A potential strategy of carbon dioxide separation using supersonic flows

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ARTICLE INFO

Keywords:
Carbon capture
CO2 separation
Supersonic flow
Energy conversion
Carbon emission

ABSTRACT

Carbon capture and storage (CCS) is one of the most promising technologies to tackle climate challenges. The separation of carbon dioxide (CO2) is the key step to achieve the economic and technical objectives of CCS. The present study proposes a potential strategy to separate CO2 using the phase change behavior in supersonic flows, which is not only a clean process of CO2 processing but also provides an efficient way to maximize utilize the thermal energy. To this end, a condensation flow model based on the real gas thermodynamics is developed to obtain an accurate evaluation of the heat and mass transfer due to the homogeneous condensation process of CO2 in supersonic flows. The prediction accuracy of the ideal gas model and real gas model is compared, and the result shows that the real gas condensation model presents a more accurate prediction of CO2 supersonic condensation with the root mean square error (RMSE) of 0.0147. The sensitivity of the two models to inlet pressure is analyzed, which shows that the ideal gas model under-estimated the liquid fractions of CO2 condensation by 2.8% of the total mass as well as over-estimated the latent heat by 20.1% at Wilson point during the heat transfer process. The condensation performances and Wilson point characteristics of CO2 are analyzed by using the real gas model. The prediction model of the relationship between the degree of supercooling, pressure, and expansion rate at the Wilson point was established with the mean relative error of 0.176% and the relative RMSE of 2.275% respectively, which is of great help for further forecasting to obtain the regularity of known data for CO2 separation in supersonic flows.

1. Introduction

The National Energy and Climate Plans (NECPs) and the Long-Terms Strategy (LTS) plans of the Member States of the European Union determine the national contributions toward the European Union’s (EU) energy–climate target. They are the main tools to promote EU decarbonization. In NECPs, however, many EU Member States still have no plans to phase out coal by 2030, while others are planning to replace coal with natural gas and are pushing for the use of EU funds to finance natural gas infrastructure investment. It has to be mentioned that natural gas, as green energy, is considered to be the key energy to achieve carbon neutrality. The European Commission released the proposal “REPowerEU: Joint European Action for more affordable, secure and sustainable energy”. The proposal states that REPowerEU will seek to diversify natural gas supplies and accelerate the promotion of renewable natural gas [1,2]. As a signatory to the Paris Agreement [3] and the largest emitter of CO2, China aims to peak its CO2 emissions by 2030 and achieve carbon neutrality by 2060 [4]. Decarbonization of energy systems has been a key measure to combat climate change. In the long term, the breakthrough technologies to achieve energy decarbonization are essential for climate change mitigation [4,5]. Sequestration of carbon dioxide as much as possible to achieve net-zero or even negative carbon dioxide emissions is the key link to be urgently realized in the long run [6]. At present, innovative technologies such as carbon capture and storage (CCS) have a great potential to reduce CO2 emissions, which received increasing attention [7]. And closer international collaboration in CCS will be essential to meeting that challenge [8]. Take it a step further, carbon capture, utilization, and storage (CCUS) is a sustainable technology promising in terms of reducing CO2 emissions [9] that would otherwise contribute to climate change. It’s worth noting that, natural gas has a great contribution to reducing CO2 emissions. As a key link in the process of carbon neutralization, the clean utilization and improvement of the production quality of natural gas have become particularly important.

As mentioned above, natural gas is currently recognized as a high-quality green energy [10] for its lower harmful gas emissions when burning compared with fossil energy [11,12]. The use of natural gas is
undoubtedly an important way to slow down the greenhouse effect and reduce environmental pollution [13]. However, in the natural gas extraction and storage process, CO2 gas impurities [14] mixed in natural gas will corrode the transportation pipeline [15], which poses great challenges to the transportation and preservation of natural gas. Therefore, it is an urgent problem to separate CO2 from natural gas [16,17]. At present, industrial CO2 removal methods are mainly chemical absorption method [2,18–20], physical absorption method [21], pressure swing adsorption method [22,23], low-temperature separation method [24,25], and membrane separation method [19,26,27], but these methods have more shortcomings, such as complex process, especially membrane separation technology [28,29], intermediate process pollutants cause secondary pollution to the environment [30], large energy consumption, low recovery rate of CO2 problems. Different from the proposed industrial method [31], supersonic separation technology is a promising separation technology [32] in recent years which utilizes the phase transition phenomenon in supersonic flow to achieve condensation separation [33]. Compared with the traditional CO2 separation technology, the supersonic separation technology has the advantages of its simple and reliable system, low-pressure loss, high separation efficiency, and no secondary pollution. Considering the superiority of the supersonic separation technology [34], it is expected that the supersonic separation technology can be applied to the separation of CO2 from natural gas [35], which will be a relatively desired frontier technology for removing CO2 [36]. But to date, most of the relevant studies are focused on the phase change of CO2 [37], and there are few studies on the removal of CO2 in natural gas [38], especially the condensation mechanism of CO2 in supersonic nozzle [39] still needs to be investigated. That is most of the research on CO2 has focused on its phase transition, but the study of the removal mechanism of CO2 from natural gas in supersonic nozzles is not yet mature, especially the CO2 condensation mechanism based on real gas models has not been fully explored, such as the Wilson point position characteristics of the real gas, which will hinder the utilization of supersonic separators for the removal of CO2 in natural gas, and cannot guide the large-scale production design of supersonic separators applied to the natural gas industry.

