Prediction of dehydration performance of supersonic separator based on 1 a multi-fluid model with heterogeneous condensation 2 3 Hongbing Ding¹, Chunqian Sun¹, Chao Wang^{1,*}, Chuang Wen², Yuhe Tian¹ 4 5 ¹Tianjin Key Laboratory of Process Measurement and Control, School of Electrical and Information 6 Engineering, Tianjin University, Tianjin 300072, China 7 ²Faculty of Engineering, University of Nottingham, University Park, Nottingham NG7 2RD, UK 8 *Corresponding author: Chao Wang, Email: wangchao@tju.edu.cn 9 10 Abstract: Supersonic separation is a novel technology. A multi-fluid slip model for swirling flow with 11 homogenous/heterogenous condensation and evaporation processes in the supersonic separator was built 12 to estimate the separation efficiency. This model solves the governing equations of compressible turbulent 13 gas phase and dispersed homogenous/heterogenous liquid phase considering droplet coalescence and 14 interphase force. Its prediction accuracy for condensation and swirling flows was validated. Then, the 15 flow field, slip velocity and droplet trajectory inside the separators with different swirl strengths were 16 investigated. The maximum values of radial slip velocity are 29.2 and 8.26 m/s for inlet foreign droplet 17 radius of 1.0 and 0.4 micron. It means the larger foreign droplet has a better condensation rate. However, 18 the residence time of larger foreign droplet in core flow is shorten. Thus, the inlet radius of foreign 19 droplet has to be moderate for best separation efficiency. Finally, the dehydration performances of 20 separator were evaluated. The optimal radius of inlet foreign droplet to maximize the dehumidification 21 and efficiency was found. For the separator with swirl strength of 22%, the optimal radius is 0.85 micron 22 at inlet pressure of 250 kPa, where the maximum dew point depression is 42.41 °C and the water removal 23 rate is 87.82%.

24

Keywords: Supersonic separator; Condensation and evaporation; Multi-fluid model; Natural gas
 dehydration; Separation efficiency

Nomencla	Nomenclature					
Α	area, m ²	$x_{\rm a}, x_{\rm r}$	axial and radial coordinates, m			
a _k	heat transfer coefficient, W $m^{\text{-}2}\ K^{\text{-}1}$	Y_k, Y_ω	the dissipations of k and ω			
$C_{\rm c}$	Cunningham slip correction factor, -	Greek				
с	sound speed, m s ⁻¹	α	volume fraction, -			
C_p	specific heat capacity, J kg ⁻¹ K ⁻¹	β	gas-liquid mass ratio, -			
Cs	species mass fraction, -	Г	specific heat ratio, -			
D_{s}	Mass diffusion coefficient, m ² s ⁻¹	γ	pressure loss ratio, -			
D_{T}	subcooling, °C	ΔT	dew point depression, °C			
D_ω	cross-diffusion term, kg m ⁻³ s ⁻²	$\delta_{ m ij}$	Kronecker delta, -			

d	throat diameter of nozzle, mm	η	water removal rate, %	
Ε	total energy, J kg ⁻¹	λ	thermal conductivity, W m ⁻¹ K ⁻¹	
$F_{\rm D}$	drag force, kg m ⁻² s ⁻²	μ	dynamic viscosity of fluid, Pa s	
f	collision frequency, Hz	ρ	density of fluid, kg m ⁻³	
G_k, G_ω	the generations of k and ω	σ	surface tension, N m ⁻¹	
$h_{ m lg}$	latent heat of water vapor, J kg ⁻¹	σ_k, σ_ω	turbulent Prandtl numbers, -	
J	homogeneous nucleation rate, m ⁻³ s ⁻¹	$ au_{ m ij}$	deviatoric stress tensor, Pa	
Κ	bulk elastic modulus, Pa	υ	single water molecule volume, m ³	
Kn	Knudsen number, -	Φ	relative humidity, $p_v/p_s(T_g) \times 100 \%$	
k	turbulence kinetic energy, J kg ⁻¹	χ	mole fraction of water vapor, -	
k _B	Boltzmann's constant. 1.38 \times 10 ⁻²³ J K ⁻¹	ψ	recovery of dry gas at the outlet	
М	dimensionless mass flow rate, -	Ω	magnitude of strain rate, s ⁻¹	
Ма	Mach number, -	ω	specific dissipation rate, s ⁻¹	
m_m	mass of water molecule, 2.99×10^{-26} kg	Subscripts		
т	liquid mass changing rate, kg m ⁻³ s ⁻¹	*	stagnation condition	
n	droplet number concentration, m ⁻³	a, r, t	axial, radial, tangential	
Pr	Prandtl number, -	c	critical	
p	pressure, Pa	d	dew point	
Q	mass flow-rate, kg s ⁻¹	eff	effective	
Re _p	Reynolds number	g	gas	
R_g	gas constant of air, J kg ⁻¹ ·K ⁻¹	het	heterogeneous	
R	specific gas constant of water vapor, J	hom	homogeneous	
n.,	kg ⁻¹ ·K ⁻¹	nom		
r	droplet radius, m	i, j, k	tensor notation	
S	swirl strength, -	k	species	
$S_{ m s}$	supersaturation of water vapor, -	l	liquid	
$S_{ m i,j}$	mean strain rate, s ⁻¹	rel	relative	
Т	fluid temperature, °C	S	saturation	
$T_{\rm R}$	reduced temperature, -	tu	turbulent	
T _r	droplet surface temperature, °C	V	water vapor	
t	time, s	Superscripts		
и	velocity of fluid, m s ⁻¹	in, out	Inlet, outlet	
Vs	interphase slip velocity, m s ⁻¹	nt	nozzle throat	
xj	Cartesian coordinates (tensors), m	dry, wet	dry and wet gas outlets	

1 **1. Introduction**

2 Natural gas as a popular and cleaner alternative to coal and other fossil fuel, plays a crucial role in 3 the next decades and reduces the carbon and other emissions leading to the long-term benefits for public 4 health and the environment [1]. However, the presence of water vapor, heavy hydrocarbons and carbon 5 dioxide (CO₂) [2] in raw natural gas causes several problems, such as reduction of heating value [3], 6 corrosion of water combined with the sour gases including CO₂ and H₂S, formation of hydrate, the 7 blockage of equipment and pipelines, and CO_2 emission [4]. Therefore, separation technology is crucial 8 for natural gas processing [5]. Several separation techniques can be utilized for the natural gas processing, 9 including adsorption, absorption, cryogenic separation, turbine expansion, and Membranes [6]. However, 10 these technologies have some disadvantages, such as complex structure, large equipment, huge 11 investment and possibility of environmental pollution.

12 The supersonic separator operated without rotating parts and chemicals is a revolutionary technique 13 for removing water vapor and heavy hydrocarbons from natural gas [7]. It also potentially uses for CO_2 14 removal in CCS (carbon capture and storage). As a simple, reliable and environmentally friendly 15 separator [8], the condensable vapor is condensed instantaneously during the gas expansion, and then 16 separated from the natural gas because of the strong centrifugal force [9]. It can prevent the hydrate 17 problem without any inhibitor and regeneration system because of the low temperature and short 18 residence time inside the supersonic separator [10]. Although many works have been done for optimizing 19 the structure and performance of supersonic separator, the actual dehydration performance is still far from 20 being satisfactory, as the flow inside supersonic separator is quite complex which includes condensation, 21 evaporation, vorticity, turbulence, shockwave and interphase slip.

The goal of supersonic separator is to remove condensable vapors from the gas flow and achieve a lower dew point or strip the gas of heavy hydrocarbons. The dew point depression and water removal rate of the supersonic separator are really desired. Currently, there are two approaches for predicting its separation performance, the computational fluid dynamics using Fluent software [4] and the process simulation conducted in Aspen HYSYS [11].

27 For process simulation, Karimi and Abdi [12] investigated the flow field of single-phase gas in a 28 Laval nozzle without swirl by using Aspen HYSYS, and found the gas could potentially be dehydrated to 29 very low water dew point. Wen et al. [13] compared the temperature and pressure profiles obtained by 30 FLUENT with phase envelope diagrams by HYSYS and found the supersonic separators is suitable for 31 liquefied natural gas. Hammer et al. [14] investigated CO2 removal of supersonic separator from dry 32 2.98% CO2 exhausts by using Aspen HYSYS. Niknam et al. [15] used Aspen HYSYS to predict the 3S 33 unit performance by conventional unit operations, then analyzed the performance of nozzle and proposed 34 an efficiency model for supersonic separation by integrating COMSOL, HYSYS and MATLAB software 35 [16]. Arinelli et al. [17] developed two steady state Unit Operation Extensions (UOE) and the vapor-liquid equilibrium (VLE) envelopes for HYSYS 8.8 to simulate supersonic separator and 36 37 membrane permeation for treating humid natural gas with 44% mol CO2. Bian et al. [18] proposed a novel 38 gas liquefaction process and the liquefaction efficiency under different condition were calculated by using

MATLAB and HYSYS. Rezakazemi et al. [19] carry out a series of process simulation by Aspen HYSYS to compare recovery of ethane from typical JT Valve, Turbo-Expander and Twister Technology . Brigagão et al. [20] developed a new CCS unit by using a supersonic separator based on HYSYS 8.8. CO2 emissions can be reduced by 43% with economic performance. de Medeiros et. al [21]-[22] proposed UOE module for estimating sound speed of two-phase systems in supersonic reactors for multiphase multi-reactive equilibrium system via HYSYS. However, it is recognized that their results were not validated against experimental data.

