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Preliminary Study on Supersonic Two-phase Expansion Refrigeration Technology in Liquid Hydrogen Temperature Region

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ABSTRACT

As a clean energy carrier, hydrogen has attracted extensive international attention. Hydrogen liquefaction is the key solution of large-scale utilization of hydrogen energy. How to realize the high-efficiency and low-cost liquefaction of hydrogen is one of the key technologies that need to be solved urgently. In the current mainstream hydrogen liquefaction technology, the high-speed rotating turbine may have an adverse impact on the stable operation of the bearing. Therefore, the supersonic two-phase expander in liquid hydrogen temperature zone is innovatively employed for the first time to complete expansion refrigeration, condensation phase change, gas-liquid separation and pressure recovery in a compact space. It has the advantages of gas-liquid two-phase operation, direct liquefaction, easy high power, simple structure and low processing cost. In the hydrogen supersonic two-phase expander, Laval nozzle is the key component. The main research contents in this paper include: (1) Establish the design criteria of hydrogen Laval nozzles. (2) The design law of hydrogen Laval nozzles under different working conditions. (3) The cooling characteristics of hydrogen Laval nozzles under different operating conditions. This paper preliminarily investigates the liquefaction possibility of supersonic two-phase expansion refrigeration technology in liquid hydrogen temperature region, and supports the development of new hydrogen liquefaction technology. It has important strategic value for promoting the realization of carbon neutralization goal in clean energy industry.

Keywords: Hydrogen liquefaction, Hydrogen supersonic two-phase expander, Hydrogen Laval nozzle

NONMENCLATURE

Abbreviations	
STPE	Supersonic two-phase expander
Symbols	
T	Temperature
P	Pressure
Ma	Mach number

1. INTRODUCTION

As supersonic two-phase expander (STPE) has respectable refrigeration and gas-liquid separation effect, many researchers have carried out a series of research.

Russia's ENGO oil company and the Dutch Shell Oil Company first introduced this technology into the field of natural gas processing, which was mainly used for dehydration and heavy hydrocarbon removal of natural gas [1]. Russian Translang company established an industrial test device in Moscow, with a natural gas processing capacity of 17×104~28×104 m^3/d. Subsequently, it was built in Calgary, Canada, with a processing capacity of 110×104~140×104 m^3/D industrial demonstration plant [2]. The first set of "3S" industrial device was built in Siberia, Russia in September 2004, realizing the leap from experimental research to industrial application [3]. Jassim et al. [4] conducted numerical research on the gas phase flow characteristics of high-pressure natural gas in the separation device, and obtained the influence law of real gas and nozzle geometry on supersonic flow field. Karimi et al. [5] predicted the pressure, temperature, dew point and other parameters of the internal flow field of the separation device through numerical simulation.

Malyshkina [6] used Euler's two-dimensional model to numerically calculate the fluid characteristics of natural gas in the expansion separation device after swirling, and analyzed the influence law of aerodynamic shock wave on supersonic flow field. In addition, they also analyzed the influence of different Mach number and temperature on the condensation composition of natural gas.

To sum up, supersonic two-phase expander can achieve good gas-liquid separation effect, but the research content mostly takes wet water steam or hydrocarbon gas as working medium, and mainly focuses on hydrocarbon gas dehydration. However, in the lower temperature region of liquid hydrogen, there is still a lack of research on supersonic two-phase expander in the field of hydrogen liquefaction.

In the hydrogen supersonic two-phase expander, Laval nozzle is the key component. The high-speed expansion of gas happens in Laval nozzle to produce low-temperature effect, which promotes the expansion and cooling of gas.

In this paper, the main aims are to establish the design criteria of hydrogen Laval nozzles under different working conditions, and to investigate the cooling characteristics of hydrogen Laval nozzles with different operating parameters.

2. METHODOLOGY

The density-based coupled CFD solver ANSYS-Fluent v19.0 has been employed to perform steady-state and transient 3D viscous simulations of the hydrogen supersonic two-phase expansion. In this paper, Reynolds-Averaged Navier Stokes (RANS) equations for viscous compressible flows are applied in a finite volume solver adapted to accommodate dense gas simulations.

