shapes of Laval nozzle. It is found that the physical quantities of the nozzle flow show a positive correlation trend with different throat positions. In terms of the temperature, density, and pressure, they increase during the initial evolutions, then reach the maximum point and produce significant fluctuations, indicating the flow flows into the transonic stage. Subsequently, those physical properties gradually tend to a stable value during the supersonic stage. Moreover, it is observed that the closer the throat is to the exit, the lower the Mach number at which it eventually stabilizes. Finally, a suggestion about the best shape of the nozzle which can realize the max efficiency is concluded. Despite using an inviscid flow model, the steady pressures are quite satisfactorily predicted over the range of frequencies studied.

1. Introduction
Computational fluid dynamics (CFD) is a group of computational methodologies to solve the fluid flow related governing equations, an area of study in solving complex problems which cannot be solved by direct calculation [1-2]. The fundamental of almost all CFD problems is the Navier–Stokes equations, which could be combined with the optimization techniques to fulfill complex engineering design tasks. The Euler equations can be derived by neglecting the viscous effect. Moreover, by removing the term describing vorticity, the full potential equation can be obtained. Finally, for small perturbations in subsonic and supersonic flows (not transonic or hypersonic), the full potential equation can be linearized to obtain the linearized potential equations [1-2]. CFD can be applied to a variety of disciplines. For example, CFD can be used to evaluate the physical performance of spacecraft [3], aero-engines [4], nozzles [5], etc., to replace part of the experimental results so as to shorten the equipment development cycle and reduce the development cost. The CFD method is also often used to study the numerical simulation of the Laval nozzle. The Laval nozzle is an important part of the thrust chamber. The cross-sectional area of the front half of the nozzle decreases from large to small and shrinks towards the middle...
to a narrow throat. After passing the narrow throat, the cross-sectional area of the front half of the nozzle expands outwards to the end of the nozzle. The gas from the front component of the nozzle flows into the front half of the nozzle under high pressure and escapes from the back half after passing through the narrow throat. This allows the airflow velocity to vary depending on the cross-sectional area, accelerating the airflow from subsonic to sonic to supersonic.

In clean energy applications, Bian et al. [6] proposed a new Laval nozzle natural gas liquefaction process to enhance the superior performance of supersonic natural gas dehydration separators. The supersonic flow and liquefaction process of the methane-ethane binary system in the nozzle was numerically studied. The effects of inlet temperature, inlet pressure, back pressure, and composition on the hydraulic process were analysed. The results show that the methane-ethane binary system's critical liquefaction temperature and pressure decrease under low inlet temperature and high inlet pressure, and the range of liquid phase increases, which promotes the liquefaction process. With the increase of the nozzle back pressure, the position of the shock wave moves forward, and the liquefaction environment is destroyed more thoroughly.

In the field of metallurgy, coherent jet technology is needed to achieve a better mixing effect. One of the key features of this technology is to use combustion flame to protect the main oxygen jet. Liu et al. [7] introduced a Laval nozzle with preheating technology and established a computational fluid dynamics model of a coherent jet flow field to simulate the study. The conclusions are as follows: the liner jet forms shock waves at the outlet of the Laval nozzle, resulting in the loss of kinetic energy after the main oxygen jet passes through. The results show that the axial velocity of a coherent jet is less than that of a conventional jet. The variation of velocity increases with the increase of velocity.

Because of the nature of the Laval nozzle, which accelerates inlet speeds up to supersonic speeds, it is widely used. It has been well studied and based on the work of others, and we find that the Laval nozzle can still be studied further. In this paper, to further optimize the shape of the Laval nozzle, we deeply explore the influence of different positions of the nozzle throat to improve its working efficiency.

The objective of this study is the numerical simulation of the flow field in the Laval nozzle based on the one-dimensional Euler equation. This study mainly explores the different physical properties in the flow field where it is under different calibres of the nozzle, positions of the throat, and Mach numbers. The physical properties are obtained by numerical solving the Euler equation via finite difference method, and the results can play a certain enlightening role in some engineering problems.

