Please find the published version at: https://doi.org/10.1016/j.ijheatmasstransfer.2021.122315

1	The droplets and film behaviors in supersonic separator by using
2	three-field two-fluid model with heterogenous condensation
3	Hongbing Ding ^{1, *} , Chunqian Sun ¹ , Chuang Wen ² , Zhenxin Liang ¹
4	¹ Tianjin Key Laboratory of Process Measurement and Control, School of Electrical and Information
5	Engineering, Tianjin University, Tianjin 300072, China
6	² College of Engineering, Mathematics and Physical Sciences, University of Exeter, Exeter EX4 4QF,
7	United Kingdom
8	*Corresponding author: Hongbing Ding, Email: hbding@tju.edu.cn
9	Abstract:
10	Supersonic separator is a kind of natural gas dehydration device with great potential, but its internal mass
11	and heat transfer process has not been fully studied. In this study, a novel three-field two-fluid model
12	described by Eulerian-Eulerian approach for supersonic separator considering the heat and mass transfer
13	between gas, liquid droplets, and liquid film was developed and validated. The interphase slip, latent heat,
14	film heat flux, and film phase change rate were studied. It revealed that the maximum centrifugal slip
15	velocity of droplets can reach 24.9 m s ⁻¹ . The maximum latent heat is 5.3×10 ⁸ J m ⁻³ from droplets to gas
16	phase during condensation, and the minimum latent heat is -3.4×10 ⁸ J m ⁻³ during evaporation. The thickness
17	of swirling liquid film at wet gas outlet is 21 µm, 47 µm, 74 µm and 89 µm, respectively. The liquid film
18	temperature decreases to a minimum 304.1 K due to droplets deposition, where the maximum heat flux is
19	0.74 MW m ⁻² . Besides, the frequency and velocity of the interfacial wave of liquid film were obtained by
20	using the cross-correlation algorithm, and their maximum values was 11.07 Hz and 1.49 m s ⁻¹ , respectively.
21	In addition, for achieving higher dehydration efficiency, the optimal value of effective density of foreign
22	droplets should be 0.01 kg m ⁻³ . The maximum separation efficiency and dew point depression of separator
23	A are 85.11% and 40.32°C, respectively. The model without considering the liquid film over-predicts the
24	separation efficiency.
25	

Keywords: Three-field two-fluid model; Heterogenous condensation; Supersonic flows; Liquid film;
 Interfacial wave.

Nomen	nclature		
ac	centrifugal acceleration, m s ⁻²	$T_{ m w}$	wall temperature, °C
а	heat transfer coefficient, W m ⁻² K ⁻¹	ū	velocity vector, m s ⁻¹
Cc	Cunningham slip correction factor, -	${ec U}_{d}$	momentum source term of film, Pa
$C_{\rm D}$	drag coefficient, -	$u_{ m w}$	interfacial wave velocity, m s ⁻¹
C_{phase}	phase change constant, -	Vs	slip velocity, m s ⁻¹
d	cell-center-to-wall distance, m	x	Cartesian coordinate, mm
D_{T}	subcooling, °C	x_1, x_2	film collecting point 1 and 2, mm

Ε	total energy, J kg ⁻¹	x_l	transit distance, mm
f	collision frequency, Hz	<i>y</i> 1, <i>y</i> 2	fluctuation of film thickness at x_1 ,
J			<i>x</i> ₂ , µm
$f_{ m w}$	interfacial wave frequency, Hz	Yi	mass fraction of species, -
$\vec{F}_{ m D}$	drag force, kg m ⁻² s ⁻²	Greek	
ġ	gravity vector, m ⁻¹ s ⁻²		
\vec{g}_{τ}	gravity component parallel to film, m ⁻¹ s ⁻²	α	volume fraction, -
h_f	enthalpy of film, J kg ⁻¹	ρ	density, kg m ⁻³
$h_{ m i}$	enthalpy of specie, J kg ⁻¹	$\overline{\overline{\tau}}$	effective stress tensor, Pa
$h_{ m lg}$	latent heat of water vapor, J kg ⁻¹	$ au_0$	transit time, s
T	homogeneous nucleation rate m ⁻³ c ⁻¹	$\vec{ au}$	viscous shear stress on gas-film
5	nonlogeneous nucleation rate, in * s	t fs	interfaces, Pa
\vec{J}	diffusion flux, kg s ⁻¹ m ⁻²	λ	thermal conductivity, W m ⁻¹ K ⁻¹
k _B	Boltzmann's constant. 1.38×10 ⁻²³ J K ⁻¹	μ	molecular dynamic viscosity, Pa s
Kn	Knudsen number, -	δ	film thickness, µm
ṁ	droplet mass changing rate, kg m ⁻³ s ⁻¹	υ	water molecule volume, m ³
112	mass source term due to collision and	σ	liquid surface tonsion N m ⁻¹
m _c	coalescence, kg m ⁻³ s ⁻¹		
$\dot{m}_{\rm d}$	deposition rate, kg m ⁻² s ⁻¹	${\Phi}$	relative humidity, $p_v/p_s(T_g) \times 100\%$
m _{evap}	film evaporation rate, kg s ⁻¹	χ	mole fraction of water vapor, -
110	water molecular mass, 2.99×10 ⁻²⁶ kg	$\eta_{ m v}$	water removal rate (i.e., separation
mm			efficiency), %
$\dot{m}_{\rm phase}$	film phase change rate, kg m ⁻² s ⁻¹	$\Delta T_{ m d}$	dew point depression, °C
М	mass diffusivity of water vapor, m ² s ⁻¹	Subscripts	
n	volumetric concentrations of droplet, m ⁻³		
N _c	source term due to collision, m ⁻³ s ⁻¹	*	stagnation condition
р	pressure, Pa	a, r, t	axial, radial, tangential
q_w	surface heat flux, kW m ⁻²	eff	effective
Q	droplet flow rate, ml min ⁻¹	f	liquid film
r	droplet radii, µm	g	gas
rc	critical radii of homogenous nucleus, µm	het/hom	hetero- and homogeneous
$R_{12}(\tau)$	cross-correlation function, -	i	species
Re _p	relative Reynolds number, -	l	liquid

$R_{\rm v}$	specific gas constant, J kg ⁻¹ ·K ⁻¹	max	maximum
S	swirl strength, -	S	saturation
Si	mass source term of species, kg m ⁻³ s ⁻¹	tu	turbulent
Ss	water vapor supersaturation, -	v	water vapor
t	time, s	W	interfacial wave
Т	temperature, °C	Superscripts	
T _d	dew point temperature, °C		
T _m	film half depth temperature, °C	dry, wet	dry and wet gas outlets
Ts	film surface temperature, °C	in, out	inlet, outlet
T _r	droplet surface temperature, °C		

2 1 Introduction

3 As a kind of clean energy, natural gas contains almost no sulfur, dust and other harmful substances, 4 and produces less carbon dioxide when burned than other fossil fuels, so it can reduce carbon emissions 5 and environmental pollution [1]. Natural gas contains saturated water that leads to many hazards. For 6 example, the formation of hydrates during transportation causes pipelines and valves to block [2], moreover, 7 the action of water with carbon dioxide, hydrogen sulfide, and other acid gases will corrode pipelines and 8 equipment [3]. Therefore, natural gas dehydration processing is very important. The supersonic separator 9 is a new type of natural gas dehydration device. Because of its simple structure, small size, and no rotating parts [4], it is more suitable for offshore natural gas processing [5], which has attracted the attention of 10 11 many scholars in recent years.

12 The two main processes of the supersonic separator are condensation and swirl separation [6]. The 13 components producing these two processes are the supersonic nozzle and the swirl generator, respectively. 14 As shown in Fig. 1, due to the complex three-field (gas, droplets, and liquid film) two-fluid (gas and liquid) 15 [33] characteristics in the supersonic separator, including complex phase changes (condensation and 16 evaporation), interphase slip, liquid film, swirl flow, and shockwave phenomenon [8], even though many 17 scholars have performed flow field analysis and structural optimization of supersonic separators, there are 18 still many problems that need to be fully studied, especially the droplets and liquid film behaviors in 19 supersonic separators.



Fig. 1 Three-field characteristics of gas, droplets, and liquid film in supersonic separator.