The condensation characteristics of CO2 in a supersonic nozzle are very important for the investigation of CO2 supersonic separation, and many scholars have done a lot of analysis on this technology. Chen et al. [40] established the condensation flow model of CO2-CH4 two-component gas by computational fluid dynamics software based on the ideal gas, which gives important numerical opinions on CO2 separation. However, only numerical studies under a single pressure condition were carried out. Jiang et al. [41] calculated the efficiency of CO2 separation but lack of real gas model. Niknam et al. [42] conducted numerical analysis of condensation parameters in the supersonic flow process, such as pressure and temperature, and made a certain study of the fluidity inside the supersonic separator. Wen et al. [43] put forward an efficient approach to separate CO2 using supersonic flows for carbon capture and storage. Cao et al. [44] established a CO2 condensation model in supersonic flow and analyzed the use of supersonic separation technology to remove CO2 and hydrogen sulfide from natural gas. Li et al. [45] studied the expansion state of the nozzle and its influence on the performance of the steam ejector numerically based on the ideal gas model. In all the above studies, CO2 was assumed as an ideal gas. However, in high-pressure environments such as the separation of natural gas, the physical properties of CO2 are not ideal gas actually, but real gas. For higher simulation accuracy, it is necessary to take into account the influence of real gas condensation which is different from ideal gas. Cruz et al. [46] have studied the uncertainty quantification of the real gas model in supersonic flow of CO2, they found the sources of uncertainty are input parameters of real gas models. Yang et al. [47] simulated the flow of the real gas model in supersonic separation of natural gas dehydration numerically and made a correlation with ideal gas. Wen et al. [48] studied the dehydration of natural gas in high-pressure supersonic flow numerically and analyzed the influence of the thermodynamic model on non-equilibrium condensation of ideal gas and real gas. Wen et al. [49] also studied the condensation of CO2 in supersonic flow of real gas and ideal gas at low pressure and found that the ideal gas model greatly underestimates the mass flow. Croquer et al. [50] firstly extended the compound-choking criterion analytically to real gases and they solved the problem that the performance of supersonic ejector was limited by the choking of the flow. However, the above studies related to the condensation of real gas CO2 are limited to low-pressure environments and have not been extended to supercritical

### Nomenclature

| Term | Definition |
|------|------------|
| $c_p$ | specific heat capacity, J kg$^{-1}$ K$^{-1}$ |
| $F$ | safety factor |
| $h_l$ | latent heat of vapor, J kg$^{-1}$ |
| $h_G$ | latent heat of vaporization, J kg$^{-1}$ |
| $l$ | nucleation rate, m$^{-3}$ s$^{-1}$ |
| $k_B$ | Boltzmann’s constant, 1.38 × 10$^{-23}$ J K$^{-1}$ |
| $Kn$ | Knudsen number, – |
| $l_0$ | average free path of the molecule, m |
| $m_0$ | single molecular mass, kg |
| $m_v$ | liquid mass changing rate, kg m$^{-3}$ s$^{-1}$ |
| $N$ | number of droplets per volume, m$^{-3}$ |
| $N_A$ | Avogadro number |
| $P$ | pressure, Pa |
| $Pr$ | Prandtl number, – |
| $q_c$ | condensation coefficient |
| $r$ | droplet radius, m |
| $r_c$ | critical radius, m |
| $R_{CO2}$ | gas constant of CO2, J kg$^{-1}$ K$^{-1}$ |
| $S_s$ | supersaturation of CO2, – |
| $t$ | reduced temperature, – |
| $T$ | fluid temperature, K |
| $V$ | volume, m$^3$ |
| $Y$ | liquid fraction, % |

### Greek

| Symbol | Definition |
|--------|------------|
| $\alpha$ | droplet growth correction coefficient |
| $\beta$ | droplet growth correction coefficient |
| $\gamma$ | specific heat capacity ratio |
| $\epsilon$ | relative error of grids |
| $\lambda$ | thermal conductivity, W m$^{-1}$ K$^{-1}$ |
| $\mu$ | laminar viscous |
| $\rho$ | density of fluid, kg m$^{-3}$ |
| $\sigma$ | surface tension, N/m |
| $\varphi$ | non-isothermal correction coefficient |
| $\omega$ | accentric factor |

### Subscripts

| Symbol | Definition |
|--------|------------|
| $c$ | critical |
| $g$ | gas |
| $l$ | liquid |
| $s$ | saturation |
| eff | effective |

### Superscripts

| Symbol | Definition |
|--------|------------|
| $p$ | the order of algorithm |
CO$_2$ gas, the condensation characteristics of real CO$_2$ gas under high pressure still need to be explored.

It is worth mentioning that the condensation position of CO$_2$ gas in the supersonic nozzle and the thermodynamic characteristics of this condensation position can’t be ignored in the research process, which could help explain the condensation behavior of CO$_2$ in a more systematic way. In particular, the location at which the CO$_2$ gas begins to condense and the degree of supercooling of the supersonic nozzle is greatest along the way, is known as the Wilson point. The prediction of the properties at the Wilson point is the key to the numerical studies of the CO$_2$ condensation. Dobbins [51] put forward an algebraic method for determining the start of condensation (Wilson line) in low-pressure steam. Huang et al. [52] proposed an analytical solution of Wilson point in homogeneous nucleation flow. The numerical study of homogeneous condensation at Wilson point is carried out based on the approximate values of parameters at Wilson point. Delale et al. [53] presented an algorithm for the flow properties of Wilson point. The asymptotic solutions of the expansion of wet air in the nozzle in each supercritical flow state under atmospheric supply condition are given. Ding et al. [54] gave an analytical method for Wilson point in nozzle flow with homogeneous nucleating. An analytical method for calculating the flow characteristics of the Wilson point was proposed and a more comprehensive understanding of the nucleation phenomenon of nozzle flow at low pressure was sought. Lettieri et al. [55] also explained the Wilson line, but only introduced the position of Wilson point in the phase change process based on condensation. Zhang et al. [56] studied the condensation flow numerically with the modified model and explained the condensation process along with the flow by Wilson point and described the variation law of condensation parameters at Wilson point. Azzini et al. [57] proposed a semi-analytical model for predicting the Wilson point of uniformly condensed steam flow. At present, most studies on Wilson point focus on algebraic methods, which are difficult to be popularized and applied due to the complexity of methods. There are few studies on Wilson point in the process of CO$_2$ condensation in supersonic flow. In particular, there is a lack of strong demonstration of Wilson point variation under different inlet conditions, in which inlet pressure is subcritical, critical, and supercritical.

As mentioned above, the main problems existing in previous studies of the CO$_2$ condensation mechanism in the supersonic nozzle are as follows: firstly, research on the condensation of real CO$_2$ gas is limited to the lower pressure environment; secondly, the research on Wilson point is not thorough enough. Based on the aforementioned knowledge gaps, the present study proposes an advanced mathematical model to predict the CO$_2$ condensation in supersonic flow using the real gas thermodynamics properties. We reveal the significant influence of the ideal gas model and the real gas model on CO$_2$ condensation characteristics at Wilson point as well as analyse the changes of typical parameters in non-equilibrium condensation process. Then, according to the position and condensation characteristics of Wilson point under different inlet conditions, a more accurate prediction formula of the degree of supercooling, pressure and expansion rate at Wilson point is obtained by using the established model.

