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Numerical Study on the Nucleation Law of Water Vapor Condensation in Laval Nozzle

Weijun Ni [1, 3], Runyu Sun [1*], Gang Liu [2], Fei Ma [2], Chaobo Fan [2], Cong Xie [2] and Yong Kang [1]
[1] College of Petroleum Engineering, Xi'an Shiyou University, Xi'an, Shaanxi, 710065, China
[2] Gas Production Plant, Yanchang Gas Field, Shaanxi Yanchang Petroleum Group, Yan'an, Shaanxi, 727500, China
[3] National Subsea Centre, Robert Gordon University, Aberdeen AB21 0BH, UK
*454051766@qq.com

Abstract: **In order to explore the formation of condensed droplets and the process of agglomeration into droplets during the gas-liquid separation in the Laval nozzle, the wet gas is taken as the research object, and the numerical simulation model and control equations for the condensation of wet gas are established, which are simulated by Fluent software the effects of three parameters, the inlet relative humidity, the inlet and outlet pressure ratio and the inlet temperature, on the law of water vapor condensation and nucleation in the supersonic nozzle were analyzed. The results show that the higher the relative humidity is, the greater the peak value of the nucleation rate is, and the location of water vapor nucleation is getting closer to the throat of the nozzle; as the pressure ratio increases, the peak value of the nucleation rate becomes larger, and the pressure ratio is It has an impact on the peak value of the nucleation rate; the lower the inlet temperature, the greater the peak value of the nucleation rate, and the inlet temperature has the greatest influence on the nucleation rate. When the inlet temperature is 285K, the nucleation rate reaches the maximum value and the nucleation position is closest to Throat, that is, the time of nucleation is the shortest, and the position of nucleation is the most forward. Therefore, in the actual application process, the length of the expansion section can be adjusted by the relative humidity of the wet gas, and the equipment can be simplified; at the same time,the dehydration efficiency of the Laval nozzle can be improved by increasing the inlet and outlet pressure ratio or reducing the inlet temperature of the nozzle.**

Keywords: Laval nozzle, condensation nucleation, dehydration, numerical simulation

I. INTRODUCTION

Natural gas is an efficient, economical and clean fossil energy. With the rapid development of the national economy and the proposal of the "dual carbon" strategic goal, the demand for natural gas has maintained a stable and continuous growth trend.[1] The natural gas extracted from the wellhead usually contains a large amount of impurities such as water vapor and acid gas, which needs to be purified before storage and utilization. The supersonic separator is a new type of natural gas processing device, which can realize the purification of natural gas at the wellhead. [2] It is the development and improvement of the existing natural gas gathering and transportation process, and has a good application prospect.

In the supersonic separator, the Laval nozzle is the core component of the condensed gas, so scholars at home and abroad have done a lot of research on it. At present, the two mainstream theories are homogeneous nucleation theory and heterogeneous nucleation theory, which mainly discuss the nucleation law of water vapor when steam reaches supersaturated state and non-supersaturated state.[3]

A. Homogeneous nucleation theory

The homogeneous nucleation theory proposes formulas to calculate the droplet nucleation rate and droplet growth rate. At the beginning of the 20th century, Volumer and Weboer [4] first established the formula of droplet nucleation rate. After that, Becker & Dorig [5], Zeklovich [6] improved the formula of droplet nucleation rate on the basis of their predecessors. The formula for numerical calculation:

$$J_{CL} = J_0 \left(\frac{2\sigma}{\pi m_m}\right)^{1/2} \frac{n(1)^2}{\rho_l} e^{-\Delta G^*/KT} \tag{1}$$

This formula is not ideal for calculating the nucleation rate, so there are still many problems to be solved in the homogeneous nucleation theory.

At present, there are two common and widely used calculation formulas:

The first one was proposed by Frenkl and revised by Feder. It is often used to calculate the spontaneous condensation flow of high-speed expanding wet steam. The formula is as follows:[7]

$$J = \frac{q_c}{1+\emptyset}\sqrt{\frac{2\sigma}{\pi m_m^3}\frac{\rho_g^2}{\rho_l}}\exp\left(-\frac{4\pi r_c^2\sigma}{3kT_g}\right) \tag{2}$$

$$\emptyset = \frac{2(\gamma-1)}{\gamma+1}\left[\frac{h_{1g}}{RT_g}-\frac{1}{2}\right]^2 \tag{3}$$

In the formula: Ø—isotherm correction coefficient; qc—coagulation coefficient, generally taken as 1; Q—surface tension, N/m; mm—mass of a single molecule, kg; rc—critical radius of condensation core, m; k—Bohr Zeman constant, generally 1.38×10-23J/K; Tg—steam temperature, K.