8 For CFD simulation, Malyshkina [23] numerically investigated the single-phase swirling flow inside 9 a supersonic separator and analyzed effects of Mach number and temperature on recovery of pressure. 10 Wen et al. [24]-[25] studied the flow characteristics and mass flux inside a supersonic separator with and 11 without swirls. Wang and Hu [26] investigate the effects of swirling generator and drainage structure 12 where the RNG k-E turbulence model was utilized. Liu [27] established a three-dimensional single-phase 13 numerical model considering the compressible and strong swirling effect to study the flow field and to 14 optimize separation performance. Alnoush and Castier [28] proposed a shortcut one-dimensional 15 single-phase numerical modeling for the conceptual preliminary design of supersonic separator.

16 On this basis, two-phase models based on the discrete particle method (DPM) were built. Wen et al. 17 [29] and Yang et al. [30] studied natural gas flow characteristics and particle separation behavior by using 18 DPM model with particle diameter constant of 1.4 micron. Liu et al. [31] also predicted the particle 19 behavior inside a supersonic separator employing the DPM model, where the particle diameter range is 20 from 10 to 50 micron, However, the typical particle size in the supersonic separator is 0.1-2 micron [32] 21 from Twister BV. Jiang [33] studied the gas flow field and CO₂ droplet trajectory inside a supersonic 22 separator employing DPM model. The size of CO₂ droplet is set to be a constant of 1.25 micron. However, 23 these researches do not consider the complex nucleation-condensation process of condensable vapor and 24 the evaporation process of droplet inside the supersonic separator.

25 Take into account the condensation process in the supersonic flow, Ma et al. [34] built an Eulerian 26 two-fluid model to investigate homogenous condensing flow in a Laval nozzle. Shooshtari and 27 Shahsavand [35] provided a new theoretical approach based on mass transfer rate to predict liquid droplet 28 growth of homogenous condensation of binary mixtures in a Laval nozzle. Ding et al. [36] proposed an 29 analytical solution to predict Wilson point of homogeneous nucleation inside the nozzle. Castier [37] 30 conducted several numerical simulations for the natural gas partial condensation inside a Laval nozzle 31 without swirl. Dykas [38]-[39] built an in-house CFD code with 3-D RANS equations for single-fluid 32 no-slip model to predict the wet steam and moist air condensation process within a Laval nozzle. Wen et 33 al. [4] developed a numerical model of homogenous nucleation to predict CO_2 condensation because of 34 condensation inside supersonic flows. The condensation model predicted 18.6% of condensed liquid 35 fraction.

Actually, raw natural gas usually contains foreign droplets before entering into the supersonic separator in practical operation and laboratory tests, and leads to the heterogeneous condensation. This process can effectively reduce the free energy barrier and promotes the condensation appearance. Ma et al. [40] experimentally investigated the effect of foreign droplets on vapor condensation by using droplet

enlargement according to heterogeneous condensation theory. Ding et al. [41] carried out a 1 2 two-dimensional multi-phase turbulence model for homogeneous/heterogeneous condensation to 3 investigate the effect of condensation on mass flow rate of Laval nozzle without swirl. Niknam et al. [42] 4 experimentally obtained dehydration of low-pressure gas in supersonic separator with heterogeneous 5 condensation of water droplets containing small foreign droplet and built a two-phase Euler-Euler model 6 in 2D asymmetric domain for analyzing the dehydration efficiency. However, they did not consider 7 homogenous nucleation process and the drag model was not provided. Shooshtari and Shahsavand [43] 8 built a heterogeneous condensation model without interphase slip for optimizing geometry of the Laval 9 nozzle which was validated by Dykas's predictions [44]. Bian et al. [45] built a physical model for 10 homogenous and heterogeneous condensations in a Laval nozzle. However, the interphase slip velocity 11 was ignored which is not suitable for the swirling flow in a supersonic separator.

12 As mentioned above, there is a lack of CFD model for accurate prediction of liquid droplets 13 trajectories inside supersonic separator with combination of swirling, nucleation, growth, evaporation, 14 slip, collision and coalescence in respect of the operation optimization of the supersonic separator. This 15 paper proposed a novel multi-fluid (slip) model for the swirling flow with the homogenous/heterogenous 16 condensation and evaporation processes in supersonic separator. The mathematical modeling and 17 performance assessment of present multi-fluid model have been conducted. It provides an effective 18 method to analyze the effects of homogeneous/heterogeneous condensation with enhanced heat transfer 19 coefficient due to strong swirl on the dehydration efficiency of supersonic separator.

20 2. Supersonic separator

In this paper, the supersonic separator is composed of a central body and some vanes were designed, as shown in Fig. 1. The annular channel between the central inner body and the shell wall forms a supersonic nozzle section, a cyclonic separation section and a diffuser with the dry and wet gas outlets [24]. The swirling flow is generated by several static vanes with specific turning angle at the subsonic section which can control the flow swirl strength.



27

- 28
- 29 Several parameters related to the separation efficiency and hydration performance were defined. The
- 30 pressure loss ratio γ is expressed as

$$\gamma = \frac{p^{\rm in} - p^{\rm out}}{p^{\rm in}} \tag{1}$$

2 where *p* is the pressure of the fluid. The superscripts in and out represent inlet and outlet conditions.

3 The recovery of dry gas at the outlet is defined as

$$\psi = \frac{Q^{\rm dry}}{Q^{\rm in}} \times 100\% = \frac{Q^{\rm in} - Q^{\rm wet}}{Q^{\rm in}} \times 100\%$$
(2)

5 where Q^{in} , Q^{dry} and Q^{wet} represent the mass flow rates at inlet, dry and wet gas outlets.

The dew point depression ΔT_d is defined as [40],

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 $\Delta T_{\rm d} = T_{\rm d}^{\rm in} - T_{\rm d}^{\rm out} \tag{3}$

8 where, *T* is gas temperature and the subscript d represents dew point. In fact, even if no separation occurs, 9 the partial pressure of water vapor and dew point at dry gas outlet will also decrease due to the gas 10 expansion. Thus, the dew point depression ΔT_d at dry gas outlet should be divided into two parts, ΔT_{d1} due 11 to expansion (without phase change) and ΔT_{d2} due to separation (with phase change), namely $\Delta T_d = \Delta T_{d1}$ 12 $+ \Delta T_{d2}$. The effective dew point depression is ΔT_{d2} due to the condensation and separation.

13 The water removal rate η_v at dry gas outlet is calculated by

$$\eta_{\rm v} = \frac{\chi_{\rm v}^{\rm in} - \chi_{\rm v}^{\rm dry}}{\chi_{\rm v}^{\rm in}} \times 100\% \tag{4}$$

15 where, χ is the mole fraction of water vapor and the subscript v represents the water vapor.

16 **3. Mathematical model**

17 3.1 Multi-fluid model for condensation-evaporation swirling flow

The multi-fluid model for condensation-evaporation swirling flow in supersonic separator was built according to the following assumptions: (i) The droplet is spherical; (ii) The released latent heat is completely absorbed by the gas phase due to the comparatively small heat capacity of droplet; (iii) both homogeneous and heterogenous condensations are considered; (iv) For the heterogenous condensation, the concentration n_{het} ⁱⁿ and radius r_{het} ⁱⁿ of the inlet foreign droplets (mainly contains water) are specified at the inlet; (v) The velocity slip between the gas and dispersed liquid phase is taken into account.