2. Problem statement

2.1. CO$_2$ capture in supersonic flows

As shown in Fig. 1, the supersonic separator consists of a supersonic nozzle, an array of vortex generator and a diffuser. As the gas mixture expands rapidly inside the nozzle, the supersonic nozzle condenses CO$_2$ from the main gas into droplets. CO$_2$ droplets will flow out of the liquid outlet due to the strong centrifugal force generated by the static vanes. The diffuser is used to recover the static pressure, and the temperature will increase to ensure efficient use of energy. This new method achieves CO$_2$ capture in a clean way through a purely physical separation process without chemicals and is expected to release no pollutant by-products into our environment.

To analyze the non-equilibrium condensation phenomenon of CO$_2$ in supersonic flow, a supersonic nozzle is deployed in this study. As shown as Fig. 2, a supersonic nozzle is composed of two parts: convergent section and expansion section. In the divergent section of the nozzle, the gas flow is subsonic, and in the expansion section, the gas flow is supersonic. The superheated steam expands along the nozzle from the inlet, and the temperature and pressure decrease accordingly. It will reach the saturation point behind the throat. If there are no foreign particles in the gas, condensation will not occur here but continue to expand, and the gas is in a supersaturated state until it reaches Wilson point, where condensation occurs suddenly. After the Wilson point, a large number of condensation cores are generated, steam molecules continuously form droplets and grow on the condensation cores. In the condensation process, a lot of latent heat is released to heat the gas molecules, and the supersonic flow slows down, causing pressure and temperature to rise. After the above condensation process, the steam will re-enter the thermal equilibrium state from the original supersaturated state, and the condensation process ends.

The geometry data of the supersonic nozzle is derived from the nozzle data of Claudio Lettieri [58]. As shown in Fig. 2, the convergence and divergence parts of nozzle are connected smoothly, which reduces the strong shock waves at the connecting angle of the two straight lines. The size parameters of each part of the supersonic nozzle are shown in Table 1. The throat is located at $x = 0$, the throat diameter is 3.086 mm, the inlet diameter and outlet diameter are 12.7 mm and 4.012 mm respectively, the length of convergence segment is 32.01 mm, and the length of divergence segment is 66.35 mm.

2.2. Mathematical model

The nucleation and condensation of CO$_2$ are overwhelmingly complicated due to the non-equilibrium state in supersonic flows [59]. The mathematical model used in this study is based on the assumption that the condensation is spontaneous [60] and there is no relative slip velocity between the two phases [61]. The basic equations are based on the two-phase non-equilibrium condensation model, including mass, momentum, and energy equations for gas–liquid mixtures. In addition, two transport equations are coupled to simulate the phase transition from gas phase to liquid phase, which are the conservation of liquid
fraction and droplet number.

The mass, momentum and energy conservation equations of the gas–liquid mixture are shown as below,

\[
\frac{∂ρ}{∂t} + \frac{∂}{∂x_i}(ρu_i) = S_m
\]  

(1)

\[
\frac{∂}{∂t}(ρu_i) + \frac{∂}{∂x_i}(ρu_ju_i) = -\frac{∂ρ}{∂x_i} + \frac{∂τ_{ij}}{∂x_i} + S_u
\]  

(2)

\[
\frac{∂}{∂t}(ρE) + \frac{∂}{∂x_i}(ρu_iE + p) = \frac{∂}{∂x_i}(k_{ij}\frac{∂T}{∂x_i}) + \frac{∂}{∂x_i}(u_ik_{ij}τ_{ij}) + S_h
\]  

(3)

where \(u_i, ρ, p, T\) and \(E\) are the velocity, density, pressure, temperature, and total energy respectively; \(u_i, u_j\) are axial and radial velocity components respectively, \(k_{ij}\) is the effective thermal conductivity, \(τ_{ij}\) is the effective stress tensor; \(S_m, S_u, S_h\) are the source terms to consider the effect of the condensation process.

The source terms are defined as follows,

\[
S_m = -m_0
\]  

(4)

\[
S_u = -m_0u_i
\]  

(5)

\[
S_h = -m_0(h - h_g)
\]  

(6)

where \(m_0\) (kg m\(^{-3}\) s\(^{-1}\)) is the liquid mass per unit volume condensation in unit time, \(h\) is the total enthalpy, and \(h_g\) (kJ kg\(^{-1}\)) is the latent heat of condensation.

As the supersonic separation process is performed at high pressure and low temperature, the properties of CO\(_2\) may be far from ideal gas.

The \(p\) in classical ideal gas law can be written:

\[
p = ρR_{CO2}T
\]  

(7)

where \(p, ρ, T\) are the pressure, density and temperature, the \(R_{CO2}\) (J kg\(^{-1}\)K\(^{-1}\)) is the gas constant of the Carbon dioxide. For higher pressures, especially near or above the critical point of the components, real gas effects must be considered. Most models describing the fugacity coefficients use a cubic equation of state with the general form, and the \(p\) is described as:

\[
p = \frac{R_{CO2}T}{V - b + c} - \frac{α(T)c}{V^2 + αV - α_2^2}
\]  

(8)

where \(p, V, T\) are the pressure, volume and temperature respectively. The coefficients \(α(T), a, b, c, λ_1\) and \(λ_2\) are given for each equation of state as functions of the critical temperature \(T_c\), critical pressure \(p_c\), acentric factor \(ω\) and critical specific volume \(V_c\). It is worth mentioning that the REFPROP database employs accurate pure-fluid equations of state that are available from NIST. These equations are based on three models which are modified Benedict-Webb-Rubin (MBWR) equation of state, Helmholtz-energy equation of state and extended corresponding states (ECS) respectively. And the real gas model referred to in this study is based on this NIST real gas model.