3

4 There are three main methods to study the supersonic separator: theory, experiment and simulation. 5 Because the use of natural gas for experiments is expensive and dangerous, air is often used as feed carrier gas in low pressure experiments instead of natural gas [9]-[10], which has little effect on the experimental 6 7 results. The experimental results of Ma et al. [11] showed that the injection of foreign droplets caused 8 heterogeneous condensation, which effectively improved the separation efficiency. Cao et al. [12] 9 conducted an experimental study on a new type of supersonic separator with ellipsoidal center body to 10 evaluate dehydration performance. The results showed that the maximum dew point depression could be 11 34.9°C at 20.6% pressure recovery coefficient. Wang et al. [13] carried out an experimental study on a novel 12 supersonic separator with reflux channel. The results showed that the cylindrical drainage structure can 13 reduce the interaction between shock wave and boundary layer, thereby improving separation performance. 14 The process simulations in Aspen HYSYS were carried out by de Oliveira Arinelli et al. [14]-[15] to study 15 the offshore natural gas processing with high CO₂ content based on supersonic separators. Simultaneously, 16 the computational fluid dynamics can simulate the distribution characteristics of the flow field by 17 establishing an appropriate numerical model. Therefore, many scholars have established different numerical 18 models for supersonic separators.

19 The first commonly used model is a two-fluid model based on the Discrete Particle Method (DPM), 20 namely Eulerian-Lagrangian approach, which can track the trajectory of droplets. Wen et al. [16] 21 established a numerical model based on RNG k-ε turbulence model and Discrete Particle Method (DPM) 22 to calculate the flow field and droplet trajectory in a supersonic separator. The results showed that when the 23 separation section length is 10 times the throat diameter, the separation efficiency can reach 95%. The 24 particle behaviors in a supersonic separator with strong swirling flow were modeled by Yang et al. [17] The 25 results showed that majority of the particles were separated by centrifugation to the wall or directly into the 26 moisture outlet, moreover, the separation efficiency reached 80% at the droplet size of 1.5 µm. Liu et al. [18] established compressible Navier-Stokes equations coupled DPM to predict the separation efficiency. 27 28 The results showed that increasing the droplet size within a certain range improved the separation efficiency.

Jiang et al. [19] analyzed the effect of droplet size and inlet velocity on separation efficiency. The results showed that the droplets were effectively separated when the droplets size was about 1 μm. A numerical model taking into account the actual droplet size distribution was established by Shooshtari et al. [20] to simulate a more realistic condensation droplet trajectory. However, the existing DPM-based two-fluid model does not consider the condensation and evaporation of droplets in the supersonic separator, thus, which has great limitations.

7 Another commonly used model is the Eulerian two-fluid model, namely Eulerian-Eulerian approach, 8 which takes into account the condensation and evaporation processes. Dykas et al. [21] used Eulerian-9 Eulerian approach to simulate the homogeneous condensing flow in low- and high-pressure supersonic 10 nozzle, and studied the performance of the numerical algorithm in terms of gas and liquid properties. Patel 11 et al. [22] using Eulerian-Eulerian model combining with modified turbulence model investigated the 12 irreversible heat and mass transfer losses in the condensation process in in nozzle and turbine cascade. 13 White et al. [23] and Ding et al. [24] performed numerical simulation to obtain the distribution of 14 polydisperse droplets of condensing flow. Edathol et al. [25] using Eulerian-Eulerian models predicted the 15 homogeneous condensing flow in a supersonic nozzle. It was found that more experimental validations under different geometric and boundary conditions were needed to validate the effectiveness of the non-16 17 equilibrium condensation model. Abadi et al. [26] established a Eulerian-Eulerian model for solving the 18 wet steam flow in the high-pressure nozzle. The results showed that the decreased superheat level makes 19 the nucleation process happen earlier. Wen et al. [27]-[28] developed a Eulerian two-fluid model to study 20 the flow field structure where non-equilibrium condensation and shock coexisted in a supersonic separator, 21 and analyzed the influence of swirl strength on the condensation process. Liu et al. [2] analyzed the 22 influence of the pressure recovery process on the condensation and evaporation of droplets. The results 23 showed that the interaction of shock waves and boundary layers would reduce the liquefaction efficiency. 24 Under actual operating conditions, saturated natural gas contains foreign liquid droplets before entering the 25 dehydration equipment, thus, it is actually heterogeneous condensation in the supersonic separator. Niknam et al. [29] conducted heterogeneous condensation experiments to study the dehydration efficiency of a 26 27 supersonic separator, moreover, who established a two-phase heat and mass transfer model in a 2D 28 asymmetric domain to predict the dehydration efficiency. Shooshtari et al. [30] assumed that certain rates 29 of salt particles were injected into the supersonic separator, thereby a Eulerian multi-fluid model 30 considering homogeneous/heterogeneous condensation was established. The results showed that the 31 particle injection rate had a profound effect on the separation efficiency. However, the above Eulerian two-32 fluid models do not consider interphase slip and droplet drag. In our previous research, Ding et al. [8] established a homogeneous/heterogeneous condensation model considering interphase slip and droplet drag, 33 34 which was verified to have high calculation accuracy and was used to obtain droplet behavior characteristics. However, the above numerical models only model the two fields (gas and droplets), ignoring the formation
 of liquid film. Recently, no scholar has established a three-field (gas, droplets, and liquid film) two-fluid
 model considering liquid film for supersonic separator.

4 Eulerian-Lagrangian coupled Eulerian wall film model and Eulerian-Eulerian coupled Eulerian wall 5 film model are applied to the modeling of the annular-mist flow. Deng et al. [31] used Eulerian-Lagrangian 6 coupled Eulerian wall film model to simulate the heat and mass exchange between gas, liquid droplets and 7 liquid film in an axial flow cyclone. The results showed that under the centrifugal action of the guide vanes, 8 the droplets moved to the wall and formed a thin liquid film. As time goes by, and the liquid film thickness 9 gradually increased with time. Han et al. [32] established the Eulerian-Lagrangian two-phase model 10 coupled Eulerian wall film model for the gas-water separator to obtain the droplet trajectory and liquid film 11 distribution, and validated the model experimentally. A three-field two-fluid model was developed by Li et 12 al. [33] to simulate the post-dryout heat and mass transfer in a vertical pipe including liquid film evaporation, 13 droplets deposition, and droplets entrainment, which was a Eulerian-Eulerian coupled Eulerian wall film 14 model. The comparison between the simulation results of the liquid film flow rate and the experimental results of the steam-water pipe flow validated the model. Yue et al. [34] used Eulerian-Eulerian coupled 15 Eulerian wall film model to study the influence of liquid flow rate on liquid film flow in a Gas-Liquid 16 17 Cylindrical Cyclone. The results showed that high liquid flow rate impairs the uniformity of the liquid film. 18 As mentioned above, the existing numerical models of supersonic separators do not consider the 19 formation of liquid film, moreover, the existing three-field two-fluid model does not consider the 20 condensation effect, thereby it cannot be directly applied to supersonic separators. In order to study the 21 complicated heat and mass exchange mechanism among the three fields of gas, liquid droplets and liquid 22 film in the supersonic separator, this research proposes a novel three-field two-fluid model based on 23 Eulerian-Eulerian approach considering homogeneous/heterogeneous condensation and interphase slip. 24 This model has not been reported. Subsequently, the coupled heat and mass transfer was studied, and the 25 separation performance was predicted. It provides an effective method for analyzing the three-field heat 26 and mass transfer with the characteristics of condensation and strong swirl and optimizing the supersonic 27 separator.

28

29 2 Three-field two-fluid model

The three-field two-fluid model based on the Eulerian-Eulerian approach for the supersonic separator includes the gas-phase governing equations, the homogeneous/heterogeneous condensation model, the Eulerian wall film model, and the heat and mass coupling between the three fields of gas, liquid droplets, and liquid film. The schematic diagram of three-field two-fluid in the supersonic separator is shown in Fig. 2 (a). The three-field two-fluid is established based on the following assumptions: (i) The liquid droplets are spherical; (ii) The latent heat released by condensation is completely absorbed in the gas phase; (iii)
The homogeneous/heterogeneous condensation and interphase slip are considered; (iv) Due to the strong
swirling flow, the influence of the drag force on the two-phase momentum equations is considered. (v) Due
to the strong swirling flow, only the droplet deposition is considered, while the droplet entrainment is
ignored.