The limitation of the above formula is that it does not consider the influence of non-condensable components in the mixed gas on the droplet nucleation. On the basis of the above formula, a new calculation formula is calculated. This formula includes the influence of the supersaturation of steam and the surface tension of liquid droplets on its nucleation. Nucleation rate for spontaneous condensation of components:[8]

$$J = \frac{vn^2}{S}\sqrt{\frac{2\sigma}{\pi m_m}}\, exp\left(-\frac{16\pi}{3}\frac{v^2\sigma^3}{(kT)^3(lnS)^2}\right) \tag{4}$$

Where: v—the volume of a single liquid molecule, m^3; n—the molecular density of water vapor, kg/m^3; S —the steam supersaturation.

B. Heterogeneous nucleation theory

Heterogeneous nucleation may occur when the steam does not reach a supersaturated state, but homogeneous nucleation can only occur when the steam reaches a supersaturated state, which is the biggest difference between homogeneous nucleation and heterogeneous nucleation. [9] Scholars at home and abroad have done a lot of research on the heterogeneous nucleation of condensable components. In 2016, Keisari and Shams carried out structural optimization of the wet steam Laval nozzle and compared the condensation performance of wet steam under different nozzle Laval structural conditions.[10] In 2019, Sharapov et al. studied and experimentally verified the main characteristics of non-uniform two-phase flow in the nozzle, and described the calculation method of the Laval nozzle based on the two-phase discrete flow integral energy equation.[11] In 2011, Han Zhonghe proposed a water droplet growth model based on the heat and mass transfer equilibrium coupling solution method, and compared the established model with the growth model widely used in the calculation of wet steam two-phase flow. The results show that different water droplet growth rate models have obvious effects on liquid phase nucleation rate, water droplet number and water droplet radius, but have little effect on steam humidity.[12] In 2019, Bian Jiang et al. established a mathematical model for the supersonic condensation flow of a two-component natural gas mixture to study the spontaneous condensation process of methane-ethane mixture gas in the Laval nozzle at different inlet temperatures. The results show that lowering the inlet temperature can advance the nucleation position of the mixed gas, increase the nucleation rate, and improve the condensation and liquefaction efficiency.[13]

In this paper, the law of condensation and nucleation of wet gas in supersonic nozzle is studied, and a mathematical model suitable for supersonic condensation flow of wet gas is established on the basis of the theory of droplet nucleation and growth. The influence of the three parameters of outlet pressure ratio and inlet temperature on the condensation and nucleation of wet gas in Laval nozzle, in order to obtain the law of condensation and nucleation of wet gas, improve the dehydration efficiency of Laval nozzle, shorten the length of expansion section, and simplify equipment.

II. CONDENSATION MODEL

The condensation flow of water vapor in the supersonic nozzle is very complicated, so the following assumptions are made to the model during the research process:

①Use air containing water vapor as the medium, and the condensed component in it is only water.

②Assume that the condensed liquid droplets in the nozzle are distributed orderly in the mixed air flow, and they will not collide with each other.

After the water vapor enters the nozzle, it expands at a high speed to produce a low-temperature effect, and gradually changes from an unsaturated state to a saturated state. At this time, it is still unable to condense to form droplets. It must reach a supersaturated state and exceed a certain value before it can begin to form condensation cores. condensation phenomenon.[14]The nucleation rate in the condensation process is an exponential function of free energy, and the homogeneous nucleation rate formula used in this paper is as follows:

$$J = \frac{v n_w^2}{S}\sqrt{\frac{2\sigma}{\pi m_m}}exp(-\frac{16\pi}{3}\frac{v^2\sigma^3}{(kT_r)^3(lnS)^2}) \tag{5}$$

In the formula:v—the volume of a single water vapor liquid molecule, m-3; n_w —the density of a single water vapor molecule, kg/m^3; S —degree of supersaturation; σ —droplet surface tension, N/m; k —Boltzmann constant, generally 1.38×10-23J/K; T_r—Temperature on the molecular surface of the droplet, K; m_m—the mass of a single water molecule, kg;

III. DROPLET GROWTH MODEL

After the water vapor is condensed and nucleated in the nozzle, the uncondensed and nucleated water vapor in the mixed gas will gather on the surface of the condensed droplet, making the droplet gradually become larger.[15] This process is called droplet growth. The mass of gas condensed on the surface of a single droplet per unit time is:

$$\frac{dm_p}{dt} = 4\pi r^2\rho_l\frac{dr}{dt} \tag{6}$$

In the formula: m_p—droplet mass, kg;ρ_l—the density of liquid water, kg/m3;r—the radius of the droplet particle, m.