Two transport equations are used to describe the condensation process of CO\(_2\) in supersonic flow. Two scalar equations are used to describe the droplet number (\(N\)) and liquid fraction (\(Y\)).

\[
\frac{∂}{∂t}(ρY) + \frac{∂}{∂x_i}(ρu_iY) = S_Y
\]  

(9)

\[
\frac{∂}{∂t}(N) + \frac{∂}{∂x_i}(u_iN) = I
\]  

(10)

where the source term \(S_Y\) describes the condensation rate of the wet steam and \(S_Y = m_0; N (m^{-3})\) is the number of droplets per volume; \(I (m^{-4} s^{-1})\) is the spontaneous condensation nucleation rate.

The mass production rate \(m_0\) is determined by nucleation and droplet growth in the process of non-equilibrium condensation.

\[
m_0 = \frac{λρ4πr^3}{3} + 4πNρ_{d}r^2\left(\frac{dr}{dt}\right)
\]  

(11)

where \(ρ_l\) is the liquid density, \(r\) (m) is the droplet radius, \(dr/dt\) is the growth rate of droplets, the \(r_c\) is the critical droplet radius. The droplet radius and critical droplet radius are defined as:

\[
r = \left(\frac{3Y}{4πρ_{d}N}\right)\frac{1}{2}
\]  

(12)

\[
r_c = \frac{2σ}{ρR_{CO2}T_{CO2}ln(S_l)}
\]  

(13)

where \(σ\) (N/m) is the surface tension. \(T_{CO2}\) is current temperature in supersonic flows. The \(S_l\) is the degree of supersaturation. It’s defined as
where \( p_s \) is the saturation pressure of CO\(_2\) at this temperature. \( \rho_{\text{CO}_2} \) is the current pressure of CO\(_2\) gas.

The surface tension coefficient \( \sigma \) for CO\(_2\) is implemented based on the following equation from Miqueu et al. [62]:

\[
\sigma = k_B T_c \frac{N_A V_c}{W_c} \left[ 4.35 + 4.14 \omega \right]^{1.26} \left[ 1 + 0.19 \gamma^{0.5} - 0.25 \right]
\]

where \( k_B \) (1.38 \times 10^{-23} \text{J K}^{-1}) is the Boltzmann constant; \( N_A \) is the Avogadro number; \( V_c \) is the critical volume; \( T_c \) is the critical temperature; \( \omega \) is the eccentric factor. And the \( \tau = 1 - T/T_c \) is reduced temperature. \( \omega = -1 - \log \left( (p_0 - p_s)/p_s \right) \) [62], \( p_0 = 0.7 p_s \).

In supersonic nozzle, the CO\(_2\) condensation process can be divided into two stages, nucleation process and droplet growth process.

Considering the effect of non-isothermal effects, the nucleation rate \( \mathcal{I} \) (m\(^5\) s\(^{-1}\)) expression corrected by Kantrowitz [63] is used.

\[
\mathcal{I} = \frac{q_c \rho_{\text{CO}_2}^2}{1 + \phi} \frac{2g}{\rho_{\text{water}}} \exp \left( -\frac{4 \pi m \gamma^2}{3 k_B T_{\text{CO}_2}} \right)
\]

The \( m_0 \) (kg) is single molecular mass, and the \( q_c \) is condensation coefficient. \( q_c \) approximately equal to 1 [64]; \( \rho_{\text{CO}_2} \) is the density of steam at current temperature \( T_{\text{CO}_2} \).

And the \( \phi \) is the non-isothermal correction coefficient proposed by Kantrowitz [63] and defined as follows:

\[
\phi = \frac{2(\gamma - 1) h_{b_0}}{\gamma + 1} \frac{h_{b_0}}{R_{\text{CO}_2} T_{\text{CO}_2}} \left( \frac{h_{b_0}}{R_{\text{CO}_2} T_{\text{CO}_2}} - \frac{1}{2} \right)
\]

where \( \gamma \) represents the specific heat ratio. The latent heat of CO\(_2\) at the arbitrary temperature is computed by

\[
h_t = h_{b_0} \left( \frac{1 - T/T_s}{1 - T_s/T_c} \right)^{0.38}
\]

where \( h_{b_0} \) represents the latent heat of vaporization at standard boiling point.

The growth rate of droplets due to evaporation and condensation, \( \frac{dr}{dt} \), is calculated as follows.

\[
\frac{dr}{dt} = \frac{k(T_c - T_{\text{CO}_2})(1 - \gamma)}{\rho_{\text{water}} r^{(\gamma + 1) / \rho_{\text{water}}} \left( 1 - \gamma - 1 + \frac{4 \pi m \gamma^2}{3 k_B T_{\text{CO}_2}} \right)}
\]

In this formula,

\[
v_c = \frac{R_{\text{CO}_2} T_s}{h_{b_0}} \left( a - 0.5 \frac{2 - q_c \gamma + 1 + \varepsilon p_s}{2 q_c \gamma} \right)
\]

where \( K_a \) is the Knudsen number; \( Pr \) is the Prandtl number; \( T_s \) is the saturated temperature; \( a \) and \( \beta \) are droplet growth correction coefficient; \( c_p \) is specific heat capacity (J kg\(^{-1}\) K\(^{-1}\)); \( a = 1, \beta = 0; \) For CO\(_2\) steam, \( \gamma = 1.3 \).

## 2.3. Numerical implementation and grid independence verification

The supersonic nozzle was meshed with two-dimensional structural grids, as shown in Fig. 3. The boundary layer and throat were locally refined, and grid-independent validation was also carried out to ensure the accuracy of the model calculation. For the goal of ensuring the predicting precision of the modified wet steam model, the grid independence of this study is evaluated by the grid convergence index (GCI). The verification of GCI is the refined error estimation on the foundation of Richardson’s extrapolation. The formula of GCI is:

\[
\text{GCI} = \frac{F_{1,3} \left| e \right|}{p_r} \times 100\%
\]

where \( F \) is the safety factor, usually taken as 3. \( \varepsilon \) is the relative error of two groups of grids, and \( p \) is the ratio of refinement factor, with \( p \) means the order of algorithm. And a small GCI means that the grid is closer to the optimal.