11 2.1 Governing equations

12 2.1.1 Gas phase model

13 The mass, momentum, and energy conservation equation of gas phase (air and water vapor mixture)14 is governed by

15
$$\frac{\partial}{\partial t} \left(\alpha_{g} \rho_{g} \right) + \nabla \cdot \left(\alpha_{g} \rho_{g} \vec{u}_{g} \right) = -\left(\dot{m}_{hom} + \dot{m}_{het} \right)$$
(1)

16
$$\frac{\partial}{\partial t} \left(\alpha_{g} \rho_{g} \vec{u}_{g} \right) + \nabla \cdot \left(\alpha_{g} \rho_{g} \vec{u}_{g} \vec{u}_{g} \right) = -\alpha_{g} \nabla p + \nabla \cdot \left(\alpha_{g} \overline{\overline{\tau}}_{eff} \right) + \alpha_{g} \rho_{g} \vec{g} - \left(\dot{m}_{hom} + \dot{m}_{het} \right) \vec{u}_{g} - \vec{F}_{D}$$
(2)

17
$$\frac{\partial}{\partial t} \left(\alpha_{g} \rho_{g} E \right) + \nabla \cdot \left[\alpha_{g} \left(\rho_{g} E + p \right) \vec{u}_{g} \right] = \nabla \cdot \left[\alpha_{g} \lambda_{eff} \nabla T_{g} - \alpha_{g} \sum_{i} h_{i} \vec{J}_{i} + \alpha_{g} \left(\overline{\vec{\tau}}_{eff} \cdot \vec{u}_{g} \right) \right] + \left(\dot{m}_{hom} + \dot{m}_{het} \right) h_{lg} \quad (3)$$

where the subscript 'g', 'hom', 'het', and 'i' represent gas phase, homogenous nucleus, heterogenous nucleus, and species, respectively. α_{g} is the volume fraction of gas phase, $\alpha_{g} = 1 - \alpha_{hom} - \alpha_{het}$. \vec{u} and \vec{g} is the velocity and gravity vector. \vec{J}_{i} is the diffusion flux of species i. The ρ , p, T, E, h_{i} , and h_{lg} denote the density, pressure, temperature, total energy, enthalpy of species i, and latent heat, respectively. The drag 1 force is $\vec{F}_{\rm D} = \vec{F}_{\rm D,hom} + \vec{F}_{\rm D,het}$. The $\dot{m}_{\rm hom}$ and $\dot{m}_{\rm het}$ (kg m⁻³ s⁻¹) is droplet mass changing rate for 2 homogenous and heterogenous condensation, respectively. $\lambda_{\rm eff}$ is the effective thermal conductivity, 3 $\lambda_{\rm eff} = \lambda + \lambda_{\rm tu}$, where $\lambda_{\rm tu}$ represents turbulent thermal conductivity. The effective stress tensor is described 4 by

$$\overline{\overline{\tau}}_{\text{eff}} = \mu_{\text{eff}} \left[\left(\nabla \vec{u}_{\text{g}} + \nabla \vec{u}_{\text{g}}^{T} \right) - \frac{2}{3} \nabla \cdot \vec{u}_{\text{g}} I \right]$$
(4)

6 where *I* is the unit tensor, μ_{eff} is the effective molecular viscosity, $\mu_{eff} = \mu + \mu_{tu}$. The turbulent viscosity 7 μ_{tu} and turbulent thermal conductivity λ_{tu} is calculated by the turbulence model. In this research, the 8 Reynolds stress model is applied to calculate the turbulence flow.

9 The species transport equation of gas phase is

$$\frac{\partial}{\partial t} \left(\alpha_{g} \rho_{g} Y_{i} \right) + \nabla \cdot \left(\alpha_{g} \rho_{g} \vec{u}_{g} Y_{i} \right) = -\nabla \cdot \left(\alpha_{g} \vec{J}_{i} \right) + S_{i}$$

$$\tag{5}$$

where Y_i represents the mass fraction of species i. S_i is source term where the value is $-(\dot{m}_{hom} + \dot{m}_{het})$ for the species of water vapor.

13 2.1.2 Dispersed droplet model

5

10

14 The volumetric concentration of dispersed homogeneous and heterogeneous droplet number, n_{hom} and 15 n_{het} (m⁻³) are expressed by

16
$$\frac{\partial n_{\rm hom}}{\partial t} + \nabla \cdot \left(n_{\rm hom} \vec{u}_{\rm hom} \right) = J - N_{\rm c} \tag{6}$$

17
$$\frac{\partial n_{\rm het}}{\partial t} + \nabla \cdot \left(n_{\rm het} \vec{u}_{\rm het} \right) = 0 \tag{7}$$

18 where $J(m^{-3} s^{-1})$ is homogeneous nucleation rate. N_c is the source term due to collision.

19 The volume fractions of homogeneous and heterogeneous droplets, α_{hom} and α_{het} are expressed as

20
$$\frac{\partial}{\partial t} (\alpha_{\rm hom} \rho_l) + \nabla \cdot (\alpha_{\rm hom} \rho_l \vec{u}_{\rm hom}) = \dot{m}_{\rm hom} - \dot{m}_{\rm c}$$
(8)

21
$$\frac{\partial}{\partial t} (\alpha_{\rm het} \rho_l) + \nabla \cdot (\alpha_{\rm het} \rho_l \vec{u}_{\rm het}) = \dot{m}_{\rm het} + \dot{m}_{\rm c}$$
(9)

where ρ_l is the droplet density. \dot{m}_c is the mass source term due to collision and coalescence. The effective density of homogenous and heterogeneous droplets is $\rho_{\text{hom}} = \alpha_{\text{hom}} \rho_l$ and $\rho_{\text{het}} = \alpha_{\text{het}} \rho_l$.

24 The momentum conservation equations of homogenous and heterogeneous droplets are expressed by

25
$$\frac{\partial}{\partial t} \left(\alpha_{\rm hom} \rho_l \vec{u}_{\rm hom} \right) + \nabla \cdot \left(\alpha_{\rm hom} \rho_l \vec{u}_{\rm hom} \vec{u}_{\rm hom} \right) = -\alpha_{\rm hom} \nabla p + \alpha_{\rm hom} \rho_l \vec{g} + \left(\dot{m}_{\rm hom} - \dot{m}_{\rm c} \right) \vec{u}_{\rm hom} + \vec{F}_{\rm D,hom}$$
(10)

$$26 \qquad \qquad \frac{\partial}{\partial t} \left(\alpha_{\rm het} \rho_l \vec{u}_{\rm het} \right) + \nabla \cdot \left(\alpha_{\rm het} \rho_l \vec{u}_{\rm het} \vec{u}_{\rm het} \right) = -\alpha_{\rm het} \nabla p + \alpha_{\rm het} \rho_l \vec{g} + \left(\dot{m}_{\rm het} + \dot{m}_{\rm c} \right) \vec{u}_{\rm het} + \vec{F}_{\rm D,het} \tag{11}$$

1 where $\vec{F}_{D,hom}$ and $\vec{F}_{D,het}$ are drag force between gas and water droplet.

2 2.1.3 Eulerian wall film model

5

3 The mass, momentum, and energy conservation equation of the two-dimensional film in three-4 dimensional domain are as follows

$$\frac{\partial}{\partial t} (\rho_l \delta) + \nabla_{\rm s} \cdot (\rho_l \delta \vec{u}_f) = \dot{m}_{\rm d} - \dot{m}_{\rm phase}$$
(12)

$$6 \qquad \qquad \frac{\partial}{\partial t} \left(\rho_l \delta \vec{u}_f \right) + \nabla_s \cdot \left(\rho_l \delta \vec{u}_f \vec{u}_f \right) = -\delta \nabla_s p + \rho_l \delta \vec{g}_r + \frac{3}{2} \vec{\tau}_{fs} - \frac{3\mu_l}{\delta} \vec{u}_f + \vec{U}_d + \left(\dot{m}_d - \dot{m}_{phase} \right) \vec{u}_f \tag{13}$$

$$7 \qquad \qquad \frac{\partial}{\partial t} \left(\rho_l \delta h_f \right) + \nabla_{\rm s} \cdot \left(\rho_l \delta h_f \vec{u}_f \right) = \frac{\lambda_l}{\delta} \left(T_{\rm s} + T_{\rm w} - 2T_{\rm m} \right) + \left(\dot{m}_{\rm d} - \dot{m}_{\rm phase} \right) h_{\rm lg} \tag{14}$$

8 where ∇_s is the surface gradient. δ is the film thickness. \vec{u}_f is film velocity vector. \dot{m}_d and \dot{m}_{phase} 9 represent deposition rate, film phase change rate (kg m⁻² s⁻¹), respectively. \vec{g}_{τ} is the gravity component 10 parallel to the film. The third and fourth terms on the right-hand side of Eq.(13) represent viscous shear 11 stress on gas-film and film-wall interfaces. \vec{U}_d is the momentum source term of film. T_s , T_w , and T_m are 12 the film surface, wall, and film half depth temperature, respectively.