The Reynolds-Averaged Navier Stokes (RANS) equations for viscous compressible flows are presented below, and solved using a finite volume solver adjusted for high-density fluid numerical simulations[7].

$$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x_j}(\rho u_i)=0 \tag{1}$$

$$\begin{aligned}\frac{\partial}{\partial t}(\rho u_i)+\frac{\partial}{\partial x_j}(\rho u_i u_j) &= -\frac{\partial p}{\partial x_j} \\ &\quad+\frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_j}-\frac{2}{3}\delta_{ij}\frac{\partial u_j}{\partial x_j}\right)\right] \\ &\quad+\frac{\partial}{\partial x_j}\left(-\rho\overline{u_i' u_j'}\right)\end{aligned} \tag{2}$$

$$\begin{aligned}\frac{\partial}{\partial t}(\rho E)+\frac{\partial}{\partial x_j}(\rho u_j E+u_j p) &= \frac{\partial}{\partial x_j}\left(k_{eff}\frac{\partial T}{\partial x_j}+u_i\tau_{eff}\right)\end{aligned} \tag{3}$$

Where ρ is gas density. $u_i u_j$ is velocity component; $\rho\overline{u_i' u_j'}$ is Reynolds stress; δ_{ij} is Kronecker delta number; E is Total energy; k_{eff} is effective thermal conductivity; τ_{eff} is effective stress tensor.

The suitability of the SST *k-ω* model for the supersonic two-phase expander and allows us to maintain a good balance between accuracy and computational cost [6].

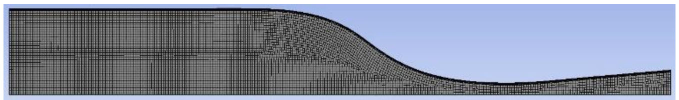

Fig. 1. 2D view of the grid for half hydrogen Laval nozzle.

For all of the simulations, the convergence is achieved once the Root Mean Squared (RMS) for mass, momentum, and turbulence variables approaches the residual target of 1×10^{-6}. The unstructured grid for the model is built with a total grid number of 229,907 nodes with the mesh independent study regarding Mach number as the evaluated result. The two-dimensional computational grid for the numerical study of the Laval nozzle is presented in Fig. 1.

The average non-dimensional grid space at the wall is $y_w^+=703$, which is close to the recommended value of 500 for RANS simulations using wall function-based turbulence models at approximately Reynolds number = 107 [8]. This value is sufficient to conduct pioneering numerical investigations of the supersonic flow.

3. RESULTS

3.1 Brief introduction of the hydrogen supersonic two-phase expander

The hydrogen supersonic two-phase expander is mainly composed of Swirl generator, Laval nozzle, Cyclone separation section, Drainage structure, and Diffuser, as shown in Fig.2.

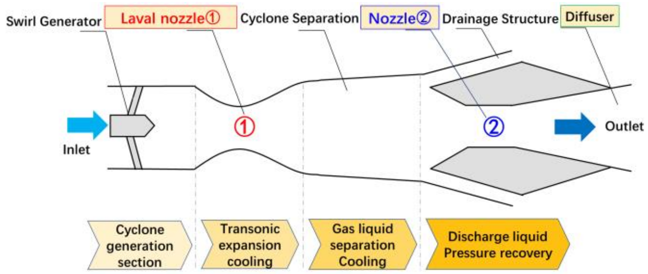

Fig. 2. Schematic diagram of the hydrogen supersonic two-phase expander.

Laval nozzle is the most important component in the STPE, which realizes the expansion and cooling of hydrogen. Laval nozzle ① with isentropic expansion produces refrigeration effect and makes gas flow be supersonic. The condensation phase change occurs, and low-temperature droplets are thrown to the wall in the cyclone separation section to realize gas-liquid separation. The remaining supersonic gas passes through the second nozzle ② to the diffuser to realize the conversion from kinetic energy to pressure energy.

3.2 Design of the hydrogen Laval nozzle

The calculation flow chart of throat critical flow parameters is shown in Fig.3. Based on the input basic data, such as inlet temperature, pressure, and mass flow, it calculates the inlet gas density, enthalpy and entropy. It needs to give an initial value to the throat temperature. Then it enters a loop to solve the local throat temperature and local sound velocity at throat. Then, the throat size will be determined.

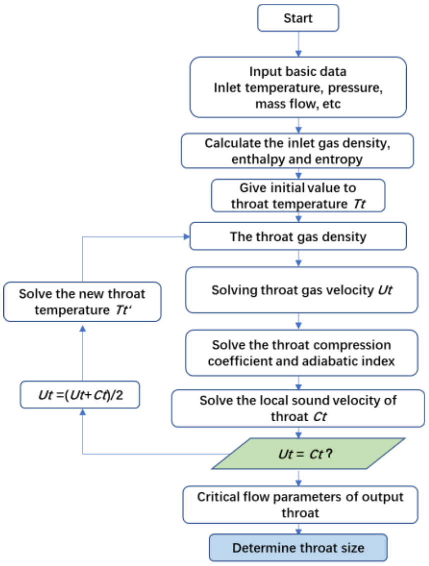

Fig. 3. Calculation flow chart of throat critical flow parameters.