In this study, the established CFD model is used for analysis with three sets of grids: 1: superior (87,200 quadrilateral elements), 2: moderate (71,880 elements) and 3: inferior (56,600 elements). Taking the outlet pressure as the test parameter, the test data of GCI is shown in Table 2. Regarding the discretization of grid computing, the refinement of the grid cannot adequately improve the exactitude of CFD calculations. The outcome obtained by set 1 is very similar to those of 2. Thus, 71,880 grids of moderate refinement are utilized to further investigate which can ensure the computation accuracy as well as the calculating speed.

In addition, the standard k-epsilon model is used for the turbulence model in this study. Considering the compressible flow characteristics of CO\(_2\) gas in the nozzle, the density-based solver is used to solve the equation, and the second-order upwind scheme is used to discrete the turbulent flow energy equation, the turbulent dissipation rate equation, and the flow control equation. When we need to carry out numerical simulation of condensation, the source term of gas phase control equation and liquid phase control equations should be added. The source term of the gas phase control program is compiled through user-defined function (UDF). Liquid phase governing equations and source terms are implemented by user-defined scalars (UDS), and the mass, momentum and energy changes are calculated in the governing equations. The pressure inlet condition is assigned for the nozzle entrance, while the nozzle exit utilizes the pressure outlet condition. Also, the wall boundary conditions are set as no seepage, no slip and adiabatic boundary.

### Table 2

| Grids | GCI (%) | ε (\%) |
|-------|--------|--------|
| 1-2   | 0.13   | 0.69   |
| 2-3   | 0.45   | 1.78   |

![Fig. 3. Grids of the supersonic nozzle.](image-url)
3. Thermodynamics modelling of CO₂ condensation

3.1. Accuracy validation of thermodynamics models

To validate the usability of the established model and compare the simulated quality of thermodynamics modelling based on real gas model and ideal gas model, the nozzle structure and data in Claudio Lettieri’s [58] experiment results are chosen, which the inlet pressure is 57.24 bar and inlet temperature is 314.78 K. Condensation model of real gas was validated in this paper, the validation results are shown in Fig. 4(a). The condensation occurs approximately 2 mm after the nozzle throat, where the pressure jump appears due to the release of latent heat during condensation. However, it can be observed that the condensation position of ideal gas is later, and the prediction of condensation characteristics is worse. Below, the mean relative error (MRE) and the root mean square error (RMSE) are used to evaluate the prediction accuracy of the two models quantitatively.

\[
\begin{align*}
\text{MRE} & = \frac{1}{n} \sum_{i=1}^{n} \frac{(y_i - \hat{y}_i)}{y_i} \\
\text{RMSE} & = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (\hat{y}_i - y_i)^2}
\end{align*}
\]

(22)

where \(\hat{y}_i\) is the simulation data under real gas model and ideal gas model, \(y_i\) is the experiment data respectively, and \(n\) is the amount of the data. The MRE value of real gas model calculated by Eq. (22) is 0.90% and that of ideal gas model is 14.37%. The validation result will be better when the RMSE is close to 0. It can be obtained that the RMSE of real gas model is 0.01471 and RMSE of the ideal gas model is 0.07626 after further calculation, which is shown in Fig. 4(b). Therefore, it is found that the real gas model has more advantages in the supersonic flow of CO₂, which is in good agreement with the experimental results, indicating that the geometric model and mathematical model used in this paper can be used to simulate the condensation process of CO₂ in supersonic nozzle. Subsequently, nucleation rate distribution of the real gas and ideal gas is given, as shown in Fig. 5, the peak position of the nucleation rate is called Wilson point, it can be seen clearly that the peak position of nucleation rate of real gas model is closer to the Wilson point of the experimental data in Fig. 4(a), while the peak position of nucleation rate of ideal gas is far away from the experimental Wilson point, which further confirms that the real gas model is more accurate using to simulate the condensation process of CO₂.

3.2. Analysis of the swirling effect of the vortex generator

In the structural composition of the supersonic separator, in addition to the need for the thermodynamic condensation accuracy validation of the supersonic nozzle, another important structure is the vortex generator. In order to make this study further in line with the working principle of supersonic separator, the effect of the swirling performance on the condensation process of the supersonic nozzle was also validated in this section.

For the effect of the swirling action of the vortex generator on the CO₂ condensation separation process, a two-dimensional axisymmetric Laval nozzle was used for model validation. The mesh and the three-dimensional structures of the Laval nozzle is shown in the Fig. 6. Because the swirling strength of the vortex generator determines the magnitude of the centrifugal acceleration, this study will set up four different sets of centrifugal acceleration from the perspective of swirling strength, which are 1e5 m²/s, 4e5 m²/s, 8e5 m²/s and no swirling for contrasting. As can be seen from Fig. 7 (a), as the centrifugal acceleration increases, the liquid phase fraction along the central axis will be greater than the liquid phase fraction corresponding to the case where the centrifugal acceleration is small, and the droplets will condense first when the centrifugal acceleration is greater, that is, the condensation position in the supersonic nozzle will be advanced. The relationship between the outlet liquid fraction and the centrifugal acceleration was then analyzed, as shown in Fig. 7 (b). With the increase of the inlet centrifugation acceleration, the liquid fraction of the outlet will be greater, on the contrary, in the absence of swirling action, that is, when the inlet centrifugal acceleration is zero, the liquid fraction is only 3.4%, and the condensation effect is significantly weaker. The Fig. 7(c) and (d) focused on the analysis of the swirling velocity at centrifugal acceleration of 1e5 m²/s and 4e5 m²/s respectively, and it can be seen in Fig. 7(c) that the swirling velocity increases significantly when the centrifugal acceleration is greater. As shown in Fig. 7(d), it can be seen that on the circular section after the axisymmetric rotation of the two-dimensional nozzle, the swirling velocity at the center of the circular section is the smallest, and the swirling velocity near the nozzle wall is the largest, which is caused by the inlet swirling action.

Therefore, in summary, the introduction of swirling action makes the condensation effect of CO₂ stronger, and the condensation position will be advanced.

Fig. 4. Numerical and experimental results of two models in supersonic nozzle.
3.3. Comparison of ideal gas and real gas models

Based on the accuracy validation of the two models, this study attempts to compare the condensation characteristics of the ideal gas model and the real gas model in supersonic flow from more perspectives. The mass transfer and heat transfer mechanisms are worth exploring in the process of condensation and nucleation. Therefore, in this investigation, the differences of the condensation characteristics, mass transfer and heat transfer between the two gas models under different inlet conditions will be proposed to solve the problem of lacking demonstration about investigating CO$_2$ supersonic separation using real gas model in previous studies.