24 The mass conservation equation of the gas phase (humid gas) is expressed as

25
$$\frac{\partial \alpha_{\rm g} \rho_{\rm g}}{\partial t} + \frac{\partial}{\partial x_{\rm j}} \left(\alpha_{\rm g} \rho_{\rm g} u_{\rm gj} \right) = -\left(m_{\rm hom} + m_{\rm het} \right)$$
(5)

where the subscript g represent gas phase. α_{g} , ρ_{g} and u_{gj} are the volume fraction, density and mean velocity component of gas phase. $\alpha_{g} = 1 - \alpha_{hom} - \alpha_{het}$. The source items m_{hom} and m_{het} are liquid mass changing rates from homogenous and heterogenous condensations, respectively, kg m⁻³ s⁻¹. The momentum conservation equation of the gas phase is computed by

$$30 \qquad \frac{\partial \alpha_{g} \rho_{g} u_{gi}}{\partial t} + \frac{\partial}{\partial x_{j}} \left(\alpha_{g} \rho_{g} u_{gi} u_{gj} \right) = -\alpha_{g} \frac{\partial p}{\partial x_{i}} + \frac{\partial}{\partial x_{j}} \left[\alpha_{g} \mu_{g} \left(\frac{\partial u_{gi}}{\partial x_{i}} + \frac{\partial u_{gi}}{\partial x_{j}} - \frac{2}{3} \delta_{ij} \frac{\partial u_{gk}}{\partial x_{k}} \right) \right] + \frac{\partial}{\partial x_{j}} \left(-\alpha_{g} \rho_{g} \overline{u'_{gi} u'_{gj}} \right) - \left(m_{\text{hom}} + m_{\text{het}} \right) u_{gi} - F_{\text{Di}} (6)$$

1 where μ_{g} is the dynamic viscosity of gas phase, i, j and k are tensor notations. u'_{gi} is the fluctuating 2 component of the fluid velocity. F_{Di} is the component of drag force. δ_{ij} is the component of Kronecker 3 delta. The energy conservation equation of the gas phase is described by

$$4 \qquad \qquad \frac{\partial \alpha_{g} \rho_{g} E}{\partial t} + \frac{\partial}{\partial x_{j}} \Big[\alpha_{g} \big(\rho_{g} E + p \big) u_{gj} \Big] = \frac{\partial}{\partial x_{j}} \Big[\alpha_{g} \big(\lambda_{eff} \big) \frac{\partial T_{g}}{\partial x_{j}} + \alpha_{g} u_{gi} \big(\tau_{ij} \big)_{eff} \Big] + \big(m_{hom} + m_{het} \big) h_{lg} \qquad (7)$$

5 where the total energy is *E* and h_{lg} is the latent heat, J kg⁻¹. The effective turbulent thermal conductivity is 6 $\lambda_{eff} = \lambda_g + \frac{c_{pg}\mu_{tu}}{Pr_{tu}}$. The deviatoric stress tensor $(\tau_{ij})_{eff}$ is defined by

7
$$\left(\tau_{ij}\right)_{\rm eff} = \mu \left(\frac{\partial \bar{u}_{gj}}{\partial x_i} + \frac{\partial \bar{u}_{gi}}{\partial x_j}\right) - \frac{2}{3}\mu_{\rm eff}\frac{\partial \bar{u}_{gk}}{\partial x_k}\delta_{ij}$$
(8)

8 where the effective turbulent viscosity is $\mu_{eff} = \mu + \mu_{tu}$ and the turbulent viscosity μ_{tu} is described by

9
$$\mu_{\rm tu} = \frac{\rho_{\rm g}k}{\omega} \frac{1}{\max\left[\frac{1}{a^*}, \frac{\Omega F_2}{a_1\omega}\right]}$$
(9)

10 where k and ω are turbulence kinetic energy, J·kg⁻¹ and specific dissipation rate, s⁻¹, respectively. The 11 strain rate magnitude is $\Omega = \sqrt{2S_{i,j}S_{i,j}}$ and the component of mean strain rate $S_{i,j}$ is computed by

- 12 $S_{i,j} = \frac{1}{2} \left(\frac{\partial \bar{u}_j}{\partial x_i} + \frac{\partial \bar{u}_i}{\partial x_j} \right)$. The coefficient a^* is a low-Reynolds number correction. a_1 is a constant 0.31. F_2 is
- 13 the blending function.

19

14 The species transport equation for gas phase is expressed by

15
$$\frac{\partial}{\partial t} (\alpha_g \rho_g c_s) + \frac{\partial}{\partial x_j} (\alpha_g \rho_g u_j c_s) = \frac{\partial}{\partial x_j} \left(D_s \alpha_g \rho_g \frac{\partial c_s}{\partial x_j} \right) + S_{cs}$$
(10)

16 where c_s is the species mass fraction and D_s is mass diffusion coefficient. S_{cs} is source term in species

- 17 transport equation. If the species is water vapor, $S_{cs} = -(m_{hom} + m_{het})$.
- 18 The turbulence kinetic energy and specific dissipation rate for gas phase are expressed as:

$$\frac{\partial}{\partial t} \left(\rho_{g} k \right) + \frac{\partial}{\partial x_{j}} \left(\rho_{g} k u_{gj} \right) = \frac{\partial}{\partial x_{j}} \left[\left(\mu + \frac{\mu_{tu}}{\sigma_{k}} \right) \frac{\partial k}{\partial x_{j}} \right] + G_{k} - Y_{k}$$
$$\frac{\partial \rho_{g} \omega}{\partial t} + \frac{\partial}{\partial x_{j}} \left(\rho_{g} \omega u_{gj} \right) = \frac{\partial}{\partial x_{j}} \left[\left(\mu + \frac{\mu_{tu}}{\sigma_{\omega}} \right) \frac{\partial \omega}{\partial x_{j}} \right] + G_{\omega} - Y_{\omega} + D_{\omega}$$

(11)

where,
$$G_k$$
 and G_{ω} are the generation of k and ω . Y_k and Y_{ω} are the dissipations of k and ω . D_{ω} is
cross-diffusion term. σ_k and σ_{ω} are the turbulent Prandtl number.

22 The dispersed homogeneous and heterogeneous (foreign) droplet number concentrations n_{hom} and 23 n_{het} (m⁻³) are calculated by

24
$$\frac{\partial n_{\rm hom}}{\partial t} + \frac{\partial}{\partial x_{\rm j}} \left(n_{\rm hom} u_{\rm j, hom} \right) = J - n_{\rm het} f \tag{12}$$

$$\frac{\partial n_{\text{het}}}{\partial t} + \frac{\partial}{\partial x_{j}} \left(n_{\text{het}} u_{j,\text{het}} \right) = 0 \tag{13}$$

where, the subscripts hom and het represent homogenous and heterogenous. f is the mean collision frequency of one heterogenous droplet with others homogenous droplets. J is nucleation rate, m⁻³ s⁻¹. The homogeneous and heterogeneous volume fraction α_{hom} and α_{het} are computed as follows,

5
$$\frac{\partial \alpha_{\text{hom}} \rho_l}{\partial t} + \frac{\partial}{\partial x_j} \left(\alpha_{\text{hom}} \rho_l u_{j,\text{hom}} \right) = m_{\text{hom}} - n_{\text{het}} f \rho_l \frac{4\pi r_{\text{hom}}^3}{3}$$
(14)

$$\frac{\partial \alpha_{\rm het} \rho_l}{\partial t} + \frac{\partial}{\partial x_j} \left(\alpha_{\rm het} \rho_l u_{\rm j,het} \right) = m_{\rm het} + n_{\rm het} f \rho_l \frac{4\pi r_{\rm hom}^3}{3}$$
(15)

7 where ρ_l is density of water droplet. Thus, the effective densities of homogenous and heterogenous 8 droplet are

9
$$\rho_{\rm hom} = \alpha_{\rm hom} \rho_l, \quad \rho_{\rm het} = \alpha_{\rm het} \rho_l \tag{16}$$

10 The velocity components $u_{j,hom}$ and $u_{j,het}$ for the homogenous and heterogenous droplets in liquid 11 phases are calculated by

12
$$\frac{\partial \alpha_{\rm hom} \rho_l u_{\rm i,hom}}{\partial t} + \frac{\partial}{\partial x_j} \left(\alpha_{\rm hom} \rho_l u_{\rm i,hom} u_{\rm j,hom} \right) = m_{\rm hom} u_{\rm gi} + F_{\rm Di,hom}$$
(17)

13
$$\frac{\partial \alpha_{\rm het} \rho_l u_{\rm i,het}}{\partial t} + \frac{\partial}{\partial x_{\rm j}} \left(\alpha_{\rm het} \rho_l u_{\rm i,het} u_{\rm j,het} \right) = m_{\rm het} u_{\rm gi} + F_{\rm Di,het}$$
(18)

where, $F_{\text{Di,hom}}$ and $F_{\text{Di,het}}$ are the components of drag force between the continuous and the dispersed phases.

16 3.2 Nucleation rate and droplet growth model

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17 In this study, classical nucleation rate J (m⁻³ s⁻¹) is calculated by [46]

18
$$J = \frac{\nu \rho_s^2}{S_s} \sqrt{\frac{2\sigma}{\pi m_m^5}} \exp\left(-\frac{16\pi}{3} \frac{\nu^2 \sigma^3}{\left(k_B T_g\right)^3 \left(\ln S_s\right)^2}\right)$$
(19)

19 where, v, σ , $m_{\rm m}$ and $k_{\rm B}$ represent the volume of single water molecule (m³), liquid surface tension (N m⁻¹), 20 the mass of single water molecule (2.99×10⁻²⁶ kg), and Boltzmann's constant (1.38×10⁻²³ J K⁻¹) 21 respectively. The supersaturation of vapor is $S_s = p_v / p_s(T_g)$, where $p_s(T_g)$ is the water vapor saturation 22 pressure at temperature T_g .