According to the hydrogen Laval nozzle flow chart design, the design condition (inlet temperature, pressure and mass flow rate is 60K, 8Mpa and 10kg/s respectively) of the hydrogen Laval nozzle geometry with main dimensions are presented as Fig.4.

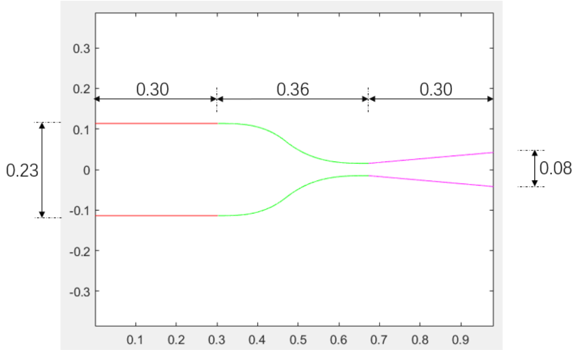

Fig. 4. The main dimentions of hydrogen Laval nozzle at design conditions.

The different mass flow rate, inlet pressure, and inlet temperature in terms of different Laval nozzles are presented in Fig.5, Fig.6, Fig.7 respectively.

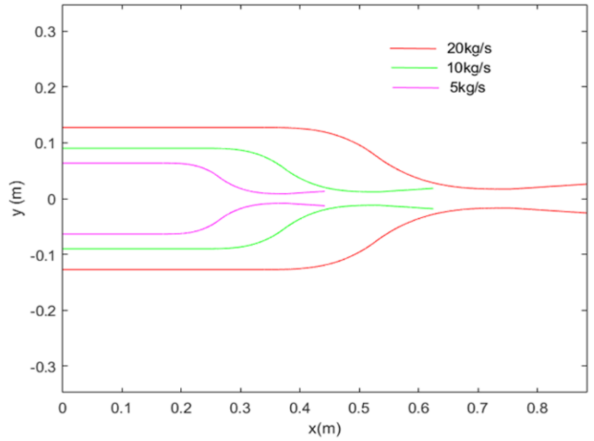

Fig. 5. Different mass flow rate for different Laval nozzle.

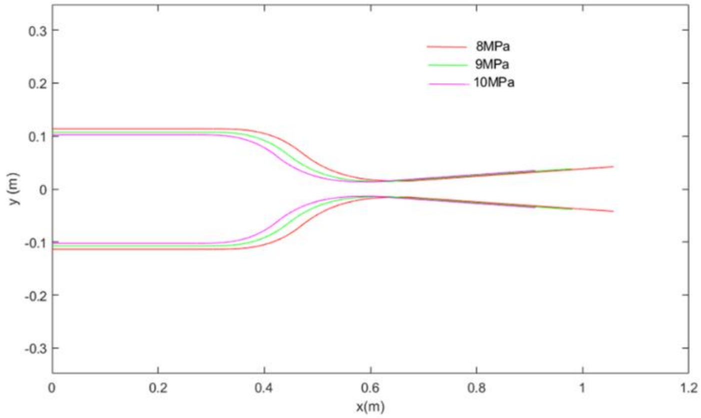

Fig. 6. Different inlet pressure for different Laval nozzle.

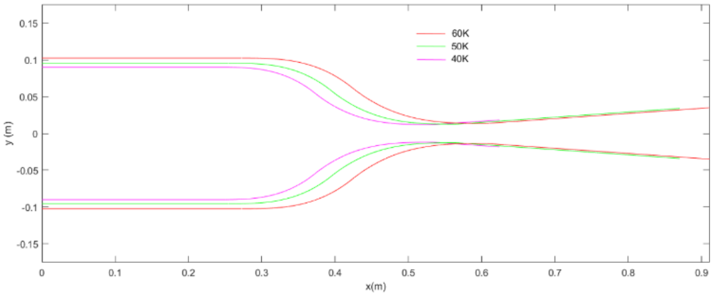

Fig. 7. Different inlet temperature for different Laval nozzle.

It can be seen from above results, when the inlet mass flow or inlet temperature is larger, the Laval nozzle size is also larger. On the contrary, while the inlet pressure is larger, the Laval nozzle size is smaller.

3.3 *Design condition results*

The boundary condition of the hydrogen Laval nozzle design: inlet temperature, pressure, and mass flow rate are 60K, 8MPa and 10kg/s respectively.