Section 2 presents the deconstruction and analysis of the one-dimensional Euler equation. Section 3 details the Construction of the numerical model of the Laval nozzle. The computer simulation experiment and its details are introduced in Section 4. Conclusions are drawn in Section 5.

2. Method

Firstly, we consider the case where the velocity \( u(x,t) \) is a vector and \( A \) is a constant matrix with distinct real eigenvalues:

\[
\frac{\partial u}{\partial t} + A \frac{\partial u}{\partial x} = 0 \tag{1}
\]

To understand the solution of such equations, we introduce the diagonalization of \( A \). Let \( S \) be a matrix whose columns are the eigenvectors of \( A \), then we have \( AS = \Gamma S \) or equivalently \( S^{-1} AS = \Gamma \), where \( \Gamma \) is a diagonal matrix with the eigenvalues of \( A \) on the diagonal. Multiply the time dependent equation by \( S^{-1} \) we get that equation is:

\[
S^{-1} \frac{\partial u}{\partial t} + S^{-1} \frac{\partial u}{\partial x} = 0 \tag{2}
\]

Or

\[
S^{-1} \frac{\partial u}{\partial t} + S^{-1} ASS^{-1} \frac{\partial u}{\partial x} = 0 \tag{3}
\]
Then we introduce $\delta \omega = S^{-1} \delta u$ gives

$$\frac{\partial \omega}{\partial t} + \Gamma \frac{\partial \omega}{\partial x} = 0 \quad (4)$$

There are three dependent equations,

$$\frac{\partial \omega_j}{\partial t} + \lambda_j \frac{\partial \omega_j}{\partial x} = 0 \quad (5)$$

The $\omega$'s are called characteristic variables.

From the above analysis of the vector case, we see that each of the $\omega$'s might need a different scheme, positive eigenvalue, and negative eigenvalue. In a positive eigenvalue situation, the wave goes from left to right. While in a negative situation, the wave goes from right to left. In these wave propagation directions, it tells us where we need to give physical boundary conditions, which will be used later. In a positive eigenvalue situation, the boundary condition is specified on the right boundary. The other issue is the proper treatment of shocks. Shocks are correctly described only in conservation form. But waves are properly described in characteristic form.

Now we introduce the one-dimensional Euler equations in conservative form. The conservative unknowns are:

$$U = \begin{pmatrix} \rho \\ \rho u \\ \rho e \end{pmatrix} = \begin{pmatrix} \rho \\ m \\ e \end{pmatrix} \quad (6)$$

And the corresponding flux vector is

$$F = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u H \end{pmatrix} = \begin{pmatrix} m \\ m^2 / \rho + p \\ m(e + p) \end{pmatrix} \quad (7)$$

$$p = (\gamma - 1) \rho \left( E - \frac{1}{2} u^2 \right), \quad \gamma = 1.4 \quad (8)$$

$$H = E + \frac{p}{\rho} \quad (9)$$

Then the equation is written in conservation form as

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0 \quad (10)$$

or as

$$\frac{\partial U}{\partial t} + A \frac{\partial U}{\partial x} = 0 \quad (11)$$

where

$$A = \begin{pmatrix} 0 & 1 & 0 \\ -(3 - \gamma) u^2 / 2 & 3 - \gamma & \gamma - 1 \\ (\gamma - 1) u^3 - \gamma u E & \gamma E - 3 \gamma - 1 u^2 / 2 & 2 \gamma \end{pmatrix} \quad (12)$$

This equation uses the conservative variables.