3.3.1. Nucleation and Wilson point

In terms of the global condensation characteristics of the two models, this study focused on the parameters in the process of condensation, which is shown in Fig. 8. With the same entry conditions, the degree of supercooling $\Delta T = T_s - T_{CO2}$, which is defined as the difference between saturation temperature ($T_s$) and current temperature ($T_{CO2}$) at Wilson point of ideal gas is greater than that of real gas, and the position of the maximum degree of supercooling occurs further back. With the increase of inlet pressure, the degree of supercooling of ideal gas and real gas tends to decrease. In addition, it can be seen that the nucleation region decreases in the process of inlet pressure changing from critical to supercritical, and there is a great difference in the location of condensation and nucleation between the two models. As shown in Fig. 8, for the real gas with an inlet condition of 30 bar and 268 K, the Wilson point position is $x = -6.806$ mm, while the Wilson point position of the ideal gas is $x = -3.038$ mm. When the inlet condition is 60 bar and 310 K, the Wilson point position of real gas is $x = -0.0825$ mm, and that of ideal gas is $x = 16.0128$ mm. When the inlet condition is 100 bar and 340 K, the Wilson point of real gas is $x = 4.843$ mm, and the Wilson point of ideal gas is $x = 27.110$ mm. This illustrates that compared with the real gas, the location of condensation and nucleation of the ideal gas will be further back.

3.3.2. Mass transfer performance in condensation flow

The mass change during the phase transition determines the mass...
transfer between gas and liquid phases in the condensation of CO$_2$. Comparison of real gas and ideal gas at different inlet conditions, in addition to the real gas and ideal gas have great differences in typical condensation characteristics parameters, the mass transfer during the phase transition process is also a great difference between them. The following Fig. 9 shows the mass change rate $m_1$ (kg m$^{-3}$ s$^{-1}$) during nucleation and the mass change rate $m_2$ (kg m$^{-3}$ s$^{-1}$) during droplet growth under different inlet conditions of real gas and ideal gas. Taking the inlet pressure of 30 bar and the inlet temperature of 278 K as an example, shown as Fig. 10, the difference between the nucleation position of real gas and ideal gas is reflected in the mass generation of $m_1$ in the nucleation process. The peak values of real gas $m_1$ and ideal gas $m_1$ are consistent with the Wilson point between them mentioned above. Compared with the condensation model of ideal gas, the mass generation in nucleation and droplet growth of real gas is higher. For example, under the inlet condition of 30 bar and 278 K, $m_1$ of ideal gas is only about 0.01 kg m$^{-3}$ s$^{-1}$, while $m_1$ of real gas is about 0.25 kg m$^{-3}$ s$^{-1}$. The $m_2$ of ideal gas is only about $3.6 \times 10^3$ kg m$^{-3}$ s$^{-1}$, while the $m_2$ of real gas is about $1.21 \times 10^4$ kg m$^{-3}$ s$^{-1}$. Observe the other two inlet pressures, the same change law still holds. According to the mass change rate values and the order of magnitude relationship between the values of $m_1$ and $m_2$, it can be found that in the mass transfer process of phase transition, its contribution basically comes from the mass generation $m_2$ of droplet growth.

This study also compared and analyzed the liquid fraction of ideal CO$_2$ gas and real gas at the exit of supersonic flow. As shown in Fig. 11, it is obvious that the ideal gas model and the real gas model significantly affect the liquid fraction. When the inlet pressure is 30 bar, the liquid fraction predicted by the real gas condensation model reaches 3.5% of the total mass, while the liquid fraction predicted by the ideal gas model is only 1.3%. When the inlet pressure is 60 bar, the liquid fraction predicted by the real gas condensation model reaches 4.1%, which increases in a small scale compared with 30 bar, while that of the ideal gas model is just 1.4% of total mass. And the difference in liquid fraction between the two models increases significantly with the increase of the inlet pressure. It can be confirmed that when the inlet pressure rises to 100 bar, the liquid fraction predicted by the real gas model is 3.5%. However, the liquid fraction predicted by the ideal gas model is only 0.7%, underestimating the CO$_2$ condensation of 2.8% of the total mass in the liquid fractions. With all the said, it indicates that the ideal gas model greatly underestimates the outlet liquid fraction compared with real gas model.

Fig. 7. Effect of the introduction of swirling on the condensation phenomenon.
3.3.3. Heat transfer property at Wilson point

The different condensation performances and mass transfer characteristics of the two gas models in supersonic nozzle have been summarized above. Similarly, the different heat transfer characteristics generated by the two models in the process of condensation flow are also worthy of attention. Table 3 lists the degree of supercooling corresponding to Wilson point under the same inlet conditions for the two gas models. It can be clearly concluded that under the same conditions, the degree of supercooling of the ideal gas model at Wilson point is always larger than that of the real gas model. And, with the increase of pressure, the difference in the value of the degree of supercooling will increase to a limited extent.

Furthermore, the latent heat released at the condensation onset location of two gas models was calculated and plotted in Fig. 12. It can be obtained that the Latent heat released at the condensation onset location decreases with the increase of inlet pressure, which exists in
both the ideal gas model and the real gas model. However, compared with real gas, the prediction of latent heat release of ideal gas has a great deviation. The Latent heat released at the condensation onset location of ideal gas is obviously larger than that of real gas. As expected, the relative error of latent heat of ideal gas and real gas will increase with the increase of inlet pressure. When the inlet pressure is 30 bar, the relative error is about 8.8%. When the inlet pressure is 60 bar, that is 13.6%. In supercritical state where the inlet pressure is 100 bar, the relative error between the two models reaches as high as 20.1%, which indicates that the ideal gas model does have great limitations in simulating condensation flow under high-pressure inlet environment.

4. Results and discussion

After the superiority of the real gas model in the process of CO$_2$ supersonic flow was expounded from multiple perspectives, the real gas model will continue to be used in this study to discuss the condensation mechanism of CO$_2$ in supersonic nozzle and the condensation characteristics at Wilson point, especially the variation rule of condensation parameters at Wilson point under different inlet conditions. Subsequently, from the perspective of a functional relationship, it is planned to establish a prediction model for the degree of supercooling, pressure, and expansion rate at Wilson point in the supersonic flow process of CO$_2$.