13 2.2 Interphase exchange between gas and droplet

14 The droplet mass changing rate (condensation and evaporation rate) between the gas phase and 15 dispersed droplets are calculated by

16
$$\dot{m}_{\rm hom} = J \rho_l \frac{4\pi r_{\rm c}^3}{3} + n_{\rm hom} \rho_l 4\pi r_{\rm hom}^2 \frac{dr_{\rm hom}}{dt}, \quad \dot{m}_{\rm het} = n_{\rm het} \rho_l 4\pi r_{\rm het}^2 \frac{dr_{\rm het}}{dt}$$
(15)

17 The homogeneous nucleation rate $J(m^{-3} s^{-1})$ is calculated by [35]

18
$$J = \frac{\upsilon \rho_g^2}{S_s} \sqrt{\frac{2\sigma}{\pi m_m^5}} \exp\left(-\frac{16\pi}{3} \frac{\upsilon^2 \sigma^3}{\left(k_{\rm B} T_g\right)^3 \left(\ln S_s\right)^2}\right)$$
(16)

where, v and m_m represent volume and mass of single water molecule. k_B represents Boltzmann's constant, σ (N m⁻¹) is liquid surface tension. S_s is the supersaturation of water vapor, $S_s = p_v / p_s(T_g)$, where $p_s(T_v)$ is the saturation pressure of water vapor at T_v . The critical droplet size of homogenous nucleation is calculated by

23 $r_{\rm c} = \frac{2\sigma}{\rho_l R_{\rm v} T_{\rm g} \ln(S_{\rm s})}$ (17)

24 where R_v represent specific gas constant. The mean radii r_{hom} and r_{het} are expressed as

25
$$r_{\rm hom} = \left(\frac{3\alpha_{\rm hom}}{4\pi n_{\rm hom}}\right)^{\frac{1}{3}}, \quad r_{\rm het} = \left(\frac{3\alpha_{\rm het}}{4\pi n_{\rm het}}\right)^{\frac{1}{3}}$$
(18)

The growth rate of droplet in condensation and evaporation processes is calculated by

2

5

 $\frac{dr}{dt} = \frac{1}{\rho_l h_{\rm lg}} \left(T_{\rm r} - T_{\rm v} \right) \sum_{\rm i=1}^2 a_{\rm i}$ (19)

(22)

where the subscript 'v' represents water vapor. a_i is the heat transfer coefficient between the water droplet and species i [8]. The droplet surface temperature T_r is calculated by

$$T_{\rm r} = T_{\rm d} \left(p_{\rm v} \right) - D_{\rm T} \frac{r_{\rm c}}{r} \tag{20}$$

6 where $D_{\rm T}$ is subcooling, $D_{\rm T} = T_{\rm d}(p_{\rm v}) - T_{\rm g}$. $T_{\rm d}(p_{\rm v})$ is the dew point temperature at $p_{\rm v}$.

Generally, the size and slip velocity of heterogeneous droplets (foreign droplet) are significantly
greater than those of homogeneous droplets, since the diameter of homogeneous droplets is generally below
0.1 µm [30][36]. Thus, the heterogeneous droplets as collectors collide with the surrounding smaller size
homogeneous droplets. The mean collision frequency *f* is expressed as [37]

11
$$f = n_{\rm hom} \pi \left(r_{\rm het} + r_{\rm hom} \right)^2 \left| \vec{u}_{\rm het} - \vec{u}_{\rm g} \right|$$
(21)

12 Therefore, the source term of Eq.(6) is

14

15

The homogeneous droplets are collected by heterogeneous droplets, whose mass is transferred to the heterogeneous droplets, thereby the heterogeneous droplet radius increases up gradually. The mass source

 $N_{\rm c} = n_{\rm het} f$

16 term due to coalescence is calculated by

17
$$\dot{m}_{\rm c} = n_{\rm het} f \rho_l \frac{4\pi r_{\rm hom}^3}{3}$$
(23)

18 The drag force between the continuous and dispersed droplets in Eq.(2) is defined as [38]

19
$$\vec{F}_{\text{D,hom}} = \frac{9\mu_{\text{g}}}{2r_{\text{hom}}^2} C_{\text{D}} \frac{\text{Re}_{\text{p,hom}}}{24} \alpha_{\text{hom}} \left(\vec{u}_{\text{g}} - \vec{u}_{\text{hom}}\right), \quad \vec{F}_{\text{D,het}} = \frac{9\mu_{\text{g}}}{2r_{\text{het}}^2} C_{\text{D}} \frac{\text{Re}_{\text{p,het}}}{24} \alpha_{\text{het}} \left(\vec{u}_{\text{g}} - \vec{u}_{\text{het}}\right)$$
(24)

20 where the relative Reynolds number Re_{p,hom} and Re_{p,het} are expressed as

21
$$\operatorname{Re}_{p,hom} = 2\rho_{g}r_{hom} \left|\vec{u}_{hom} - \vec{u}_{g}\right| / \mu_{g}, \quad \operatorname{Re}_{p,het} = 2\rho_{g}r_{het} \left|\vec{u}_{het} - \vec{u}_{g}\right| / \mu_{g}$$
 (25)

22 The drag coefficient C_D is expressed as [39]

23
$$C_{\rm D} = \begin{cases} \frac{24}{{\rm Re}_{\rm p}}, & {\rm Re}_{\rm p} \le 1 \\ \frac{24}{{\rm Re}_{\rm p}} \left(1 + 0.15 {\rm Re}_{\rm p}^{0.687}\right), & 1 < {\rm Re}_{\rm p} \le 1000 \\ 0.44, & {\rm Re}_{\rm p} > 1000 \end{cases}$$
(26)

For smaller Reynolds numbers, the molecular viscous force dominates. However, when the particle size is small enough to approach the gas molecules free path length (Knudsen number Kn > 1), the drag coefficient should be corrected by Cunningham slip correction factor, $C_{\rm D} = \frac{24}{\text{Re}_{\rm p}C_{\rm c}}$, where Cunningham slip correction factor is calculated by [40]

$$C_{\rm c} = 1 + 2 \,{\rm Kn}_{\rm g} \left(1.257 + 0.4 e^{-1.1/(2 \,{\rm Kn}_{\rm g})} \right) \tag{27}$$

2.3 Coupling of the gas core with liquid film 2

3 The deposited droplets to the wall will gradually form a liquid film, that is, their mass and momentum 4 will be removed from the dispersed phase and added to the liquid film equations as source terms. The 5 droplet deposition rate, that is, the mass source term of liquid film \dot{m}_{d} (kg m⁻² s⁻¹) is given by [41]

$$\dot{n}_{\rm d} = \dot{m}_{\rm d,hom} + \dot{m}_{\rm d,het} = \alpha_{\rm hom} \rho_{_{I}} \vec{u}_{\rm hom} \cdot \vec{n} + \alpha_{\rm het} \rho_{_{I}} \vec{u}_{\rm het} \cdot \vec{n}$$
(28)

(0.0)

7 where \vec{n} is film area normal.

The momentum source term of liquid film is

13

8

6

 $\vec{U}_{d} = \vec{U}_{d \text{ hom}} + \vec{U}_{d \text{ het}} = \dot{m}_{d \text{ hom}} \vec{u}_{t \text{ hom}} + \dot{m}_{d \text{ het}} \vec{u}_{t \text{ het}}$ (29)

10 where film tangential velocity vector is $\vec{u}_t = \vec{u} - (\vec{u} \cdot \vec{n})\vec{n}$. The tangential and normal directions of thin liquid 11 film are shown in Fig. 2 (b).

The phase change rate between wall film and gas phase (kg $m^{-2} s^{-1}$) is calculated by [42] 12

$$\dot{m}_{\rm phase} = \frac{\rho_{\rm g} M/d}{\rho_{\rm g} M/d + C_{\rm phase}} C_{\rm phase} \left(Y_{\rm s} - Y\right) \tag{30}$$

14 where d represents cell-center-to-wall distance. M is the mass diffusivity of water vapor. C_{phase} is the phase 15 change constant. Ys represent saturation mass fraction of water vapor. Y is the mass fraction of water vapor at the cell-center of near-wall cell. 16

17

3 CFD validation 18

19 3.1 Numerical scheme

20 ANSYS FLUENT software is used for numerical simulation. The conservation equations of dispersed 21 droplets are implemented through the User-Defined-Scalar interface. The mass and thermal coupling 22 between the discrete droplets and the gas phase and it between the liquid film and the discrete droplets are 23 realized by establishing source terms through the User-Defined-Function interface. Because the conditions 24 of this study are low pressure and normal temperature, it is reasonable to approximate the gas phase as an 25 ideal gas. The separator and applies Reynolds stress model (RSM) to calculate turbulence, and other cases 26 apply transition SST model. The density-based solver is employed to calculate the supersonic flow, and the 27 pressure-based solver is used to calculate the low-speed flow. Coupling Eulerian wall film model must 28 adopt a pressure-based solver. For the supersonic nozzle, the solution method adopts implicit formulation 29 and Roe-FDS flux type. The least squares cell-based format is chosen for the gradient discretization. The 30 second order upwind discrete scheme is applied to ensure higher calculation accuracy. For other cases, the 31 solution method adopts SIMPLE scheme pressure-velocity coupling, and the pressure discretization adopts