Now we will perform a diagonalization procedure to discover the characteristic variables. We need the eigenvalues and eigenvector of matrix $A$. This is done as follows:
\[
\begin{pmatrix}
    u - \lambda & \rho & 0 \\
    0 & u - \lambda & \frac{1}{\rho} \\
    0 & \rho c^2 & u - \lambda
\end{pmatrix}
\] = 0

(13)

Giving
\[
det = (u - \lambda)[(u - \lambda)^2 - c^2] = 0
\]

(14)

There are three roots(eigenvalues)
\[
\lambda_1 = u \\
\lambda_2 = u + c \\
\lambda_3 = u - c
\]

(15)

And eigenvectors
\[
\mathbf{l}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \mathbf{l}_2 = \begin{pmatrix} \frac{\rho}{2c} \\ 1 \\ 0 \end{pmatrix}, \mathbf{l}_3 = \begin{pmatrix} \frac{\rho c}{2} \\ \frac{1}{2} \\ -\frac{\rho c}{2} \end{pmatrix}
\]

(16)

The characteristic variables are obtained from the inverse matrix and obtained as,
\[
\delta \omega_1 = \delta \rho - \frac{1}{c^2} \delta p \\
\delta \omega_2 = \delta y + \frac{1}{\rho c} \delta p \\
\delta \omega_3 = \delta \rho - \frac{1}{\rho c} \delta p
\]

(17)

Then the equations for characteristic variables become
\[
\frac{\partial}{\partial t} \begin{pmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \end{pmatrix} + \begin{pmatrix} u & 0 & 0 \\ 0 & u + c & 0 \\ 0 & 0 & u - c \end{pmatrix} \frac{\partial}{\partial x} \begin{pmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \end{pmatrix} = 0
\]

(18)

If we denote the cross section of Laval nozzle as \( S(x) \). The equations are
\[
\frac{\partial (\rho S)}{\partial t} + \frac{\partial (\rho u S)}{\partial x} = 0
\]
\[
\frac{\partial (pu S)}{\partial t} + \frac{\partial (pu^2 + p)S}{\partial x} = p \frac{dS}{dx}
\]
\[
\frac{\partial (\rho ES)}{\partial t} + \frac{\partial (\rho u HS)}{\partial x} = 0
\]

(19)

With primitive variables, the above equation can be expressed as
The right hand side is arranged as:

\[
\tilde{Q} = \begin{pmatrix}
-\rho u \\
0 \\
-\rho c^2 u
\end{pmatrix}
\]

So the equations can be written as

\[
\begin{pmatrix}
\omega_1 \\
\omega_2 \\
\omega_3
\end{pmatrix} + \begin{pmatrix}
u & 0 & 0 \\
0 & u + c & 0 \\
0 & 0 & u - c
\end{pmatrix}\begin{pmatrix}
\omega_1 \\
\omega_2 \\
\omega_3
\end{pmatrix} = \begin{pmatrix}
0 \\
-uc \\
uc
\end{pmatrix}
\]

Using the expressions for the characteristic variables, we can obtain:

\[
\delta \omega_1 = \delta \rho - \frac{1}{c^2} \delta p
\]

\[
\delta \omega_2 = \delta u + \frac{1}{\rho c} \delta p
\]

\[
\delta \omega_3 = \delta u - \frac{1}{\rho c} \delta p
\]

Then we get

\[
d^0 \rho - \frac{1}{c^2} d^0 p = 0
\]

\[
d^0 u + \frac{1}{\rho c} d^0 p = -\frac{uc}{S} \frac{dS}{dx}
\]

\[
d^0 u - \frac{1}{\rho c} d^0 p = \frac{uc}{S} \frac{dS}{dx}
\]

And

\[
d^0 = \partial_i + u \partial_i \]

\[
d^0 = \partial_i + (u + c) \partial_i
\]

\[
d^0 = \partial_i + (u - c) \partial_i
\]

In this way, we have a set of one-dimensional Euler equations for the nozzle flow. Then we adapt the finite difference method, which divides the solution domain into a difference grid (rectangular grid), replaces the continuous solution domain with finite nodes (discrete points). And then replaces the derivative of the partial differential equation with the difference quotient to derive the difference equations containing finite unknowns on the discrete points. The solution of the equations of difference (the algebraic equations) is regarded as the approximate numerical solution of the definite solution of the differential equation.
Figure 1 summarizes the steps to solve the Euler equations for the nozzle flow. In the first step, we build up the model. The control body is selected, and the Euler equation of one-dimensional flow is derived from the integral equation. Then we define the nozzle inlet boundary conditions and outlet boundary conditions. It is assumed that the initial conditions of the other nodes are the same as the inlet boundary conditions. In the same section position, each parameter is uniformly distributed. When meshing, we grid along the circumferential direction of the pipe. MacCormack scheme is widely used in solving flow equations. It is a two-step scheme.
The discrete format of the one-dimensional Euler equation in this paper is:

\[
Q_{i+1}^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x} (F_{i+1}^n - F_i^n) + \Delta t S_i^n + \frac{\alpha \Delta t}{\Delta x^2} Q_{i+1}^{n+1} - 2Q_i^n + Q_{i-1}^{n+1} \quad (26)
\]

\[
Q_i^{n+1} = \frac{1}{2} [Q_i^n + Q_i^{n+1} - \frac{\Delta t}{\Delta x} (F_{i+1}^{n+1} - F_i^{n+1}) + \Delta t S_i^{n+1} + \frac{\alpha \Delta t}{\Delta x^2} Q_{i+1}^{n+1} - 2Q_i^{n+1} + Q_{i-1}^{n+1}] \quad (27)
\]

For space difference discretization, the time-forward difference is used in the estimation step, and the post-difference is used in the correction step.

3. Results and discussion

The shape function of the baseline nozzle is defined as:

\[
S(x) = \sqrt{1 + \frac{(x-a)^2}{27}} \quad (28)
\]

where \(a\) is the distance between the throat and the nozzle outlet. In order to clearly and simply represent the changes of various physical attributes of airflow in the nozzle, we first took the throat as the main research object to explore the changes of density, temperature, pressure, and Mach number with the increase of iteration steps. To make the following figures clearer, the \(y\)-axes here are normalized by the quantities at the inlet. In detail, the normalized density \(\rho\), temperature \(t\), pressure \(p\), and Mach number \(Ma\) shown in the figure is calculated by:

\[
\rho = \frac{\rho_i}{\rho_o}, t = \frac{t_i}{t_o}, p = \frac{p_i}{p_o}, Ma = \frac{Ma_i}{Ma_o} \quad (29)
\]

The physical quantities at the inlet are denoted by subscript \(i\), and the physical quantities at the outlet are denoted by subscript \(o\). Next, we would analyze the physical quantities of the different throat positions of the ordinary Laval nozzle. According to [2], when the throat position of the Laval nozzle is too close to the inlet or outlet, the effect of the Laval nozzle will degenerate to an ordinary nozzle. Therefore, the middle part of the nozzle, 1/3, 5/12, 7/12, and 2/3 of the nozzle are selected as the positions of the test throat to explore the differences in the physical quantities of the airflow on it. The four nozzles mentioned above, along with the baseline one, are illustrated in Figure 2. For convenience, we set the central throat position to the original case (Case 0), and each position from the entrance is represented by Case 1 through 4 in turn.

As shown in Figure 2, when we change the value of \(a\), that is, adjust the distance between the throat and the outlet, so as to adjust the shape of the nozzle.
Figure 3 (a) and (b) show the normalized parameter evolution of throat density and temperature for five different nozzles. It can be seen that the physical quantities at these five different positions are roughly positively correlated. For the density of the original case as well as Case 3 and 4 shown in Figure 3 (a), when the evolution reaches the interval of 40 to 60 steps, the airflow density at the throat will appear two maximum values, and the first maximum value is also the maximum value in this evolution. Then the density at these positions will rapidly drop to a minimum of about 0.6 after just over 100 steps of evolution. The stage indicates that the velocity of flow at the throat has completed a transonic transition. Subsequently, the closer the throat is to the outlet, the greater the fluctuation will occur. However, after satisfying the number of evolutionary steps over a long period, the density at these positions tends to be stable (generally between 0.6 and 1). For Case 1 and Case 2, with the throat near the inlet, the airflow density at the throat will show a slightly decreasing trend at the initial stage. But their later evolution trend is basically consistent with the changing trend of the three cases mentioned above. This trend is similar to that of ordinary supersonic nozzles [1]. For the temperature shown in Figure 3 (b), the variation trend of each position is roughly consistent with that in Figure 3 (a). However, the range of change between the maximum value and the minimum value is relatively smaller than before (the difference of about 0.25). The final convergent value is almost similar to that shown in Figure 3 (b).