4.1. Condensation characteristics of CO$_2$ in supersonic nozzle

To explain the condensation characteristics of CO$_2$ in supersonic flow, the pressure, degree of supercooling, nucleation rate, droplet number and latent heat parameters along the nozzle centerline of a typical condition are given in Fig. 13.

Superheated steam with the superheat of about 20 K enters the nozzle and expands. In this process, the temperature and pressure gradually decrease, when the inlet pressure is known to be 60 bar, the saturation temperature is about 295 K. However, as the temperature is still above saturation, condensation does not occur, the nucleation rate and droplet number are 0, and the CO$_2$ steam continues to expand. Until the saturation point is reached, the degree of supercooling is 0 K, and condensation still does not occur because there are no external cores. When the gas continues to expand into supersaturated steam and the degree of supercooling is about 2 K, condensation occurs, and the nucleation rate rises rapidly from 0 in a short time. The nucleation rate, droplet number and latent heat of condensation all reach the maximum state. The process of nucleation rate increasing from 0 to the maximum is called the nucleation zone. As can be seen from Fig. 13, the nucleation zone is very short and the nucleation rate is relatively fast, and the steam

| Degree of supercooling (K) | $P_{\text{in}} = 30$ bar | $P_{\text{in}} = 60$ bar | $P_{\text{in}} = 100$ bar |
|--------------------------|--------------------------|--------------------------|--------------------------|
|                          | $T_{\text{in}} = 268$ K  | $T_{\text{in}} = 305$ K  | $T_{\text{in}} = 340$ K  |
| Real Gas                 | 4.99                     | 1.92                     | 1.22                     |
| Ideal Gas                | 5.99                     | 3.44                     | 3.25                     |
is in a non-equilibrium state during the nucleation process. After the Wilson point, the nucleation rate decreases rapidly and the number of droplets remains unchanged, but the droplets grow rapidly on the condensation nucleus. Because there have critical dimension condensing cores, a large number of \( \text{CO}_2 \) molecules can be reunited at the droplet surface causing the droplet radius to increase, and since the release of latent heat to heat the gas molecules cause the temperature to rise, degree of supercooling to decrease. After the nucleation environment was damaged, though no new condensation nuclei, the nuclei that have been created keep growing, which restores the steam to the equilibrium state.

In addition, a lot of latent heat will be released when the steam molecules condense, and the flow of the heated steam molecules in the nozzle will slow down, thus the pressure and temperature of the nozzle will rise along the process. Eventually, the degree of supercooling is maintained at about 2 K, the nucleation rate drops to 0, the condensation process ends, and the steam returns to equilibrium.

Fig. 14 shows the phase change in the condensation process of supersonic flow, that Lettieri et al. [65] presented the phase change of the condensation in supercritical \( \text{CO}_2 \) compressors. As can be seen from the temperature and pressure diagram in the above typical case, the superheated steam enters the nozzle at the initial state of 60 bar and 315 K. At point A, \( \text{CO}_2 \) reaches the gas–liquid two phase saturation point, at which the temperature and pressure have dropped below the saturation state, and the phase change begins to occur. If expands fast, it will be in non-equilibrium state for a certain time at point B, which is Wilson point. When the phase change is over, it will be in an equilibrium state again at point C.

### 4.2. Effect of different inlet conditions on condensation characteristics of Wilson point

Different inlet temperature and pressure have a great influence on the condensation characteristics at Wilson point. In this study, three groups of inlet pressures were used for comparison, which are 30 bar, 60 bar and 100 bar respectively. Meanwhile, the inlet superheat \( DT \) was compared, which was defined as \( DT = T_{\text{CO}_2} - T_n \). When the inlet pressures are 30 bar and 60 bar, \( DT \) are 10 K, 15 K and 20 K, respectively. When the inlet pressure is 100 bar, \( DT \) are 31 K, 36 K and 41 K respectively.

It can be seen from Fig. 15 that under the same inlet pressure, with the increase of inlet superheat, the degree of supercooling and latent heat at Wilson point will increase accordingly. These are also shown in Fig. 17, where the \( \Delta T_w \) is used to represent the degree of supercooling at Wilson point. This is because, with the increase of inlet temperature, the greater the degree of supercooling required for condensation, and condensation is more difficult to achieve. In other words, the higher the inlet temperature, the higher the superheat, the further back the condensation position.

Some condensation parameters are also quantitatively analyzed. Tables 4, 5 and 6 show the comparison of condensation parameter values under different inlet conditions respectively. The degree of supercooling, degree of supersaturation, pressure, and expansion rate \( k_p \) at Wilson point are compared within and between groups. The data shows that with the increase of superheat, the pressure at Wilson point will decrease, and the expansion rate \( k_p \) at this position will also decrease, which \( k_p \) is defined as \( -(\nu/p) \) (dp/dx), and \( \nu \) is velocity. The degree of supersaturation will increase with the increase of superheat, which is degree of supercooling. It’s defined as \( S_v = p_{\text{CO}_2}/p_s \) and it can represent the extent to which steam continues to expand in a metastable supersaturated region. The greater the supersaturation, the deeper the continued expansion, and vice versa. In addition, it can be seen from Fig. 16 that under different inlet pressures and the same superheat, the condensation position will move forward. For example, when the inlet superheat is 25 K and \( P_{\text{in}} = 30 \) bar, the condensation onset Wilson point position \( x = 38.57 \text{ mm} \); when \( P_{\text{in}} = 60 \) bar, the Wilson point position \( x = 13.96 \text{ mm} \); when \( P_{\text{in}} = 100 \) bar, the Wilson point position \( x = 0.827 \text{ mm} \). This is because with the increase of the inlet pressure, the partial pressure of \( \text{CO}_2 \) will also increase, and the supersaturation will also increase, resulting in a larger expansion degree. Therefore, under the same superheat, the spontaneous condensation of \( \text{CO}_2 \) is easier to occur.