PRESTO! format. In this study, the convergence criteria for all dependent variables are lower than 1.0×10⁻
For the supersonic separator and supersonic nozzle, the air-water vapor two-phase flow as working fluid.
The inlet boundary condition is set to pressure-inlet, and the outlet boundary condition is set to pressureoutlet. The air as working fluid in the cyclone separator. The inlet boundary condition is the velocity-inlet,
and the outlet boundary condition is the outflow. There is an air-water vapor two-phase flow in the
rectangular channel, the inlet boundary condition is the velocity-inlet. The outlet boundary condition is the

8 3.2 Experimental validation

9 According to the characteristics of the flow and heat transfer in the supersonic separator, the 10 experimental validation can be divided into the following three parts: validating the supersonic condensing 11 flow in the supersonic nozzle; validating the strong swirling flow in the cyclone separator; validating the 12 liquid film flow and liquid film phase change in the rectangular channel. Consequently, the calculation 13 accuracy of the model for condensate flow, swirl separation, and liquid film flow is validated successively.

14 *3.2.1 Condensation flow in supersonic nozzle*

The geometry of the 3D axisymmetric supersonic nozzle is shown in Fig. 3 (a), and the nozzle throat diameter is 10 mm. The experimental platform for homogeneous condensation of the supersonic nozzle had been explained in our previous article [8]. The grid is structured hexahedral grid, which is refined on the wall to satisfy the requirement $y^+ < 1$. The grid independence tests are carried based on Grid Convergence Index (GCI) analysis [43]. The GCI is a method of mesh refinement error estimation based on generalized extrapolation theory, which is described by

$$GCI = \frac{F_s |\varepsilon|}{r^p - 1} \times 100\%$$
(31)

where F_s is the safety factor and its empirical value is 3, ε is the relative error between two grids, r is the refinement factor ratio, and p is the algorithm accuracy order. A small GCI means that the difference between the solution results of the two grids is small. The three groups of grids are grids 1: 16,200 cells, grids 2: 13,000 cells, and grids 3: 10,000 cells, respectively. Taking the outlet pressure as the test parameter, as shown in Table 1, 13,000 grid cells can gain grid-independent solutions.

27 28

Table 1 Test results of Grid Convergence Inde	x.
---	----

		Grids 1-2		Gric	ls 2-3
		(1-fine, 2-medium)		(2-medium, 3-coarse)	
F_s	р	$\varepsilon_{1,2}$ (%)	$GCI_{1,2}(\%)$	$\varepsilon_{2,3}$ (%)	$GCI_{2,3}(\%)$
3	3	0.17	0.87	0.65	2.74

29

The inlet pressure of the supersonic nozzle is 300 kPa, the inlet temperature is 50°C, and the outlet is supersonic flow. The pressure distribution along the nozzle is shown in Fig. 3 (b). It can be seen that the

- 1 simulation data of the back-pressure ratio is in good agreement with the experiment with different humidity
- 2 conditions, which validates that the established CFD model can maintain a high-precision simulation of
- 3 supersonic condensing flow.



4

5

7 8

Fig. 3 Comparison between CFD and experiment of supersonic nozzle.

9 *3.2.2 Dispersed phase behaviors in cyclone separator*

The geometry and grid of the cyclone separator are shown in Fig. 4. The structured hexahedral grid is generated. When the number of grid cells is 218277, a grid-independent solution can be obtained. The released particles are typical cement raw materials. The characteristic diameter of the particles is 29.9 μm. The air and particles enter the cyclone separator at the same speed and are separated by the centrifugal force. For other boundary conditions, please refer to the articles of Wang et al. [44]





Fig. 4 Geometry and grid diagram of cyclone separator (mm).

The tangential velocity distribution in the cyclone separator is shown in Fig. 5 (a). It can be seen that the maximum error between the simulation and the experiment data of the tangential velocity is about \pm 5%. The comparison between the simulation and the experiment results of the collection efficiency at different inlet velocities is shown in Fig. 5 (b). It can be seen that the inlet velocity is 15-30 m s⁻¹, the simulation and experiment of the collection efficiency are in the highest agreement. The above results validate that the setablished model can maintain high accuracy in simulating the particle behaviors in strong swirling flow.













4 *3.2.3 Liquid film flow and film evaporation*

5 The 3D computational domain and grid of the rectangular channel are shown in Fig. 6. The structural hexahedral grid is generated and refined in the near-wall area to meet the boundary layer calculation 6 7 requirement $y^+ < 1$. Simultaneously, in order to calculate the liquid film flow and liquid film evaporation 8 more accurately, the grid is further refined within the initial liquid film height of the bottom wall. After the 9 grid independence test, the number of grid cells is determined to be 960,687. The liquid film flows 10 downward from the top of the vertical rectangular channel into the calculation domain. The air flows 11 upward from the bottom of the channel into the calculation domain, forming a countercurrent with the liquid 12 film. The inlet air temperature is 45°C. and the outlet pressure is 1 atm. The initial film mass flux and incoming film temperature are setup. The heating temperature of the bottom wall is setup to evaporate the 13 14 liquid film. For other boundary conditions, please refer to the articles of Du et al. [45]

The average heat flux and liquid film evaporation rate of the bottom wall are shown in Fig. 7. It can be seen that the errors of their simulation and experimental results are within $\pm 10\%$. This means that the established model can simulate the liquid film flow and the heat and mass exchange between the liquid film and the moist air.



Fig. 6 3D computational domain and grid of rectangular channel.





(a) Comparison of the average surface heat flux





2

(b) Comparison of the average surface liquid film evaporation rate

Fig. 7 Comparison between CFD and experiment in the bottom wall of rectangular channel.

3 4

5

4 Results and discussion

6 The geometry and grid of the supersonic separator are shown in Fig. 8. The 3D computational domain 7 of the supersonic separator is the annular channel between the inner center body and the outer shell, and its 8 throat cross-sectional area is 105.07 mm². The type of grid is the structured hexahedron, which is refined 9 in the near-wall area to meet the boundary layer calculation requirements. According to the grid 10 independence test, the number of grid cells is 549,900.





Fig. 8 Geometry and grid diagram of supersonic separator A.

13 4.1 Flow field and droplet behaviors

14 The common boundary conditions are $p_*^{in} = 250$ kPa, $T_*^{in} = 30^{\circ}$ C, $\Phi_*^{in} = 100\%$ (namely $p_v^{in} = 4246$ 15 Pa), $p^{out} = 100$ kPa. The ρ_{het}^{in} and n_{het}^{in} is specified for the boundary conditions of heterogeneous condensation, the settings of Case 1-5 are shown in Table 2. The supersonic separator B differs from supersonic separator A in that the inlet diameter is 10 mm smaller. It can be seen from Table 2 that case1-4 have the same inlet heterogeneous nucleus radius r_{het} ⁱⁿ but the different inlet heterogeneous nucleus effective density ρ_{het} ⁱⁿ. The ρ_{het} ⁱⁿ represents the number of foreign droplets injected into the inlet. According to our previous research, the optimal foreign droplet radius of separator A and separator B are about 1.0 µm and 0.3 µm [8], respectively.

7 8

 Table 2 Cases of different foreign droplets in supersonic separators.

Cases	Separators	$r_{\rm het}{}^{\rm in}(\mu { m m})$	$ ho_{\rm het}{}^{\rm in}({ m kg}~{ m m}^{-3})$	$n_{\rm het}^{\rm in}$ (m ⁻³)	$Q_{\rm het}{}^{\rm in}$ (ml min ⁻¹)
Case 1	Separator A	1.0	0.001	2.39×10 ¹¹	1.73
Case 2	Separator A	1.0	0.01	2.39×10 ¹²	17.09
Case 3	Separator A	1.0	0.05	1.19×10 ¹³	84.14
Case 4	Separator A	1.0	0.1	2.39×10 ¹³	165.97
Case 5	Separator B	0.3	0.01	8.86×10 ¹³	19.03

9

10 The velocity streamline of the supersonic separator A is shown in Fig. 9. After the expansion and 11 cooling process of the supersonic nozzle, the moist gas maintains supersonic speed in the divergent section 12 of the nozzle. The maximum gas phase velocity and subcooling degree can reach 514.4 m s⁻¹ and 45.2°C, 13 respectively. At the liquid separation position, a sudden decrease in velocity can be observed from Fig. 9 14 which means that a shock wave has occurred there. However, the velocity at the liquid separation position 15 is not completely reduced to subsonic speed, so which in the diffuser further increase to supersonic speed. 16 The shock wave phenomenon at the liquid separation position will affect the heat and mass exchange 17 between gas and liquid, making the condensed droplets evaporate, which should be avoided as much as 18 possible to obtain a higher separation efficiency.