23 The critical nucleation radius r_c of the droplet is described by

24
$$r_{c} = \frac{2\sigma}{\rho_{l}R_{v}T_{v}\ln(S_{s})}$$

25 where, R_v represent specific gas constant of water vapor. The mean radii r_{hom} and r_{het} are expressed as

26
$$r_{\text{hom}} = \left(\frac{3\alpha_{\text{hom}}}{4\pi n_{\text{hom}}}\right)^{\frac{1}{3}}, \quad r_{\text{het}} = \left(\frac{3\alpha_{\text{het}}}{4\pi n_{\text{het}}}\right)^{\frac{1}{3}}$$
(21)

(20)

27 Thus, the liquid mass changing rates m_{hom} and m_{het} are calculated by

28
$$m_{\rm hom} = J \rho_l \frac{4\pi r_c^3}{3} + n_{\rm hom} \rho_l 4\pi r_{\rm hom}^2 \frac{dr_{\rm hom}}{dt}, \quad m_{\rm het} = n_{\rm het} \rho_l 4\pi r_{\rm het}^2 \frac{dr_{\rm het}}{dt}$$
(22)

The growth rate of droplet (both condensation and evaporation) is expressed as

$$\frac{dr}{dt} = \frac{\sum_{k=1}^{3} a_k}{\rho_i h_{ig}} \left(T_r - T_v \right)$$
(23)

(24)

2

3 where a_k is heat transfer coefficient. The subscript k represents different species in gas phase. The droplet

4 surface temperature T_r is calculated by

5

6

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

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

7 The flow inside the supersonic separator is strongly rotational and turbulent. The centrifugal 8 acceleration can achieve $10^6 - 10^7$ m s⁻² [24]. The velocity slip between the gas and liquid phase has to be 9 taken into account, for purpose of calculating the heat transfer coefficient accurately. The heat transfer 10 coefficients a_k between the water droplet and each gas species are calculated by

11
$$a_{k} = \left(2 + 0.6 \operatorname{Re}_{p}^{0.5} \operatorname{Pr}_{g}^{0.33}\right) \frac{\lambda_{k}}{2r} \frac{1}{1 + \frac{2\sqrt{8\pi}}{1.5 \operatorname{Pr}_{k}} \times \frac{\Gamma_{k}}{1 + \Gamma_{k}} \operatorname{Kn}_{k}}$$
(25)

where Re_{p} , Γ , λ and Kn are Reynolds number, specific heat ratio, thermal conductivity and Knudsen number, respectively. For the water vapor, Kn is expressed as

14
$$\operatorname{Kn}_{v} = \frac{3\mu_{v}\sqrt{R_{v}T_{g}}}{4p_{v}r}$$
(26)

15 The relative Reynolds number Re_{p, het} is described as

16
$$\operatorname{Re}_{p, het} = 2\rho_{g}r_{het}\left|\vec{u}_{het} - \vec{u}_{g}\right| / \mu_{g} = 2\rho_{g}r_{het}\left|Vs\right| / \mu_{g}$$
(27)

17 where Vs is the slip velocity, = u_{het} - u_g . Besides, the liquid surface tension σ is calculated by [47]

18
$$\sigma = \left(85.27 + 75.612T_{\rm R} - 256.889T_{\rm R}^2 + 95.928T_{\rm R}^3\right) \times 10^{-3}$$
(28)

where, $T_{\rm R} = T_{\rm g}/T_{\rm c}$ is the reduced temperature and $T_{\rm c}$ is critical temperature (647.3 K). The dew point temperature $T_{\rm d}$ is deduced by [48]

21
$$T_{\rm d} = \begin{cases} 2663.5/(12.537 - \lg p_{\rm v}), & T_{\rm d} \le 213.65 \text{ K} \\ -60.45 + 7.0322 \ln p_{\rm v} + 0.37 (\ln p_{\rm v})^2 + 273.15, & 213.15 \text{ K} \le T_{\rm d} \le 273.15 \text{ K} \\ -35.957 - 1.8726 \ln p_{\rm v} + 1.1689 (\ln p_{\rm v})^2 + 273.15, & T_{\rm d} > 273.15 \text{ K} \end{cases}$$
(29)

22 The latent heat of vapor at the arbitrary temperature is computed by [49]

23
$$h_{\rm lg} = h_{\rm lg}^0 \left(\frac{1 - T_{\rm g} / 647.3}{1 - 0.5767} \right)^{0.38}$$
(30)

24 where the latent heat of water h_{lg} at the normal boiling point h_{lg}^{0} is 2262.2 kJ·kg⁻¹.

25 3.3 Droplet coalescence and drag model

The mean collision frequency f of one heterogeneous foreign droplet (collector) with surrounding smaller homogeneous droplets is described by (O'Rourke [50])

8

$$f = n_{\rm hom} \pi \left(r_{\rm het} + r_{\rm hom} \right)^2 u_{\rm rel} \tag{31}$$

where $u_{rel} = |u_{j,het}-u_{j,hom}|$ is relative velocity between homogeneous and heterogeneous droplets. After the collisions, these smaller homogeneous droplets are collected by heterogeneous droplet, and the heterogeneous droplet radius increases up gradually. It is necessary to consider the effect of drag force in two-phase momentum equations for the swirling flow with strong centrifugal force. For smaller Reynolds numbers, the molecular viscous force dominates [51]. Thus, according to the Stokes' law, the drag force $F_{\rm D}$ is given by [52]

$$\vec{F}_{\text{D,hom}} = \frac{9\mu_{\text{g}}}{2r_{\text{hom}}^2 C_{\text{c}}} \alpha_{\text{hom}} \left(\vec{u}_{\text{g}} - \vec{u}_{\text{hom}} \right), \quad \vec{F}_{\text{D,het}} = \frac{9\mu_{\text{g}}}{2r_{\text{het}}^2 C_{\text{c}}} \alpha_{\text{het}} \left(\vec{u}_{\text{g}} - \vec{u}_{\text{het}} \right)$$
(32)

9 where, C_c is the empirical Cunningham slip correction factor which is calculated by

10
$$C_{\rm c} = 1 + 2 {\rm Kn}_{\rm g} \left(1.257 + 0.4 e^{-1.1/(2 {\rm Kn}_{\rm g})} \right)$$
(33)

11 4. Experimental validation

12 4.1 Numerical implementation

13 All the cases were simulated by ANSYS FLUENT, while the governing equations and the source 14 terms were performed with C code by the User-Defined-Scalar (UDS) and User-Defined-Function (UDF) 15 interfaces. The density-based solver with implicit formulation and the Roe-FDS for flux type were 16 utilized for calculating governing equations of multi-fluid flows including the gas and liquid phases. The 17 second-order upwind scheme was employed for discretization. The gradients of flow variables for spatial 18 discretization were calculated by the least squares cell based gradient evaluation. For turbulence model, 19 the SST k- ω model was selected as the viscous model of gas phase. The structured quad-map meshes 20 were utilized for better convergence. For inlet boundary conditions, the total temperature and pressure of fluid were given. The static pressure was set at the outlet. The concentration n_{het} in of inlet foreign droplet 21 22 with a given radius r_{het}^{in} were specified at the inlet. The constant-temperature condition which is equal to 23 inlet gas temperature was enforced at walls. The solutions of density ρ_{g} , velocity u_{gj} , energy E, turbulence 24 kinetic energy k, specific dissipation rate ω of the gas phase, the droplet concentration $n_{\rm hom}$ and $n_{\rm het}$, the 25 liquid phase effective density ρ_{hom} and ρ_{het} , the liquid velocity $u_{j,\text{hom}}$ and $u_{j,\text{het}}$ were converged to 26 normalized residual mean square of 10⁻⁵.

27 4.2 Experimental apparatus

This study mainly focuses on simulation analysis. The experiments are necessary to verify the accuracy of multi-fluid (slip) mathematical model. Thus, an experimental apparatus including a pure air generator, humidifier and acquisition controller [53] was built, as shown in Fig. 2. The pure air (dry gas) generator is composed of a compressor, a purifier, a gasholder, a self-operated pressure regulating valve and a motorized valve with feedback adjustment for controlling the pipeline pressure (0.1-0.6 bar, 0.2%) and flowrate (0.5-100 m³/h, 0.5%). The gas temperature (30-50 °C) is controlled by a tubular pipe heater with a silicon-controlled rectifier regulator. For controlling the relative humidity (0-100 %) of the moist

1 gas, the micron droplets are generated by a high-pressure micro-fog generator, and then evaporate within 2 the evaporator to form the moist air at the upstream of the Laval nozzle and supersonic separator. A 3 Vaisala HUMICAP humidity and temperature probe HMP110 is used to measure relative humidity and 4 temperature. The light extinction method and image method are used to confirm that there is no any water 5 droplet at the inlet. Then, the experimental data of 3D supersonic nozzle and supersonic separator can be 6 used to validate the prediction accuracy of homogenous condensation in transonic flow and mass flow 7 rate in swirling flow, respectively. For 3D supersonic nozzle, the time-averaged pressure signals along the 8 axis of nozzle and the pressure fluctuation signals at a specific point near nozzle wall are measured by 12 9 pressure probes. For supersonic separator, its mass flow rate at different swirl strength are calibrated by a 10 flow standard facility.