Through qualitative and quantitative analysis, it is found that different inlet temperature and inlet pressure have a great influence on the condensation characteristics of Wilson point, especially on the change of condensation position, which is helpful for us to predict the \( \text{CO}_2 \) condensation process in supersonic nozzle and is conducive to the perfection and improvement of \( \text{CO}_2 \) separation technology.
Fig. 13. Distribution of condensation parameters along the nozzle centerline.
4.3. The prediction model for Wilson point

In this study, the following prediction model is established for parameters at Wilson point, which is used to predict the curve relationship among the degree of supercooling, the pressure and the expansion rate under the corresponding dry gas conditions at Wilson point.

\[ \Delta T_W = b_1 + b_2 k_p + b_3 p_w + b_4 e^{b_5 k_p} + b_6 (p_w k_p)^2 \]  

(23)

where \( b \) are prediction parameters, and the \( b_1 = -90.801983155 \), \( b_2 = -72.698009114 \), \( b_3 = 0.580694882 \), \( b_4 = 102.442418210 \), \( b_5 = -0.090734535 \), \( b_6 = 0.001445394203 \), \( b_7 = 1.0509438811 \), \( b_8 = 9.43841354 \), \( b_9 = 2.93563447 \). The \( p_w \) is the pressure at Wilson point and \( k_p \) is also reflected in this formula, which is defined as the expansion.

Table 4
Quantitative analysis of condensation parameters with \( P_{in} = 30 \) bar.

| Supercooling (K) | Supersaturation (S_s) | Pressure (bar) | \( k_p \) (1/s) |
|------------------|-----------------------|---------------|-----------------|
| \( DT = 10 \) K | 7.70                  | 16.79         | 7486            |
| \( DT = 15 \) K | 9.88                  | 13.43         | 4664            |
| \( DT = 20 \) K | 11.94                 | 10.82         | 3182            |
rate at Wilson point. Considering the prediction model proposed in this study should have higher applicability and feasibility, according to the physical significance and sensitivity to the data of the mean relative error (MRE), root mean square error (RMSE) and relative root mean square error (rRMSE), the mean relative error (MRE) and relative root mean square error (rRMSE) are selected in this subsection to construct composite evaluation indexes. The main reason is that the MRE and the rRMSE can adapt to the data characteristics of the model and can better reflect the overall characteristics of the data if used in the prediction and regression model. The calculation methods of the two are given below:

\[
\begin{align*}
\text{MRE} &= \frac{1}{n} \sum_{i=1}^{n} \left( \frac{\hat{y}_i - y_i}{y_i} \right) \\
\text{rRMSE} &= \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left( \frac{\hat{y}_i - y_i}{y_i} \right)^2}
\end{align*}
\]

(24)

There MRE and rRMSE are used to evaluate the agreement between the predicted value by prediction formula Eq. (23) and the simulated value by CFD. As Eq. (24), where \(y_i\) is the simulation value by CFD, \(\hat{y}_i\) is the predicted value by prediction formula Eq. (23), and \(n\) is the amount of data. Similarly, the prediction results are in good agreement with the simulation results when the MRE and rRMSE are equal to 0 approximately. After calculation, it can be obtained that the MRE is 0.176% and the rRMSE is 2.275%.

According to the prediction results and the simulation data by CFD to do a comparison and analyze the relative error specifically. As shown in Fig. 18, the simulation values of pressure and degree of supercooling are inversely proportional relationship. This is because with the expansion of CO₂ steam in the supersonic flow, the temperature and pressure are reduced constantly, and above also points out that, the greater the inlet superheat, the deeper the continued expansion, so the greater the degree of supercooling can realize the spontaneous condensation. Then the

Fig. 16. Relationship between Wilson point and inlet superheat.

Fig. 17. Relationship between inlet superheat and degree of supercooling.
relationship between pressure and supercooling is obvious. The curves between the predicted value and simulation data show that the Eq. (23) is effective and accurate for prediction.

According to Eq. (23), the relation curve between the degree of supercooling and the expansion rate at Wilson point is obtained. In subsection 4.2, the partial numerical comparison has been made on the expansion rate at Wilson point, and the predicted value and simulation value have the same trend as shown in Fig. 19. When the degree of supercooling at Wilson point reaches a certain value, the expansion rate will decrease.

As shown in Fig. 20, the horizontal and vertical coordinates are set as 0 to 14, and the degree of supercooling under the three pressure states is divided into simulation value and predicted value. The error of the simulation and prediction results is within ±5%. According to the method mentioned in Eq. (24), the value of the MRE is calculated with 0.176%. In the meantime, the rRMSE is 2.275%, indicating that the prediction results by Eq. (23) are in good agreement with the simulation results by CFD.

The prediction model in this study provides a simple and straightforward method to predict the simulated data, which can seek the change rule of limited data. Moreover, the model has high flexibility. Where the independent variables in Eq. (23) can also be set to other condensation parameters at Wilson point. The calculation method of the mean relative error (MRE) and the relative root mean square error (rRMSE) makes the quantitative calculation for the prediction accuracy. If experimental data and simulation data are known in other studies, it also provides a way to calculate the relative error and accuracy between them.

5. Conclusion

A computational fluid dynamics (CFD) model for real gas was established to simulate the condensation and nucleation behavior of CO$_2$ in supersonic nozzle. The model was proved to have the ability to describe the condensation characteristics of real gas and ideal gas of CO$_2$ in the supersonic flows after validated with the experimental data. Then, using the proposed model, the differences in the condensation process between the real gas and the ideal gas are analyzed from multiple angles. At the same time, the significant influence on the condensation characteristics at Wilson point under different inlet conditions was expounded. The main conclusions are as follows:
in this study. Therefore, this work can effectively promote the development of CO\textsubscript{2} supersonic separation technology.

Data Availability Statement
The research data supporting this publication are provided within this paper.

**CRediT authorship contribution statement**

Hongbing Ding: Conceptualization, Supervision, Writing – original draft, Writing – review & editing. Yuanyuan Dong: Formal analysis, Investigation, Writing – review & editing. Yu Zhang: Formal analysis, Investigation, Writing – review & editing. Yan Yang: Methodology.

**Declaration of Competing Interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

**Acknowledgement**

This work is supported in part by National Natural Science Foundation of China under Grant 52276159, 51876143 and 62073135.

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