1 10, which is closely related to separation efficiency. The high tangential velocity distribution of the 2 supersonic separator A is close to the liquid separation position, which of the supersonic separator B is close 3 to the throat. The reduced height of the swirling blades decreases the swirl strength. The maximum swirl 4 strength is shown in Table 3. The maximum swirl strength S_{max} of the supersonic separator B can reach 0.42, 5 which is about twice that of the supersonic separator A.



Separators	Inlet diameter (mm)	$u_{t,max} (m s^{-1})$	$a_{\rm c,max} ({\rm m}~{\rm s}^{-2})$	$S_{\max}(-)$
А	80	71.74	1.04×10^{6}	0.23
В	70	134.43	3.08×10^{6}	0.42

13

The dehydration performance of the supersonic separator can be seen from the mole fraction and partial pressure of water vapor at the dry gas outlet. As can be seen from Fig. 11 (a) and (b), after supersonic separation, the saturated water vapor is basically discharged from the wet gas outlet, which can achieve high separation efficiency. It can be clearly observed from Fig. 11 (b) that the condensation of water vapor makes a rapid decrease in the water vapor partial pressure near the nozzle throat. In the process of approaching the liquid separation position, a large number of droplets in the near-wall area evaporate under the action of the hot gas flow and shock wave, which is not conducive to water separation.



7 The droplet distribution in the supersonic separator is shown in Fig. 12. It can be seen from Fig. 12 (a) 8 that the condensation of droplets starts near the nozzle throat, and the maximum droplet mass change rate 9 $\dot{m}_{het} = 412.0 \text{ kg m}^{-3} \text{ s}^{-1}$. The droplet evaporation occurs in the near-wall area and the wet gas outlet, and 10 the maximum droplet evaporation is -283.1 kg m⁻³ s⁻¹.

Fig. 12 (b) and Fig. 12 (c) reveal that the droplets gradually gather towards the wall and form a liquid 11 12 film under the action of centrifugal force. Different from the numerical model without considering the liquid 13 film (refer to our previous research [8]), after the dispersed droplets are centrifuged to the wall, they are not 14 absorbed into the wall and discharged along the wall in the form of dispersed droplets. Instead, they are 15 removed from the dispersed droplets and deposited to form a liquid film on the wall. The formed liquid 16 film also has a heat and mass exchange process with the gas phase. The model without considering the 17 liquid film over-predicts the separation efficiency, which will be described in the following section. 18 Therefore, as shown in Fig. 12 (b), the droplets begin to condense and grow at the throat of the nozzle. The

droplet effective density and radius gradually increase, while the droplet effective density begins to decrease after the axial position $x_a = 120$ mm, which means that most of the dispersed droplets are deposited to form a liquid film. The droplets coalesce under the action of centrifugal force, resulting in the further increase of droplet size, and the maximum droplet size is 1.6 µm.

5 Combining Fig. 12 (b) and Fig. 12 (c), it can be seen that some droplets enter the dry gas outlet. The 6 average droplet effective density at the dry gas outlet of Case1-4 is 3.85×10^{-03} kg m⁻³, 1.59×10^{-06} kg m⁻³, 7 1.45×10^{-06} kg m⁻³, 1.59×10^{-06} kg m⁻³, respectively. It means that when the effective density of foreign 8 droplets $\rho_{het}{}^{in} = 0.001$ kg m⁻³, a large number of droplets enter the dry gas outlet, resulting in low separation 9 efficiency. The droplet size distribution along the axial direction under different $\rho_{het}{}^{in}$ is shown in Fig. 12 10 (d). It can be seen that when the $\rho_{het}{}^{in}$ is small, the droplet size is larger. The maximum droplet size of Case1-4 is 2.50 µm, 1.59 µm, 1.51 µm, 1.48 µm, respectively.





7 The droplet surface temperature, the gas phase temperature, and the latent heat are shown in Fig. 13, 8 which reflects the heat transfer between the dispersed droplets and the gas phase. The gas phase expands in 9 the divergent section of the nozzle, and the gas phase temperature gradually decreases, causing the wet 10 steam to condense to form dispersed droplets. The latent heat released by the condensation is transferred to 11 the gas phase, causing the temperature of the gas phase to slightly increase. Compared with the droplet 12 surface temperature, the gas phase temperature is lower in the low temperature zone and higher in the high 13 temperature zone. The heat transfer occurs from dispersed droplets to the gas phase during the condensation process (the maximum latent heat is 5.3×10⁸ J m⁻³), which occurs from the gas phase to dispersed droplets 14 15 during the evaporation process (the minimum latent heat is -3.4×10^8 J m⁻³).



1

Fig. 13 The heat transfer of supersonic separator A.

4 The interphase slip velocity characterizes the momentum coupling between the droplet and the gas 5 phase. The slip velocity is defined as the droplet velocity minus the gas velocity. The distribution of axial 6 and centrifugal (radial) slip velocity components is shown in Fig. 14. It can be seen that the slip velocity 7 before the liquid separation position gradually increases along the flow direction, which means that the drag 8 force between the gas phase and the dispersed droplets gradually increases. The slip velocity of $\rho_{het}^{in} = 0.01$ kg m⁻³ is greater than that of $\rho_{het}^{in} = 0.1$ kg m⁻³. Combined with Fig. 12 (d), this is because the larger the 9 droplet size ($\rho_{\text{het}}^{\text{in}} = 0.01 \text{ kg m}^{-3}$), the stronger the droplet inertia. Under the action of centrifugal force, the 10 11 centrifugal slip velocity increases gradually, and the centrifugal velocity of droplet is greater than that of 12 gas phase by a maximum of 24.9 m s⁻¹, so as to realize gas-liquid separation.





6

7 4.2 Liquid film behaviors

8 The liquid film distribution of supersonic separator A is shown in Fig. 15. It can be seen from Fig. 15 9 (a) that the condensed droplets are centrifuged to the wall surface and form a liquid film, and then 10 discharged from the wet gas outlet. The liquid film is thicker at the corner of the wet gas outlet, as shown 11 in Fig. 15 (c), this is because the circular liquid film flow is formed there. The film thickness of swirling 12 liquid film flow of Case1-4 at wet gas outlet is 21 µm, 47 µm, 74 µm, and 89 µm, respectively. With the 13 increase of ρ_{het}^{in} , the thickness of liquid film increases. The maximum liquid film velocity is 1.9 m s⁻¹ at x_a 14 = 130 mm. The film phase change rate \dot{M}_{phase} represents the mass exchange between the liquid film and 1 the gas phase. A negative film phase change rate represents condensation, and a positive film phase change 2 rate represents evaporation. As shown in Fig. 15 (a), at $x_a = 120-220$ mm, vapor phase condensation 3 increases the liquid film mass.

The film temperature and heat flux reflect the heat transfer of the liquid film. As shown in Fig. 15 (b), the heat transfer of the liquid film includes the coupled heat transfer between the dispersed droplets and the gas phase, as well as the wall heat conduction. The dispersed droplets gradually form a liquid film near the axial position $x_a = 120$ mm, where the liquid film temperature decreases to a minimum 304.1 K due to the deposition of the dispersed droplets, where the maximum heat flux is 0.74 MW m⁻². Afterwards, the wall transfers heat to the cold liquid film, causing the liquid film temperature to rise. Behind the shock wave, the liquid film evaporates and reduces the liquid film temperature.





$$R_{12}(\tau) = \lim_{T \to \infty} \frac{1}{T} \int_0^T y_1(\tau) y_2(t-\tau) dt$$
(32)

1 where y_1 represents the fluctuation of film thickness at position x_1 , and y_2 represents the fluctuation of film

2 thickness at position x_2 .

- 3 The interfacial wave velocity u_w is calculated by
- 4

$$u_{\rm w} = \frac{x_l}{\tau_0} \tag{33}$$

5 where the time τ_0 corresponding to the peak of $R_{12}(\tau)$ is the transit time of the signal, $x_l = x_2 - x_1$ is transit 6 distance.