P: Pressure sensor; T: Temperature sensor; HT: Humidity and temperature probe HMP110

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Fig. 2. The experimental apparatus for the nozzle and supersonic separator.

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14 4.3 Model validation

Because the size of nozzle of supersonic separator is small and the swirling speed is fast, it is very difficult hard to measure condensation and swirling flow inside supersonic separator experimentally. Therefore, the validation of homogenous condensation and swirling flow are also performed by using supersonic nozzle and cyclone separator. Model validation can be divided into three steps. The first step is validation of homogenous condensation in a 2D nozzle and a 3D nozzle. The second step is validation of particle behavior in cyclone separator. The third step is validation of mass flow rate of gas through the supersonic separator. The experiments for model validation are shown in Table 1.

22 23

Table 1 The experiments for model validation.

Model validation	Device	Working fluid	
Homogenous condensation in transonic flow	2D nozzle [54]	moist nitrogen	
Homogenous condensation in transome now	3D nozzle	moist air	
Particle behavior in swirling flow	Cyclone separator [55]	air	
Mass flow rate in swirling flow	Supersonic separator	air	

1 4.3.1 Condensation flow in Laval nozzle

The prediction accuracy of homogenous condensation process via the present CFD model was validated by some experiments in the Laval nozzle. The first validation was derived from Wyslouzil test [54] with a 2D nozzle where the working fluid is moist nitrogen. The length, inlet diameter and throat diameter of 2D nozzle are 133 mm, 40 mm and 12.7 mm with diffuser angle of 1.8° and the ratio of the outlet area to the throat area $A^{\text{out}}/A^{\text{nt}}$ is 1.58. The inlet stagnation pressure $p_*^{\text{in}} = 60.0$ kPa and temperature $T_*^{\text{in}} = 287$ K with water vapor partial pressure $p_v^{\text{in}} = 1.00, 0.50$ and 0.26 kPa respectively.

8 A number of mesh tests were performed to guarantee a grid-independent solution. First, the effect of 9 node numbers $(N_1 \times N_2)$ was studied. The first procedure $(N_1 \text{ fixed and } N_2 \text{ varies})$ revealed that the mass 10 flow rates with grid nodes 60×280 , 60×300 and 60×320 are 1.781, 1.768 and 1.767 kg s⁻¹ m⁻¹ where the relative errors of two adjacent cases are -0.73% and -0.056%, and the mass-weighted average 11 12 velocities at outlet are 465.379, 461.247 and 460.826 m/s where the relative errors of two adjacent cases 13 are -0.98% and -0.091%, respectively. The second procedure (N_2 fixed and N_1 varies) revealed that the mass flow rates with grid nodes 50×300 , 60×300 and 70×300 are 1.782, 1.768 and 1.765 kg s⁻¹ m⁻¹ 14 15 where the relative errors are -0.79% and -0.17%, and the mass-weighted average velocities at outlet are 16 465.213, 461.247 and 460.740 m/s where the relative errors of two adjacent cases are -0.85% and -0.11%, 17 respectively. Therefore, a grid size of 60×300 ensured a grid independent solution. The meshes near the 18 throat and boundary layer were refined for better capturing the condensation and shock phenomena in the 19 transonic flow, as show in Fig. 3 (a). It is observed that the numerical results of condensation-induced 20 pressure jumps are in well agreement with the experimental data, as show in Fig. 3 (b). The present CFD 21 model can predict 2D nonequilibrium condensation process in the transonic flow accurately.







(a) The configuration and mesh of Laval nozzle



- (b) The profiles of pressure ratio at the nozzle center downstream of nozzle throat **Fig. 3.** Comparisons of CFD results with experimental data reported by Wyslouzil.
- 3 4

5 The second validation was performed in a 3D toroidal-throat supersonic nozzle with a throat 6 diameter d of 10 mm and a curvature radius of 870 mm in our own experiment, as shown in Fig. 4. The 7 grid of 3D nozzle is axisymmetric, thus, a series of grid independence analysis revealed that a grid size of 8 50×260 ensured a grid independent solution. The working fluid is moist air. In all cases, the inlet total 9 pressure is 300 kPa and the static pressure at the outlet is 1 atm. The outlet static temperature is equal to 10 the inlet value. The pressure profiles near the nozzle wall with different inlet relative humidity Φ^{in} and 11 temperature T_*^{in} are shown in Fig. 5(a) and Fig. 5(b), respectively. It also indicates that CFD data are well 12 consistent with experimental results. The pressure jump due to released latent heat inside the 3D 13 supersonic nozzle was captured accurately.





Fig. 4. The configuration of 3D toroidal-throat supersonic nozzle





1 4.3.2 Particle behavior in the cyclone separators

2 To evaluate the simulation results of swirling flow by the present model, an experiment of a cyclone 3 separator reported by Wang [55] was utilized. The configuration of the cyclone separator is shown in Fig. 6. A series of grid independence analysis revealed that the grid numbers of 53,468 ensured a grid 4 independent solution. The working fluid is dry air where $\Phi_*^{in} = 0$ %. The pressure at the top of vortex 5 finder near the exit tube is 1 atm. The inlet velocity is 20 m s⁻¹. The solid particle material was a typical 6 7 cement raw material with a concentration of 1%. The solid particle is equivalent to the inlet 8 heterogeneous droplet of multi-fluid model without condensation. A comparison of the tangential velocity 9 of gas flow field between the simulation and experiment is plotted in Fig. 7. A comparison of collection 10 efficiency of particles between the simulation and experiment is plotted in Fig. 8. The simulation values agree well with the experimental data which indicates that the present model can predict behavior of 11 12 particles in swirling flow very well.



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Fig. 6. Configuration of the cyclone separator (Unit: mm).





Fig. 7. Tangential velocity in a cyclone separator.





5 6

Fig. 8. Comparisons of collection efficiency between CFD results with experiment.

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4.3.3 Mass flow rate in supersonic separator

8 The effects of swirl strength on the mass flow rate within a supersonic separator were also validated. 9 The experimental data was derived from our experiment. The separator is 528 mm long, and has 70 10 mm/80 mm and 40 mm wall diameters at inlet and outlet. The diameters of the central body and the shell 11 wall at the throat are 14 mm and 20 mm, respectively. The drainage gap size is about 2.0 mm. The only 12 difference between supersonic separator A and B is the inlet diameter, separator A is 80 mm and separator 1 B is 70 mm.

2 The configuration and structured mesh of the supersonic separator A whose nominal swirl strength is 3 20% and the recovery of dry gas outlet is 0.72, are plotted in Fig. 9. A series of grid independence 4 analysis revealed that the numbers of hexahedral meshes 576,300 ensured a grid independent solution. 5 Besides, nominal swirl strength of supersonic separator B is 50%. The comparison of mass flow rates 6 between simulation and experiment is shown in Fig. 10. The swirl strength S is defined as the ratio of the 7 tangential velocity u_t to the axial velocity u_a (~ 318 m/s) at the throat. The dimensionless mass flow rate 8 M is normalized by the mass flow rate with no swirling flow. It is found that the maximum error is about 9 2.7 % at the swirl strength of 93.4 %. It indicates that the proposed model predicts the strongly swirling 10 supersonic flow accurately.







11 12

Fig. 10. The swirl strength effect on mass flow rate in the supersonic separator.

15 16

1 5. Results and discussion

Firstly, the detailed predictions for the gas and liquid (droplet) phases behaviors, especially for interphase velocity slip and liquid phase distribution are illustrated. Then, the results of dehydration performance (dew point depression ΔT_d and water removal rate η_v) of the supersonic separator at various conditions, i.e., total pressure, radius and concentration of inlet foreign droplet, and swirl strength were obtained.

7 5.1 Flow field, interphase slip and droplet behavior

Four cases were utilized to analyze the gas flow field, interphase slip and droplet behavior. The common conditions are $T_*^{in} = 30$ °C, $\Phi_*^{in} = 100\%$ ($p_v^{in} = 4246$ Pa), $p^{out} = 100$ kPa, $\rho_{het}^{in} = 0.01$ kg m⁻³ (volume fraction $\alpha_{het}^{in} \approx 1 \times 10^{-5}$). The differences among these cases are as follows, Case 1-Case 3: $p_*^{in} =$ 167, 200 and 250kPa ($\gamma = 0.4$ -0.6) with the same $r_{het}^{in} = 1.0 \ \mu m$ and $n_{het}^{in} = 2.39 \times 10^{12} \ m^{-3}$. Case 4: $r_{het}^{in} =$ 0.4 μm with $p_*^{in} = 250$ kPa ($\gamma = 0.6$), and $n_{het}^{in} = 3.74 \times 10^{13} \ m^{-3}$. If not specified, the supersonic separator A with nominal swirl strength S = 20% is assigned by default.