During the growth of the droplet, the heat absorbed by the droplet is far less than the heat released by the condensation of the water vapor. Therefore, in the research process, it is believed that the heat released by the condensation of the droplet is completely absorbed by other nearby non-condensable gases and uncondensed water vapor.[16] The following balance relationship:

$$4\pi r^2\rho_l\ (T_r - T_g)\ \sum_{i=1}^{3}\alpha_{ri} = h_{lg}\times\frac{dM}{dt} \tag{7}$$

In the formula:

T_r—the temperature of the outer surface of the droplet, K; Tg—gas temperature, K; hlg—heat released by condensation, J/kg; α_{ri}—The heat transfer coefficient between the water droplet and the gas phase;i—$i = 1,2,3$represent water vapor, nitrogen and oxygen, respectively.

Combining formula (6) and formula (7) to obtain the formula for calculating the growth rate of droplet radius:

$$\frac{dr}{dt} = \frac{\sum_{i=1}^{3}\alpha_{ri}}{\rho_l h_{lg}}\ (T_r - T_g) \tag{8}$$

The heat transfer coefficients of each component are derived from the gas-liquid heat transfer coefficient relationship:

$$\alpha_{ri} = \frac{\lambda_i}{r}\frac{1}{1+\frac{2\sqrt{8\pi}}{1.5Pr_i}\times\frac{\gamma_i}{1+\gamma_i}Kn_i} \tag{9}$$

In the formula: λ_i —The thermal conductivity of each component, W/(m K); r—droplet particle radius, m; Pr_i—Prandtl constant of each component, J·S;γ_i—adiabatic index.

IV. LAVAL NOZZLE STRUCTURE DESIGN AND NUMERICAL SIMULATION

The specific parameters of the three-dimensional structure used to study the influence of operating parameters on the condensation and nucleation of condensable components in the nozzle are shown in Table 1:

Table 1. Laval nozzle flow path parameter list.

Part	Parameter (mm)
Nozzle inlet diameter	40
Nozzle inlet length	60
Throat diameter	4
Throat length	5
Nozzle outlet diameter	8
Nozzle extension length	40
Wall thickness	4

In this paper, the Solidworks software is used to establish the three-dimensional structural model of the Laval nozzle, and the SpaceClaim software is used to extract the internal flow channel structure model of the Laval nozzle, as shown in Figure 1:

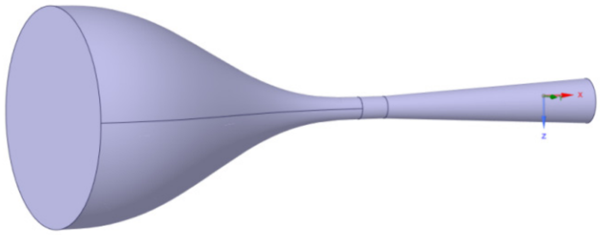

Figure 1. Laval nozzle model diagram.

The grid division of Laval nozzle is shown in Figure.2.

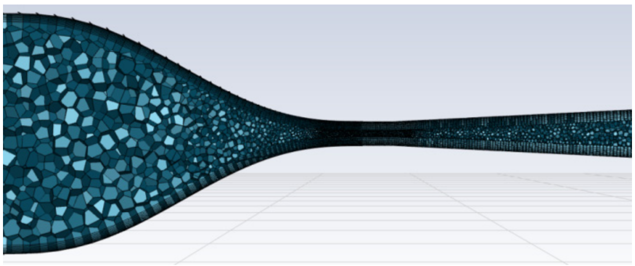

Figure 2. Laval nozzle grid.