The interfacial wave velocity calculation process of Case 4 is shown in Fig. 16. The time-dependent liquid film thickness data at wet gas outlet $x_1 = 270$ mm and $x_2 = 275$ mm ($x_l = 5$ mm) are collected in Fig. 16 (a). The fluctuation of interfacial wave can be seen from Fig. 16 (b), and y_1 is obviously lagging behind y_2 . The dominant frequency $f_w = 11.07$ Hz (Case 4) of the interfacial wave is obtained through timefrequency domain transformation. As shown in Fig. 16 (c), the transit time $\tau_0 = 3.35$ ms is calculated by the cross-correlation function. The maximum cross-correlation coefficient can reach 0.93. Thus, the interfacial wave velocity can be calculated as 1.49 m s⁻¹.

Table 4 shows the dominant frequency and interfacial wave velocity with different ρ_{het}^{in} . With the increase of the ρ_{het}^{in} , the thickness of the liquid film will increase. The large ρ_{het}^{in} increases the frequency and velocity of the interfacial wave, which increases the instability in the supersonic separator. The correlation coefficient decreases with the increase of the ρ_{het}^{in} , so as to the complexity of interfacial waves increases.



19

(a) Raw data of liquid film thickness obtained by data collection





(c) Calculation of transit time using cross-correlation function Fig. 16 The calculation process of the interfacial wave velocity (Case 4).



1 2

Table 4 Frequency and cross-correlation velocity of interfacial waves of liquid film at liquid outlet with

different ρ_{het}^{m} .					
Cases	$\delta^{\mathrm{wet}}\left(\mu m\right)$	$f_{\rm w}$ (Hz)	$ au_0$ (ms)	$R_{12}(\tau_0)$ (-)	$u_{\rm w}$ (m s ⁻¹)
Case 1	21	5.24	15.40	0.98	0.32
Case 2	47	7.97	9.60	0.97	0.52
Case 3	74	10.00	5.75	0.95	0.87
Case 4	89	11.07	3.35	0.93	1.49

4 4.3 Dehydration performance

5 The commonly used dehydration performance indicators are dew point depression ΔT_d and water 6 removal rate η_v (i.e., separation efficiency). The ΔT_d is expressed as

 $\Delta T_{\rm d} = T_{\rm d}^{\rm in} - T_{\rm d}^{\rm dry}$

 $\eta_{\rm v} = \frac{\chi_{\rm v}^{\rm in} - \chi_{\rm v}^{\rm dry}}{\chi_{\rm v}^{\rm in}} \times 100\%$

(34)

(35)

8 where, $T_{\rm d}$ (°C) is the dew point temperature of gas phase. The separation efficiency $\eta_{\rm v}$ is expressed as

10 where, χ_v is the mole fraction of water vapor.

11 The dehydration performance of supersonic separator A is shown in Table 5. The effective water vapor 12 partial pressure at dry gas outlet p_v^{dry} includes the effective partial pressure of water vapor and liquid 13 droplets, and its minimum value is 252.97 Pa. The dew point at dry gas outlet T_d^{dry} can be as low as -14 10.32°C. For supersonic separator B (Case 5), $p_v^{dry} = 200.14$ Pa, $T_d^{dry} = -12.93$ °C.

15 16

 Table 5 Dehydration performance of supersonic separator A.

Cases	$p_{\rm v}^{\rm dry}$ (Pa)	$T_{\rm d}^{\rm dry}$ (°C)	$\Delta T_{\rm d}^{\rm dry}$ (°C)	$\eta_{ m v}$ (%)
Case 1	754.63	2.93	27.07	55.58
Case 2	252.97	-10.32	40.32	85.11
Case 3	369.09	-6.01	36.01	78.27
Case 4	754.15	2.91	27.09	55.60

17

The histogram of the dehydration performance for different ρ_{het}^{in} is shown in Fig. 17. It can be seen that the optimal effective density of foreign droplets ρ_{het}^{in} is 0.01 kg m⁻³. This means that for achieving higher dehydration efficiency, the ρ_{het}^{in} should be moderate. If the ρ_{het}^{in} is too small, a better swirl separation effect cannot be achieved, and more liquid droplets cannot be separated and enter the dry gas outlet, which reduces the separation efficiency. In addition, the excessive ρ_{het}^{in} can also cause negative effects, such as thickening the liquid film against separation, increasing instability in the supersonic separator, etc. The

- 1 model without considering the liquid film over-predicts the separation efficiency. When $\rho_{\text{het}}^{\text{in}} = 0.01 \text{ kg m}^{-1}$
- 2 ³, the maximum separation efficiency and dew point depression of separator A are 85.11% (86.71% without
- 3 considering the liquid film [8]) and 40.32°C, respectively. The separation efficiency of supersonic separator
- 4 B is 88.22% (93.91% without considering the liquid film [8]), and its dew point depression is 42.93°C.



5

6

7

Fig. 17 Comparison of separation efficiency of different ρ_{het}^{in} .

8 5 Conclusion

A novel three-field two-fluid model considering the heat and mass transfer between gas, liquid droplets, and liquid film was developed and validated. Besides, the flow field, droplet behaviors, and heat transfer between the gas phase and droplets were studied. The liquid film behaviors, phase change rate, and heat flux were analyzed further. The cross-correlation algorithm was implemented to obtain the frequency and velocity of interfacial wave. Simultaneously, the effect of effective density of foreign droplets and the difference with the model without considering the liquid film was analyzed. The main conclusions are as follows:

The droplets start to condense at the nozzle throat but evaporate in the near-wall area and the wet
 gas outlet. The droplet mass change rate ranges from -283.1 kg m⁻³ s⁻¹ to 412.0 kg m⁻³ s⁻¹. The maximum
 latent heat is 5.3×10⁸ J m⁻³ from droplets to gas phase at the condensation process, and the minimum latent
 heat is -3.4×10⁸ J m⁻³ at the evaporation process.

- 20 2. The slip velocity before the liquid separation position gradually increases along the flow direction, 21 which decreases with the increase of ρ_{het}^{in} . The centrifugal velocity of the droplets is greater than that of the 22 gas phase by a maximum of 25 m s⁻¹, so as to realize gas-liquid separation.
- 23 3. The thickness of swirling liquid film flow of Case 1-4 at wet gas outlet is 21 μ m, 47 μ m, 74 μ m and 24 89 μ m, respectively. At $x_a = 120-220$ mm, vapor phase condensation increases the liquid film mass. The

1 liquid film temperature decreases to a minimum 304.1 K near the axial position $x_a = 120$ mm due to the 2 deposition of the dispersed droplets, where the maximum heat flux is 0.74 MW m⁻².

4. With the increase of ρ_{het}ⁱⁿ, the liquid film becomes thicker. Meanwhile, the frequency and velocity
of the interfacial wave increase, their maximum values are 11.07 Hz and 1.49 m s⁻¹ with ρ_{het}ⁱⁿ = 0.1 kg m⁻³,
which increases the instability in the separator.

5. The foreign droplets are beneficial to the dehydration performance, but it should be moderate. The
optimal value of effective density of foreign droplets ρ_{het}ⁱⁿ is 0.01 kg m⁻³. The maximum separation
efficiency and dew point depression of separator A are 85.11% and 40.32°C, respectively. The model
without considering the liquid film over-predicts the separation efficiency.

10

11 Acknowledgement

This work is supported in part by National Natural Science Foundation of China under Grant 51876143
 and 61873184.

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

16

17 **References**

[1] Khan MI, Shahrestani M, Hayat T, et al. Life cycle (well-to-wheel) energy and environmental
 assessment of natural gas as transportation fuel in Pakistan. Applied Energy, 2019, 242: 1738-1752.

20 [2] Liu Y, Cao X, Yang J, et al. Energy separation and condensation effects in pressure energy recovery

process of natural gas supersonic dehydration. Energy Conversion and Management, 2021, 245:
114557.

[3] Cao X, Guo D, Sun W, et al. Supersonic separation technology for carbon dioxide and hydrogen sulfide
 removal from natural gas. Journal of Cleaner Production, 2021, 288: 125689.

[4] Wen C, Ding H, Yang Y. Numerical simulation of nanodroplet generation of water vapour in high pressure supersonic flows for the potential of clean natural gas dehydration. Energy Conversion and
 Management, 2021, 231: 113853.

[5] Teixeira AM, de Oliveira Arinelli L, de Medeiros JL, et al. Recovery of thermodynamic hydrate
 inhibitors methanol, ethanol and MEG with supersonic separators in offshore natural gas processing.
 Journal of Natural Gas Science and Engineering, 2018, 52: 166-186.

[6] Wen C, Cao X, Yang Y, et al. Numerical simulation of natural gas flows in diffusers for supersonic
 separators. Energy, 2012, 37(1): 195-200.