14 5.1.1 Shock wave and swirl strength

15 The sound speed in air-water two-phase mixture fluid can be calculated by (Wood' law [56])

$$c_{gl} = \sqrt{\frac{1}{\left(\alpha_g K_g^{-1} + \alpha_l K_l^{-1}\right)\left(\rho_g \alpha_g + \rho_l \alpha_l\right)}}$$
(34)

17 Where, α_g is volume fraction of gas, and $\alpha_l = 1 - \alpha_g$ is volume fraction of liquid, *K* is bulk elastic modulus.

18 For liquid water, $K_l = 2.19 \times 10^4$ Pa. For ideal air gas, $K_g = 1.4 p_g$.

19 Another model proposed by Kieffer [57] is as follows

$$20 c_{gl} = \left(\beta \rho_{l,ref} \left(\frac{G_{g,ref}}{p}\right)^{1/\Gamma} + \exp\left(\frac{p_{ref} - p}{K_l}\right)\right) \left\{ \left[\left(1 + \beta\right) \rho_{l,ref} \right]^{1/2} \left[\frac{\beta \rho_{l,ref} G_{g,ref}^{-1/\Gamma}}{\Gamma p^{(1+\Gamma)/\Gamma}} + \frac{1}{K_l} \exp\left(\frac{p_{ref} - p}{K_l}\right) \right]^{1/2} \right\}^{-1} (35)$$

21 Where β is gas-liquid mass ratio. $G_{g,ref} = T_{ref} R_g / \rho_{ref}^{\Gamma-1}$. $\rho_{l,ref}$ and p_{ref} are chosen as 1000 kg/m³ and 1 bar.

It is found that the results of Eq. (34) and Eq. (35) are almost same. However, it should be noticed that two-phase sound speed c_{gl} is sensitive to pressure. For case of $p_*^{in} = 167$ kPa, the minimum pressure inside supersonic separator is 56.098 kPa with $T_g = 290.67$ K. if $\alpha_l = 6.5 \times 10^{-5}$, it shows $c_g = 341.78$ m s⁻¹ and $c_{gl} = 326.72$ m s⁻¹ where the error between them is 4.4 %. Thus, two-phase Mach number should be utilized to calculate Mach number, i.e. $Ma = u/c_{gl}$.

The Mach number contours for Case 1 and Case 3 inside the supersonic separator A are plotted in Fig. 11. It illustrates the complexity of shock wave, especially near the drainage channel. For Case 1 with smaller pressure loss ($\gamma = 0.4$) as shown in Fig. 11 (a), the maximum Mach number upstream of the shock is 1.239 at axial position $x_a = 91$ mm, where the maximum subcooling D_T is 25.84 °C.

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6 7

(b) Case 3: $p_*^{in} = 250$ kPa ($\gamma = 0.6$) **Fig. 11.** The Mach number contours of the gas phase inside the supersonic separator.

8 On the other hand, when the inlet pressure increases up to 250 kPa, the shock wave will move 9 downstream and reach the gas-liquid separation point with the maximum Mach number of 1.765 and 10 subcooling $D_{\rm T}$ of 48.76 °C, as plotted in Fig. 11 (b). The fluid inside the drainage channel instantaneously 11 reduces to subsonic speed, while the central fluid keeps supersonic and then a secondary shock occurs at 12 the dry gas outlet channel. This complex shock is called lambda shock-system accompanying irreversible 13 entropy production and loss of exergy [58].

14 The tangential velocity and swirl strength dominate the slip velocity and separation efficiency. 15 However, the strong swirl strength decreases Mach number and increases the static temperature inside the 16 Laval nozzle, damaging the expansion characteristics of the nozzle [24]. Fig. 12 (a) and (b) show the 17 tangential velocities and streamlines of the gas phase for Case 3 in supersonic separators A and B. Fig. 12 18 (a) illustrates that the maximum tangential velocity in the separator A is $u_t = 67.7$ m s⁻¹ and the maximum centrifugal acceleration is 8.70×10^5 m s⁻² with swirl strength of 22%. In Fig. 12 (b), the maximum 19 20 tangential velocity in the separator B reaches 136.1 m s⁻¹ and the corresponding centrifugal acceleration is 3.5×106 m s⁻² where the swirl strength achieves 45%. Then, the water vapor will be condensed and 21







(b) Separator B: maximum tangential velocity is $u_t = 136.1 \text{ m s}^{-1}$.

Fig. 12. Tangential velocities and streamlines of the gas phase for Case 3 in separators A and B.

7 5.1.2 Condensation and evaporation zones

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As we know, the water vapor will condense in the supersaturated region and the droplets will evaporate in the unsaturated region. As previously mentioned, both dry gas outlet and wet gas outlet are 10 100 kPa for Case 1 and Case 3. The heterogenous condensation is dominant and the homogenous 11 condensation can be ignored in these two cases.

The contour of the liquid mass changing rate m_{het} for Case 1 when $p_*^{in} = 167$ kPa is plotted as Fig. 13 (a). It reveals that both condensation and evaporation processes occur inside the separator. The global range of the liquid mass changing rate m_{het} is from -402.3 to 712.1 kg m⁻³ s⁻¹. According to Fig. 11 (a), the shock occurs at axial position $x_a = 91$ mm which coincides with the evaporation onset. This is because the fluid velocity begins to slow down and the static temperature recovers to high value downstream of shock wave, and then droplets evaporate into the gas phase gradually.





Fig. 13. The contours of the liquid mass changing rate m_{het} in the condensation and evaporation zones.

5 When the inlet pressure increases to 250 kPa, the rates of both condensation and evaporation are 6 bigger. The global range of liquid mass changing rate m_{het} is from -936.7 to 958.3 kg m⁻³ s⁻¹ (maximum 7 latent heat release rate is 2.51×10^9 J m⁻³ s⁻¹). The liquid mass changing rate at the near wall cells are 8 shown in Fig. 13 (b). It is found that the evaporation process occurs in two parts, the near-wall heating 9 zone and pressure recovery zone.

For the purpose of demonstrating the condensation and evaporation processes, the distributions of the droplet radius and the vapor mass fraction along the axial direction are plotted in Fig. 14 and Fig. 15. The radial positions x_r of Line 1-Line 3 are 7 mm, 8 mm and 9 mm, respectively. Fig. 14 shows radius distributions of heterogenous droplet along Line 2 at different total pressures when inlet foreign droplets $r_{het}^{in} = 1.0 \ \mu m$, and $\rho_{het}^{in} = 0.01 \ \text{kg m}^{-3}$.





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Fig. 14. The axial distributions of the droplet radius at Line 2 for Case 1, Case 2 and Case 3.

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18 It indicates that the heterogenous droplet size starts growing rapidly at the throat. Along with the

1 increasing of heterogenous droplet size, its changing rate becomes smaller. The heterogenous droplet size 2 will reach a maximum at the location of shock wave, and then begin to decrease due to the evaporation. 3 The heterogenous droplet size grows to 1.44, 1.83 and 2.26 μ m at x_a = 91.35, 174.50 and 227.40 mm for 4 $p_*^{in} = 167, 200$ and 250 kPa.

5 The mass fraction of the water vapor in the gas phase also can reflect the changes of condensation 6 and evaporation. Fig. 15 shows the results of mass fraction of water vapor for Case 3 with $r_{het}{}^{in} = 1.0 \ \mu m$ 7 and Case 4 with $r_{het}{}^{in} = 0.4 \ \mu m$. It is found that the mass fraction of water vapor at entrance of drainage 8 will increase with the decrease of the inlet foreign droplet size, which means the smaller inlet foreign 9 droplet radius $r_{het}{}^{in}$ is, the worse dehydration performance is. The differences of performance are 10 attributed to the interphase velocity slip and the uneven distribution of liquid phase.

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Fig. 15. The axial distributions of the mass fraction of water vapor for Case 3 and Case 4.

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15 5.1.3 Slip velocity and Liquid phase distribution

The slip velocity and drag force play a critical role in controlling the trajectory of droplet which can determine the separation performance in the cyclone section. As the main factor, the effect of inlet foreign droplet radius on the slip velocity distribution is discussed firstly.