When modeling, the slippage of velocity between phases is ignored, that is the generation of liquid droplets does not affect the turbulence, so only the turbulence equation of the gas phase is considered. FLUENT provides six models including K-εmodel, S-A equation model, Reynolds stress model, algebraic stress equation model, and large eddy simulation method (LES). According to the theoretical research of flow field flow in Laval and the basic characteristics of turbulent flow, the accuracy requirements of simulation, the current status of computing resources, and the limitation of solution time, etc., the K-εmodel is considered comprehensively in this paper.

The flow of gas in the Laval nozzle is a high-speed compressible flow, which is solved using a density basis. The flow governing equations, turbulent kinetic energy equations, and turbulent dissipation rate equations are all discretized using the second-order upwind method.

V. SIMULATION RESULT ANALYSIS

According to the established model, different operating parameters are adjusted to study the influence on the condensation and nucleation of condensable components in the nozzle. The main operating parameters are inlet relative humidity, inlet and outlet pressure ratio and inlet temperature.

A. *Influence of import relative humidity*

Relative humidity means the ratio of the wet gas to the saturated vapor pressure at the same temperature, expressed in. Control the inlet and outlet pressure ratio to 1.5, and the inlet temperature to 300K.By adjusting the value of relative humidity, the mass fraction of water vapor content corresponding to different relative humidity can be obtained. The formula is as follows:

$$q_m = \frac{m_{sl}}{m_{sl} + m_a} = \frac{0.622 \times \varphi \times P_s}{P - 0.378 \times \varphi \times P_s} \times 100\% \qquad (10)$$

In the formula:m_{sl}—mass of water vapor, kg; m_a—mass of dry air, kg; P_s—Saturation vapor pressure of water vapor at inlet temperature, Pa; P—Inlet pressure, Pa.

Taking φ equals 0.2,0.4,0.6,0.8, and 1 respectively. Through calculation, the corresponding water vapor mass fractions are 0.3137%,0.6287%,0.9448%,1.2621%, and 1.5807%.

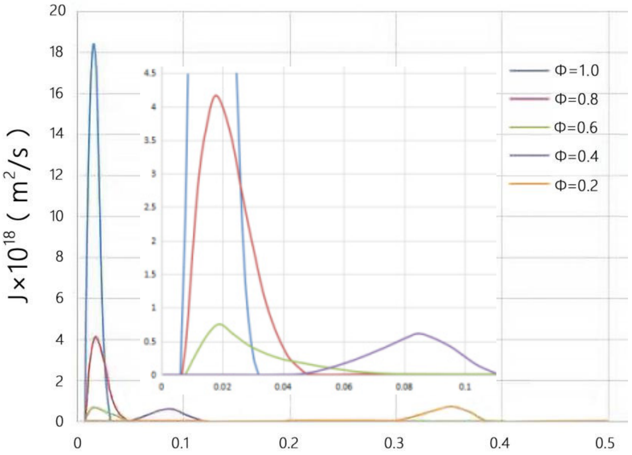

Figure 3. Variation curves of condensable gas nucleation rate(J)at different relative humidity.

Figure 3 shows the axial distribution curve of nucleation rate under different inlet relative humidity. From the nucleation change curves corresponding to different relative humidity in the figure, it can be concluded that the peak value of the nucleation rate becomes larger with the increase of relative humidity. As the relative humidity increases, the position of water vapor nucleation in the nozzle becomes closer and closer to the nozzle. Pipe throat. Among them, when =1.0, the peak nucleation rate value is 18.4. At this time, the nucleation rate reaches the maximum value and the nucleation position is closest to the throat; when =0.8, the peak nucleation rate value is 4.14; when =0.2 When the nucleation rate is ~0.6, the nucleation peak is 0.75. When the nucleation rate is 0.2, the nucleation position is farthest from the throat.

B. Influence of inlet and outlet pressure ratio

The inlet and outlet pressure ratio will affect the expansion and cooling of the mixed gas in the supersonic nozzle. The temperature drop of the mixed gas under different pressure ratios is also different. The relative humidity is controlled at 0.6, the inlet temperature remains unchanged, and the pressure ratio is adjusted to 1.4,1.5,1.6. Figure.4 is the axial distribution curve of the nucleation rate of water vapor in the supersonic nozzle under different pressure ratio conditions.