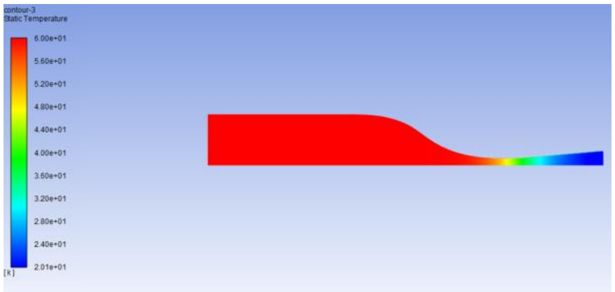

Fig. 8. Temperature distribution in hydrogen Laval nozzle.

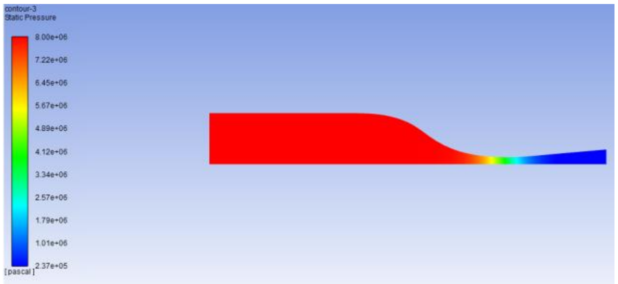

Fig. 9. Pressure distribution in hydrogen Laval nozzle.

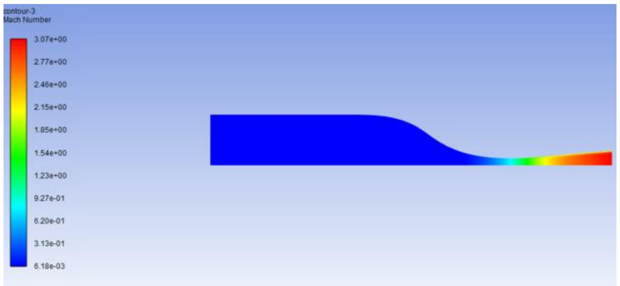

Fig. 10. Mach number distribution in hydrogen Laval nozzle.

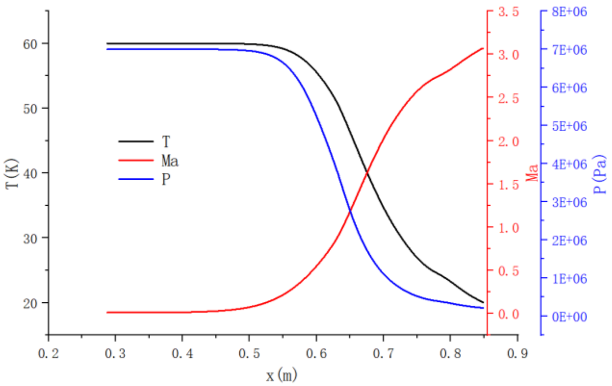

Fig. 11. Temperature, Pressure, Mach number distribution along the center line of the Laval nozzle.

After the CFD calculation, the results of the temperature, pressure, and Mach number distribution are shown in Fig.8, Fig.9, Fig.10, and Fig.11. When both the temperature and pressure decrease, the Mach number increases up above 3, which is supersonic flow. At the same time, the outlet temperature is less than 20K, reaching the hydrogen liquefaction temperature region, which shows that this design can meet the possibility of hydrogen liquefaction.

3.4 *Different operating conditions results*

The inlet operating temperatures are 75K, 70K, 65K,60K respectively, and the inlet pressure is fixed at 8MPa. The results along center line are shown in Fig.12.

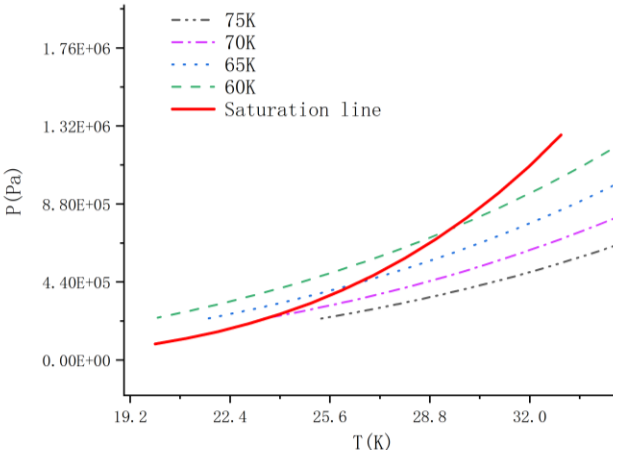

Fig. 12. Different inlet temperature *VS* saturation line along the center line of the hydrogen Laval nozzle.