Figure 4 (a) and (b) show the normalized parameter evolution of throat density and temperature for five different nozzles. It can be seen that the physical quantities at these five different positions are roughly positively correlated. For the density of the original case as well as Case 3 and 4 shown in Figure 3 (a), when the evolution reaches the interval of 40 to 60 steps, the airflow density at the throat will appear two maximum values, and the first maximum value is also the maximum value in this evolution. Then the density at these positions will rapidly drop to a minimum of about 0.6 after just over 100 steps of evolution. The stage indicates that the velocity of flow at the throat has completed a transonic transition. Subsequently, the closer the throat is to the outlet, the greater the fluctuation will occur. However, after satisfying the number of evolutionary steps over a long period, the density at these positions tends to be stable (generally between 0.6 and 1). For Case 1 and Case 2, with the throat near the inlet, the airflow density at the throat will show a slightly decreasing trend at the initial stage. But their later evolution trend is basically consistent with the changing trend of the three cases mentioned above. This trend is similar to that of ordinary supersonic nozzles [1]. For the temperature shown in Figure 3 (b), the variation trend of each position is roughly consistent with that in Figure 3 (a). However, the range of change between the maximum value and the minimum value is relatively smaller than before (the difference of about 0.25). The final convergent value is almost similar to that shown in Figure 3 (b).

According to the formula $\rho = pt$, the pressure at the throat at five different positions in Figure 4 can be obtained. As the two physical quantities (density and temperature) involved in the calculation can be seen from Figure 3 and Figure 4, the changing trend is roughly the same. The changing trend of pressure
evolution here is also roughly the same as that in Figure 3 Figure 4. The characteristics of the pressure change are exactly the same as before, except that the change is a little more drastic at the extreme values. This indicates that when the flow completes the transition from subsonic to supersonic, as the velocity increases, the pressure change at the throat tends to be a stable value from the sharp fluctuations in the transonic phase.

Figure 5. Normalized Mach Number Evolution at 5 Different Positions

According to the equation:

\[ Ma = \frac{\nu}{\rho^2} \]  \hspace{1cm} (30)

We can get the variation trend of Mach number at the throat at five different positions, as shown in Figure 5. It shows that the Mach number at the throat begins to step from a relatively high position (about 3.25) at the early stage of evolution of each position. However, for Case 1 and Case 2 with the throat close to the inlet, they would firstly evolve towards a higher Mach number for a period of steps, and then decrease after passing a maximum value. Then the change tends to be flat after experiencing a small fluctuation. From the position of the throat in the middle near the exit, the Mach number evolves directly downward, and the change tends to be flat after the minimum value of approximately the same position (after 50 steps). In general, the closer the throat is to the exit, the lower the Mach number at which it eventually stabilizes. This is a characteristic of the flow Mach number variation from the ordinary supersonic nozzle to the ordinary subsonic nozzle.

4. Conclusions and future work

Based on the Euler equation and the MacCormack finite difference method, this paper presents a numerical solution for the quasi-one-dimensional Laval nozzle flow problem at the inlet subsonic and supersonic outlet conditions. In order to derive the governing equations more simply, we consider the pipeline flow as isentropic flow. From the numerical simulation of the one-dimensional Euler equation in the Laval nozzle, it can be concluded that the physical properties of the airflow show a positive correlation trend under different positions of the nozzle throat. For the temperature, density, and pressure of the airflow, their changes all show an increasing trend during the initial evolution. After reaching the two maximum points, they quickly produce large fluctuations, which is the transonic stage. Subsequently, during the supersonic stage, these physical properties gradually tend to a stable value. Moreover, it is observed that the closer the throat is to the exit, the lower the Mach number at which it eventually stabilizes. In the future, we will build a new mathematical model to solve the optimal Laval nozzle shape.
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