[7] Li H, Anglart H. Prediction of dryout and post-dryout heat transfer using a two-phase CFD model.
 International Journal of Heat and Mass Transfer, 2016, 99: 839-850.

35 [8] Ding H, Sun C, Wang C, et al. Prediction of dehydration performance of supersonic separator based on

a multi-fluid model with heterogeneous condensation. Applied Thermal Engineering, 2020, 171:

1	115074.
1	1150/4

- [9] Wang Y, Yu Y, Hu D. Experimental investigation and numerical analysis of separation performance for
 supersonic separator with novel drainage structure and reflux channel. Applied Thermal Engineering,
 2020, 176: 115111.
- [10] Wen C, Cao X, Yang Y, et al. Swirling effects on the performance of supersonic separators for natural
 gas separation. Chemical engineering & technology, 2011, 34(9): 1575-1580.
- [11] Ma Q, Hu D, He G, et al. Performance of inner-core supersonic gas separation device with droplet
 enlargement method. Chinese journal of chemical engineering, 2009, 17(6): 925-933.
- 9 [12] Cao X, Yang W. The dehydration performance evaluation of a new supersonic swirling separator.
 10 Journal of Natural Gas Science and Engineering, 2015, 27: 1667-1676.
- [13] Wang Y, Yu Y, Hu D. Experimental investigation and numerical analysis of separation performance for
 supersonic separator with novel drainage structure and reflux channel. Applied Thermal Engineering,
 2020, 176: 115111.
- [14] de Oliveira Arinelli L, de Medeiros JL, de Melo DC, et al. Carbon capture and high-capacity
 supercritical fluid processing with supersonic separator: Natural gas with ultra-high CO2 content.
 Journal of Natural Gas Science and Engineering, 2019, 66: 265-283.
- [15] de Oliveira Arinelli L, Teixeira A M, de Medeiros J L, et al. Supersonic separator for cleaner offshore
 processing of natural gas with high carbon dioxide content: Environmental and economic assessments.
 Journal of cleaner production, 2019, 233: 510-521.
- [16] Wen C, Cao X, Yang Y, et al. Evaluation of natural gas dehydration in supersonic swirling separators
 applying the Discrete Particle Method. Advanced powder technology, 2012, 23(2): 228-233.
- [17] Yang Y, Wen C. CFD modeling of particle behavior in supersonic flows with strong swirls for gas
 separation. Separation and Purification Technology, 2017, 174: 22-28.
- [18] Liu X, Liu Z, Li Y. Investigation on separation efficiency in supersonic separator with gas-droplet flow
 based on DPM approach. Separation Science and Technology, 2014, 49(17): 2603-2612.
- [19] Jiang W, Bian J, Wu A, et al. Investigation of supersonic separation mechanism of CO2 in natural gas
 applying the Discrete Particle Method. Chemical Engineering and Processing-Process Intensification,
 2018, 123: 272-279.
- [20] Shooshtari SHR, Shahsavand A. Numerical investigation of water droplets trajectories during natural
 gas dehydration inside supersonic separator. Journal of Natural Gas Science and Engineering, 2018, 54:
 131-142.
- [21] Dykas S, Wróblewski W. Numerical modelling of steam condensing flow in low and high-pressure
 nozzles. International Journal of Heat and Mass Transfer, 2012, 55(21-22): 6191-6199.
- [22] Patel Y, Patel G, Turunen-Saaresti T. Influence of turbulence modelling on non-equilibrium
 condensing flows in nozzle and turbine cascade. International Journal of Heat and Mass Transfer, 2015,
 88: 165-180.
- [23] White AJ, Hounslow MJ. Modelling droplet size distributions in polydispersed wet-steam flows.
 International Journal of Heat and Mass Transfer, 2000, 43(11): 1873-1884.
- 39 [24] Ding H, Tian Y, Wen C, et al. Polydispersed droplet spectrum and exergy analysis in wet steam flows

1 using method of moments. Applied Thermal Engineering, 2021, 182: 116148. 2 [25] Edathol J, Brezgin D, Aronson K, et al. Prediction of non-equilibrium homogeneous condensation in 3 supersonic nozzle flows using Eulerian-Eulerian models. International Journal of Heat and Mass 4 Transfer, 2020, 152: 119451. 5 [26] Abadi SMANR, Kouhikamali R, Atashkari K. Two-fluid model for simulation of supersonic flow of wet steam within high-pressure nozzles. International Journal of Thermal Sciences, 2015, 96: 173-182. 6 7 [27] Wen C, Karvounis N, Walther JH, et al. Non-equilibrium condensation of water vapour in supersonic 8 flows with shock waves. International Journal of Heat and Mass Transfer, 2020, 149: 119109. 9 [28] Wen C, Ding H, Yang Y. Optimisation study of a supersonic separator considering nonequilibrium 10 condensation behaviour. Energy Conversion and Management, 2020, 222: 113210. 11 [29] Niknam PH, Mortaheb HR, Mokhtarani B. Dehydration of low-pressure gas using supersonic 12 separation: Experimental investigation and CFD analysis. Journal of Natural Gas Science and 13 Engineering, 2018, 52: 202-214. 14 [30] Shooshtari SHR, Shahsavand A. Optimal operation of refrigeration oriented supersonic separators for 15 natural gas dehydration via heterogeneous condensation. Applied Thermal Engineering, 2018, 139: 76-16 86. 17 [31] Deng Y, Zhang L, Hou H, et al. Modeling and simulation of the gas-liquid separation process in an 18 axial flow cyclone based on the Eulerian-Lagrangian approach and surface film model. Powder 19 Technology, 2019, 353: 473-488. 20 [32] Han J, Feng J, Hou T, et al. Numerical and experimental study on gas-water separators for a PEMFC 21 system. International Journal of Green Energy, 2021, 18(5): 490-502. 22 [33] Li H, Anglart H. Prediction of dryout and post-dryout heat transfer using a two-phase CFD model. 23 International Journal of Heat and Mass Transfer, 2016, 99: 839-850. 24 [34] Yue T, Chen J, Song J, et al. Experimental and numerical study of upper swirling liquid film (USLF) 25 among gas-liquid cylindrical cyclones (GLCC). Chemical Engineering Journal, 2019, 358: 806-820. 26 [35] Kantrowitz A. Nucleation in very rapid vapor expansions. The Journal of chemical physics, 1951, 27 19(9): 1097-1100. 28 [36] Jurski K, Géhin E. Heterogeneous condensation process in an air water vapour expansion through a 29 nozzle—experimental aspect. International journal of multiphase flow, 2003, 29(7): 1137-1152. 30 [37] O'Rourke PJ. Collective Drop Effects on Vaporizing Liquid Sprays. PhD thesis. Princeton University, 31 Princeton, New Jersey. 1981. 32 [38] Ounis H, Ahmadi G, McLaughlin J B. Brownian diffusion of submicrometer particles in the viscous 33 sublayer. Journal of Colloid and Interface Science, 1991, 143(1): 266-277. 34 [39] Wang B, Xu D, Chu K, et al. Numerical study of gas-solid flow in a cyclone separator. Applied 35 Mathematical Modelling, 2006, 30(11): 1326-1342. 36 [40] Dykas S, Wróblewski W. Two-fluid model for prediction of wet steam transonic flow. International 37 Journal of Heat and Mass Transfer, 2013, 60: 88-94. 38 [41] Yuan S, Fan Y, Chen B, et al. Forming and stripping of the wall film and the influence on gas-liquid 39 separation. Asia-Pacific Journal of Chemical Engineering. 2020, 15(3): e2447.

1	[42] Wang X, Chang H, Corradini M, et al. Prediction of falling film evaporation on the AP1000 passive
2	containment cooling system using ANSYS FLUENT code. Annals of Nuclear Energy. 2016, 95: 168-
3	175.
4	[43] Baker N, O'Sullivan P. Verification of Multiphase Flow CFD Simulation and Grid Convergence Index
5	(GCI) Analysis, 2013.
~	

- [44] Wang B, Xu D L, Chu K W, et al. Numerical study of gas-solid flow in a cyclone separator. Applied 6 7 Mathematical Modelling, 2006, 30(11): 1326-1342.
- 8 [45] Du K, Hu P, Hu Z. Numerical Investigation of Water Film Evaporation with the Countercurrent Air in
- 9 the Asymmetric Heating Rectangular Channel for Passive Containment Cooling System. Science and 10 Technology of Nuclear Installations, 2020.
- 11 [46] Wang C, Zhao N, Feng Y, et al. Interfacial wave velocity of vertical gas-liquid annular flow at different
- 12 system pressures. Experimental Thermal and Fluid Science, 2018, 92: 20-32.