Along the center line of the hydrogen Laval nozzle regarding the saturation line range (from 20K to 33K), when the inlet temperature is higher than 70K, the design Laval nozzle (with an inlet temperature of 60K) will not be prone to liquefaction, which is below the saturation line. On the contrary, if the inlet temperature is lower than 70K, hydrogen will liquefy in this design Laval nozzle, which is above the saturation line.

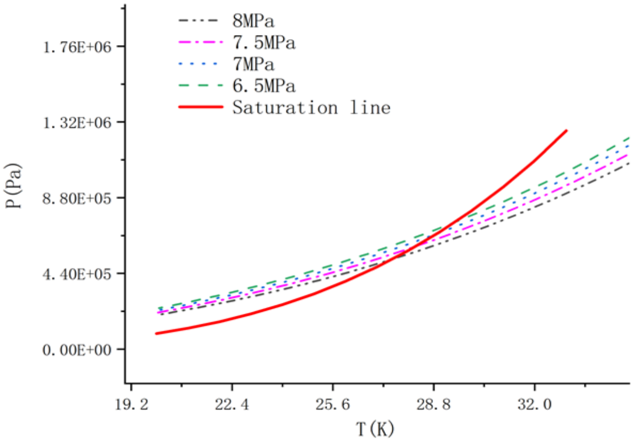

Fig. 13. Different inlet pressure *VS* saturation line along the center line of the hydrogen Laval nozzle.

As the results along center line are shown in Fig.13, when the inlet pressure is from 6.5MPa to 8Mpa and the fixed inlet temperature is 60K, the hydrogen in the Laval nozzle with 8Mpa design condition can be liquefied, which is above the saturation line. It indicates that the Laval nozzle has better adaptability to the inlet pressure compared to the inlet temperature.

4 CONCLUSIONS

A new generation of supersonic two-phase expansion refrigeration technology in liquid hydrogen temperature region without any mechanical moving part is proposed for the first time. This technology concentrates the processes of high-speed flow swirl, expansion refrigeration, condensation phase change, swirl separation and pressure recovery in one compact space.

For the innovation and contribution aspects, compared with traditional turbine expansion, it has the following advantages: gas-liquid two-phase operation, direct liquefaction, high reliability and stability, easy high power, high refrigeration efficiency, low processing cost, simple and compact structure, etc.

In this paper, the design process, parametric design and CFD calculation of hydrogen Laval nozzle in supersonic two-phase expander under different working conditions are investigated for the first time. The possibility of hydrogen liquefaction is calculated under different operating conditions. The adaptability of liquefaction cooling in the design condition of hydrogen Laval nozzle are presented. The hydrogen Laval nozzle has better adaptability to the inlet pressure compared to the inlet temperature. Further experimental validation and adding condensation two-phase flow model will be investigated in detail in the near future.

This research will enrich the connotation of low-temperature discipline, promote the development of hydrogen energy and its industrial application. It has important strategic value for promoting the realization of carbon neutralization goal in clean energy industry.

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REFERENCE

[1] M. Betting and H. Epsom, "Supersonic separator gains market acceptance," 2007.

[2] I. P. Jones, P. W. Guilbert, M. P. Owens, I. S. Hamill, and B. Prast, "The use of coupled solvers for complex multi-phase and reacting flows," 2003.

[3] V. Alfyorov, L. Bagirov, L. Dmitriev, V. Feygin, and S. Imayev, "Supersonic nozzle efficiently separates natural gas components," *Oil & Gas Journal,* vol. 103, no. 20, pp. 53-58, 2005.

[4] E. Jassim, M. A. Abdi, and Y. Muzychka, "Computational fluid dynamics study for flow of natural gas through high-pressure supersonic nozzles: Part 1. Real gas effects and shockwave," *Petroleum Science and Technology,* vol. 26, no. 15, pp. 1757-1772, 2008.

[5] A. Karimi and M. A. Abdi, "Selective dehydration of high-pressure natural gas using supersonic nozzles," *Chemical Engineering and Processing: Process Intensification,* vol. 48, no. 1, pp. 560-568, 2009.

[6] M. Malyshkina, "The procedure for investigation of the efficiency of purification of natural gases in a supersonic separator," *High Temperature,* vol. 48, no. 2, pp. 244-250, 2010.

[7] "ANSYS® Academic Research Fluent Guidance, Release 19," ed, 2019.

[8] A. Zou, J.-C. Chassaing, R. Persky, Y. Gu, and E. Sauret, "Uncertainty Quantification in high-density fluid radial-inflow turbines for renewable low-grade temperature cycles," *Applied Energy,* vol. 241, pp. 313-330, 2019.