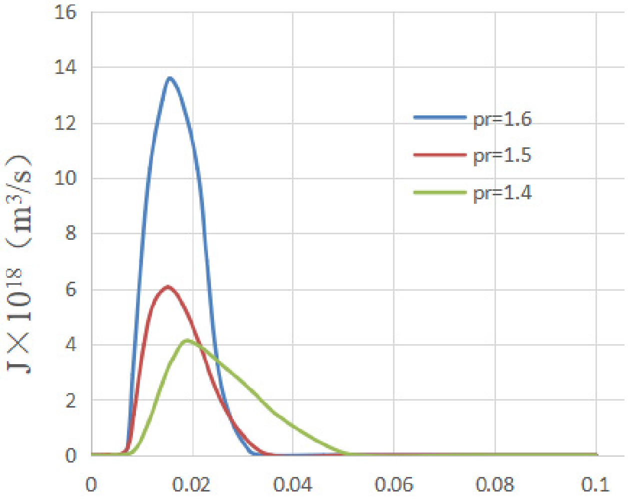

Figure 4. Variation curves of condensable gas nucleation rate(J)at different pressure ratios.

It can be seen from Figure.4 that under different pressure ratios, the nucleation position of water vapor in the nozzle is basically unchanged, but with the increase of pressure ratio, the peak value gradually increases. The nucleation rate of steam is also increasing, but when it reaches a certain value, the nucleation rate does not increase any more.

C. Influence of inlet temperature

Under the condition that the relative humidity is controlled at 0.6 and the inlet and outlet pressure ratio is 1.5, the inlet temperature is set at 285K, 294K, and 300K to study the influence of different inlet temperatures on the nucleation rate during the condensation of water vapor inside the Laval nozzle.

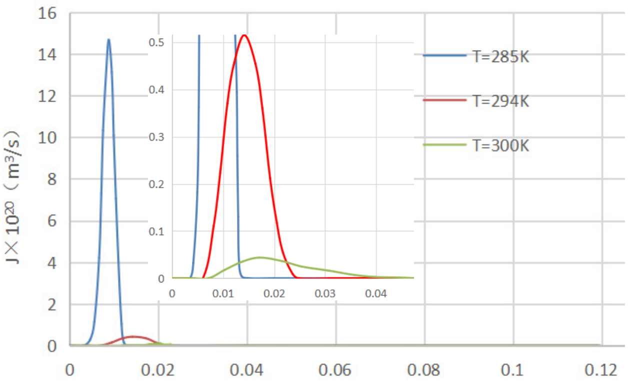

Figure 5. Variation curve of condensable gas nucleation rate(J)at inlet temperature.

It can be seen from Figure 5 that the higher the inlet temperature, the lower the nucleation rate of condensable components in the nozzle, and the nucleation position gradually shifts to the right with the increase of temperature, away from the throat, as can be seen from the figure The influence of human inlet temperature on droplet nucleation is relatively large.

VI. CONCLUSION

Taking wet gas as the research object, based on the basic theory of gas nucleation and droplet growth, a mathematical model of supersonic condensation of wet gas was established, and the influence of inlet temperature, relative humidity and inlet pressure on the condensable temperature of Laval nozzle was simulated by using Fluent software. The law of the effect of condensation and nucleation of components, the conclusions are as follows:

(1) Keeping the pressure ratio and inlet temperature constant, the peak nucleation rate becomes larger as the relative humidity of the wet gas increases, and the nucleation position of water vapor in the nozzle is closer to the throat of the nozzle. When=1.0,the peak value of nucleation reaches the maximum value and the nucleation position is closest to the throat, and when=0.2,the nucleation position is farthest from the throat.

(2) Keeping the relative humidity and inlet temperature constant, the peak value of the nucleation rate gradually increases with the increase of the pressure ratio, and the pressure ratio only affects the peak value of the nucleation rate, and does not affect the nucleation position, but controlling the relative humidity and the inlet temperature will not only affect the peak nucleation rate, but also affect the nucleation position.

(3) Keeping the relative humidity and pressure ratio constant, the lower the inlet temperature, the larger the nucleation peak, and the inlet temperature has the greatest influence on the nucleation rate. When the inlet temperature is 285K,the nucleation rate reaches the maximum and the nucleation The position is closest to the throat, that is the nucleation time is the shortest, and the nucleation position is the most forward.

Therefore, in the actual application process, the length of the expansion section can be adjusted by the relative humidity of the wet gas, and the equipment can be simplified; at the same time, the dehydration efficiency of the Laval nozzle can be improved by increasing the inlet and outlet pressure ratio or reducing the inlet temperature of the nozzle.

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