The axial and radial components of slip velocity at different locations of Case 3 and Case 4 are shown in Fig. 16. As shown in Fig. 16 (a), the magnitude of axial component of slip velocity decreases gradually along the flow direction where the maximum velocity lag of the droplet for $x_a = 90$, 140, and 190 mm is 48.2, 33.9 and 24.3 m s⁻¹ as the result of the drag force. Besides, the axial slip velocity along the radial direction is from zero (central inner body) to a negative minimum to zero again and then to positive maximum at the shell wall. Comparing Fig. 16 (a) and (c), it indicates that the bigger inlet droplet diameter is, the bigger droplet inertia is, and the larger slip speed will be. Fig. 16 (b) and (d) show the radial component of slip velocity at different locations. As we know, the radial slip speed causes the droplets to separate from primary gas fluid. It is obvious that the axial velocity of centrifugal droplet is larger than local velocity of gas phase. The maximum radial slip speed is 29.2 m s⁻¹ for Case 3 and 8.26 m s⁻¹ for Case 4.







(c) Axial component of slip velocity for Case 4

 $x_{\rm r}$ (mm)



 $x_{\rm r}$ (mm)

 1 The distribution of liquid phase in the centrifugal field was analyzed. At first, the solution accuracy 2 of the two-phase mass transfer was checked. Taking the results of Case 3 as example, the flow rate of 3 inlet foreign droplets is $Q_{het}^{in} = 2.75 \times 10^{-4} \text{ kg s}^{-1}$. For the single-fluid model, inlet total mass flow rate of 4 gas phase is $Q_g^{in} = 7.83 \times 10^{-2}$ kg s⁻¹, thus inlet mass flow rate of water vapor is $Q_v^{in} = 8.32 \times 10^{-4}$ kg s⁻¹ because inlet mass fraction of water vapor is $c_{s,v}$ =1.063×10⁻². The outlet flow rate of water contains 5 three parts, Q_{het}^{out} of heterogeneous droplets, Q_{hom}^{out} of homogeneous droplets and Q_v^{out} of vapor, where 6 7 $Q_{\text{het}}^{\text{out}} = 3.40 \times 10^{-4} \text{ kg s}^{-1}$, $Q_{\text{hom}}^{\text{out}} = 7.51 \times 10^{-4} \text{ kg s}^{-1}$ and $Q_{\text{v}}^{\text{out}} = 2.4 \times 10^{-5} \text{ kg s}^{-1}$ at the gas-liquid separation 8 section ($x_a = 240$ mm). The calculation error of total mass of water between the inlet and outlet is 0.72%. On the other hand, For the multi-fluid model, $Q_g^{in} = 7.45 \times 10^{-2} \text{ kg s}^{-1}$ and $Q_v^{in} = 7.92 \times 10^{-4} \text{ kg s}^{-1}$ at the 9 inlet. The flow rates $Q_{het}^{out} = 9.75 \times 10^{-4} \text{ kg s}^{-1}$, $Q_{hom}^{out} = 3.70 \times 10^{-8} \text{ kg s}^{-1}$ and $Q_v^{out} = 1.01 \times 10^{-4} \text{ kg s}^{-1}$ at the 10 outlet. The calculation error is 0.99 %. The results show a favorable prediction accuracy for two-phase 11 12 mass transfer.

13 The streamline and effective density of heterogeneous droplets for Case 3 with $r_{\rm het}{}^{\rm in} = 1.0 \ \mu {\rm m}$ by 14 using both single-fluid and multi-fluid models are shown in Fig. 17. In single-fluid model, no-slip fluid 15 velocity condition is assumed, thus the streamline of liquid phase goes around a circle at the cyclone as 16 shown in Fig. 17 (a) and the effective density of heterogeneous droplet is almost uniform. Due to no slip 17 in single-fluid model, the value of heat transfer coefficient of Eq. (25) is smaller than that of multi-fluid model. The droplet number of heterogenous droplet ($n_{het}^{in} = 2.39 \times 10^{12} \text{ m}^{-3}$ in this case) is not usually 18 19 enough to prevent the homogenous nucleation in single-fluid model. The percentages of heterogenous and 20 homogenous condensations are 8% and 90%. When switching to the multi-fluid slip model, the 21 streamline at the cyclone section is centrifugal motion as shown in Fig. 17 (b). The heat transfer 22 coefficient around the heterogenous droplet sharply increases as a result of the interphase slip velocity. In 23 this situation, the homogeneous condensation almost disappears. The effective density of heterogeneous 24 droplet near the shell wall increase sharply due to the centrifugal force leading to the achievement of the 25 separation performance.





(a) Single-fluid (no-slip) model (8% heterogenous +90% homogeneous condensations at $x_a = 240$ mm)





16 5.2 Dehydration performance

17 The results of the dehydration performance of supersonic separator at different inlet conditions, 18 when $T_*^{in} = 30$ °C, $\Phi_*^{in} = 100\%$ ($p_v^{in} = 4246$ Pa) and $p^{out} = 100$ kPa, are shown in Table 2-Table 4. The 19 variable p_v^{dry} is water vapor partial pressure at the dry gas outlet where the droplets evaporate again. T_d^{dry} 20 and ΔT_d^{dry} represent the dew point and the dew point depression at the dry gas outlet.

21 22

Table 2 Dehydration performance of supersonic separator A with different r_{het}^{in} and ρ_{het}^{in} of inlet foreign droplets when $p_*^{in} = 250$ kPa ($\gamma = 0.6$).

$r_{\rm het}^{\rm in}$ [µm]	$ ho_{\rm het}^{\rm in}$ [kg m ⁻³]	$n_{\rm het}^{\rm in}$ [m ⁻³]	$p_{\rm v}^{\rm dry}$ [Pa]	$T_{\rm d}^{\rm dry} [^{\circ}{\rm C}]$	$\Delta T_{\rm d}^{\rm dry} [^{\circ}{ m C}]$	$\eta_{ m v}$
1.0	0.04	9.57×10 ¹²	86.65	-21.71	51.71	94.90%
1.0	0.02	4.78×10^{12}	130.62	-17.40	47.40	92.31%

	0.01	2.39×10 ¹²	225.68	-11.48	41.48	86.71%
	0.005	1.20×10^{12}	348.99	-6.59	36.59	79.45%
	0.002	4.78×10^{11}	736.66	2.63	27.37	56.63%
	0.001	2.39×10 ¹¹	1197.13	9.49	20.51	29.53%
	0.0005	1.20×10^{11}	1532.67	13.19	16.81	9.77%
2.0		2.99×10 ¹¹	1319.60	10.93	19.07	22.32%
0.5		1.91×10^{13}	331.90	-7.16	37.16	80.46%
0.4	0.01	3.74×10^{13}	726.40	2.44	27.56	57.24%
0.3	0.01	8.86×10 ¹³	1418.75	12.02	17.98	16.48%
0.25		1.53×10^{14}	1750.03	15.24	14.76	-3.02%
0.2		2.99×10^{14}	1999.98	17.34	12.66	-17.74%

3

Table 3 Dehydration performance of supersonic separator A with different r_{het}^{in} and ρ_{het}^{in} of inlet foreign droplets when $p_*^{in} = 167$ kPa ($\gamma = 0.4$).

				u () 011)1		
$r_{\rm het}^{\rm in}$ [µm]	$ ho_{ m het}^{ m in}$ [kg m ⁻³]	$n_{\rm het}^{\rm in}$ [m ⁻³]	$p_{\rm v}^{\rm dry}$ [Pa]	$T_{\rm d}^{\rm dry} [^{\circ}{\rm C}]$	$\Delta T_{\rm d}^{\rm dry} [^{\circ}{ m C}]$	$\eta_{ m v}$ [%]
	0.04	9.57×10 ¹²	2059.43	17.80	12.19	19.05%
	0.02	4.78×10^{12}	1571.55	13.58	16.42	38.20%
	0.01	2.39×10^{12}	1446.73	12.32	17.68	43.11%
1.0	0.005	1.20×10^{12}	1483.44	12.69	17.31	41.66%
	0.002	4.78×10^{11}	1694.78	14.74	15.26	33.35%
	0.001	2.39×10 ¹¹	2113.84	18.22	11.78	16.87%
	0.0005	1.20×10^{11}	2387.42	20.19	9.80	6.13%
2.0		2.99×10 ¹¹	2027.67	17.56	12.44	20.26%
1.5		7.09×10^{11}	1539.66	13.26	16.74	39.45%
0.75	0.01	5.67×10^{12}	1831.56	15.95	14.05	27.97%
0.5	0.01	1.91×10^{13}	2241.32	19.17	10.83	11.86%
0.3		8.86×10^{13}	2984.91	23.89	6.10	-17.43%
0.2		2.99×10 ¹⁴	3368.58	25.95	4.05	-32.47%

4

Fig. 19 shows the curves of the dew point depression ΔT_d^{dry} versus inlet foreign droplet size r_{het}^{in} when $p_*^{in} = 167$ and 250 kPa, where ΔT_{d1}^{dry} due to expansion at dry gas outlet are 8.77 and 15.22 °C, respectively. It is observed that there is an optimal radius of inlet foreign droplets to maximize the dehumidification and efficiency of the device. For $p_*^{in} = 250$ kPa, the maximum of ΔT_d^{dry} is 42.41°C ($\eta_v =$ 87.82%) at the optimal radius r_{het}^{in} of 0.85 micron, while for $p_*^{in} = 167$ kPa, the maximum of ΔT_d^{dry} is 17.52°C ($\eta_v = 42.50\%$) at the optimal radius r_{het}^{in} of 1.25 micron. The residence time of droplet is the main factor leading to above result which was explained clearly in Fig. 17 (b) and Fig. 18.



1 2

Fig. 19. The dew point depression ΔT_d versus inlet foreign droplet size r_{het}^{in} when $p_*^{in} = 167$ and 250 kPa.

In addition, as shown in Table 2-Table 3 and Fig. 19, when the inlet foreign droplet size is less than a critical size, the dew point depression ΔT_d^{dry} will be smaller than ΔT_{d1}^{dry} where the water removal rate η_v is negative, the separator would be ineffective. The critical sizes of r_{het}^{in} are 0.26 micron and 0.45 micron for $p_*^{in} = 250$ and 167 kPa, respectively. When the inlet foreign droplet size continues to decrease, it will begin to evaporate into the gas phase instead of condensing, thus the water vapor partial pressure at the dry gas outlet increases and the removal rate η_v is negative, resulting in the failure of separation.

The values of dew point depression ΔT_d^{dry} at different inlet effective densities ρ_{het}^{in} are shown in Fig. 10 11 20. It is found that the curve is monotonically increasing with the ρ_{het}^{in} for $p_*^{in} = 250$ kPa, where the shock 12 wave is near the entrance of drainage as shown in Fig. 11 (b) and the evaporation is weak. On the other 13 hand, the curve has a maximum ΔT_d^{dry} at the optimal effective density of 0.008 kg m⁻³ for $p_*^{in} = 167$ kPa. 14 In this situation, the evaporation zone is quite long at the downstream of the shock shown in Fig. 11 (a) 15 and Fig. 13 (a). Although the water vapor is condensed completely at the condensation zone, it re-evaporates again after the shock. When $\rho_{\text{het}}^{\text{in}}$ is larger than the optimal value, the amount of 16 condensation remains the same but the evaporation increases gradually with the increase of $\rho_{\rm het}^{\rm in}$, 17 18 resulting in the reduction of the dehydration performance.





Fig. 20. The dew point depression ΔT_d versus effective density $\rho_{\text{het}}^{\text{in}}$ of inlet foreign droplets when $p^{*\text{in}} = 167$ and 250 kPa.





Fig. 19 and Fig. 20 also illustrate the supersonic separator will provide better dehydration performance if the pressure loss ratio increases. The dew point depression ΔT_d versus the pressure loss ratio γ is plotted in Fig. 21. The original data of Fig. 21 is also listed in Table 4. It reveals that the dew point depression ΔT_d^{dry} increases from 6.91 °C ($\eta_v = 16.23\%$) to 52.04 °C ($\eta_v = 93.42\%$) when the pressure loss ratio increases up to 0.7. The larger the pressure loss ratio inputs, the higher the separation efficiency will be. However, high pressure loss ratio means high energy consumption.

7 8

9

Table 4 Dehydration performance of supersonic separator A with different pressure loss ratio γ when $r_{\text{het}}^{\text{in}} = 1.0 \,\mu\text{m}$ and $\rho_{\text{het}}^{\text{in}} = 0.01 \,\text{kg m}^{-3} \,(n_{\text{het}}^{\text{in}} = 2.39 \times 10^{12} \,\text{m}^{-3}).$

	-		. .			
γ[-]	p_*^{in} [kPa]	$p_{\rm v}^{\rm dry}$ [Pa]	$T_{\rm d}^{\rm dry} [^{\circ}{\rm C}]$	$\Delta T_{\rm d}^{\rm dry}$ [°C]	ΔT_{d1}^{dry} [°C]	$\eta_{ m v}$ [%]
0.7	333	83.85	-22.04	52.04	19.58	93.42%
0.6	250	225.64	-11.48	41.48	15.22	86.71%
0.5	200	538.01	-1.60	31.60	11.70	74.66%
0.4	167	1449.39	12.32	17.68	8.77	43.11%
0.3	133	2285.62	19.48	10.52	6.19	23.10%
0.2	125	2845.51	23.09	6.91	3.91	16.23%

10

Besides, the effect of swirl strength on the separation efficiency was also investigated. The dehydration performance of supersonic separator B with 45% swirl strength is shown in Table 5. The optimal size of inlet foreign droplets for heterogenous condensation is 0.28 micron. Compared with the results of separator A with 22% swirl strength in Table 2, it is found that the optimal radius of inlet foreign droplets will be smaller when the separator has a stronger swirl strength. These results are helpful for designing the separator structure and optimizing the separation performance.

17

18 19

Table 5 Dehydration performance of supersonic separator B with different r_{het}^{in} of inlet foreign droplets when $\rho_{het}^{in} = 0.01$ kg m⁻³ and $p_*^{in} = 250$ kPa ($\gamma = 0.6$).

in []	in [3]	dry [D -]			
$r_{\rm het}$ [µm]	$n_{\rm het}$ [m ⁻]	p_{v} [Pa]	$I_{d}^{aay} [^{\circ}C]$	$\Delta I_{\rm d}^{\rm uny}$ [°C]	$\eta_{ m v}$
1.0	2.39×10^{12}	1619.10	14.03	15.97	4.68%
0.75	5.67×10^{12}	1075.83	7.93	22.07	36.67%
0.5	1.91×10^{13}	542.49	-1.57	31.57	68.06%
0.4	3.74×10 ¹³	275.71	-9.25	39.25	83.77%
0.3	8.86×10 ¹³	103.48	-19.86	49.86	93.91%
0.25	1.53×10^{14}	116.45	-18.65	48.65	93.14%
0.2	2.99×1014	370.46	-5.91	35.91	78.19%
0.15	7.01×10^{14}	1045.34	7.52	22.48	38.46%
0.1	2.39E×1015	1685.87	14.66	15.34	0.75%

20

21 6. Conclusion

A novel multi-fluid model with the droplet coalescence and the interphase force for the homogenous/heterogenous condensation and evaporation processes in supersonic separator was built to evaluate the dehydration performance. The flow field, slip velocity profile, droplet trajectory and liquid
 phase distribution with different pressure loss ratios, the radii and concentrations of inlet foreign droplets
 were analyzed. The dehydration performances were also investigated further. The conclusions are as
 follows:

- 5 (1) The complex lambda shock-system with maximum Mach number of 1.765 and subcooling of
 6 48.76 °C was observed in the cyclone section, where the maximum tangential velocity was
 7 136.1 m s⁻¹ and the corresponding centrifugal acceleration was 3.5×10⁶ m s⁻².
- 8 (2) The condensation begins to occur at the throat, while the evaporation appears at the near-wall 9 heating and pressure recovery zones. The liquid mass changing rate m_{het} ranges from -936.7 to 10 958.3 kg m⁻³ s⁻¹ with latent heat release rate of 2.51×10^9 J m⁻³ s⁻¹. When $r_{het}{}^{in} = 1.0$ µm, and 11 $\rho_{het}{}^{in} = 0.01$ kg m⁻³, the heterogenous droplet size grows to 1.44, 1.83 and 2.26 micron for $p_*{}^{in} =$ 12 167, 200 and 250 kPa.
- 13 (3) The magnitude of axial component of slip velocity decreases gradually along the flow direction 14 where maximum velocity lag of the droplet is 48.2 m s⁻¹ for $r_{het}^{in} = 1.0 \mu m$. The maximum 15 values of radial slip velocity are 29.2 m s⁻¹ for $r_{het}^{in} = 1.0 \mu m$ and 8.26 m s⁻¹ for $r_{het}^{in} = 0.4 \mu m$, 16 respectively. It is indicated that the larger foreign droplet will grow faster due to the enhanced 17 heat transfer coefficient.
- (4) However, large droplet will deflect faster resulting in a shorter residence time and failure of
 separation. Thus, the inlet foreign droplet radius should be moderate for the best performance.
- 20 (5) There is an optimal size of inlet foreign droplet to maximize dehumidification and efficiency. 21 When $p_*^{in} = 250$ kPa and $\rho_{het}^{in} = 0.01$ kg m⁻³, the optimal radii of inlet foreign droplet are 0.85 22 and 0.28 micron in two different separators, in which the maximum dew point depression 23 ΔT_d^{dry} is 42.41 °C and water removal rate η_v is 87.82% in separator A while maximum $\Delta T_d^{dry} =$ 24 48.65 °C and $\eta_v = 93.91\%$ are valid for separator B.
- This study provides an insight into dehydration performance of the supersonic separator considering the condensation, evaporation and interphase force. For future work, it is important to optimize the structure of supersonic separator by using present model and investigate experimentally the water separation efficiency of supersonic separator via heterogeneous condensation.
- 29 **Conflict of interest**
- 30 The authors declared that there is no conflict of interest.

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