NUMERICAL SIMULATION OF PARTICLE FLOW IN A NATURAL GAS SUPERSONIC SEPARATOR

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ABSTRACT

The supersonic separator is a new device which can be used to condense and separate water and heavy hydrocarbons from natural gas. The particle flow, representing the motion of condensed liquid droplets, in a supersonic separator was numerically calculated using the Discrete Particle Method (DPM) with the Reynolds stress model (RSM) being used to capture the strong swirling flow of the natural gas. The results showed that most of the particles either collided with the walls or entered into the liquid-collection space directly, while only a few particles escaped together with the gas from the gas outlet. The effect of the particle diameter on the collection efficiency was obtained in the newly designed supersonic separator. The separation efficiency could be over 70% when the droplet diameter was more than 2μm, demonstrating a good performance of the newly designed separator.

NOMENCLATURE

Cc	Cunningham correction coefficient
C_D	drag coefficient.
C_m	constant
C_s	constant
C_t	constant
d_{ij}	deformation tensor
d_l	particle diameter
$D_{T_{s,l}}$	thermophoretic force coefficient
E	total energy
F	gas-particle interaction force
F_a	additional force
F_d	drag force
F_s	Saffman's lift force
F_t	thermophoretic force
g	acceleration of gravity
K	conductivity ratio
K_n	Knudsen number
K_s	constant
l	liquid phase
m_l	particle mass
p	pressure
q_j	heat flux
Re	relative Reynolds number
t	time
T_g	local temperature
u_g	gas velocity
u_l	particle velocity
V_l	particle volume
δ_{ij}	Kronecker delta
λ	molecular mean free path
μ_g	gas viscosity
μ_l	liquid viscosity
v_g	gas dynamic viscosity
ρ_g	gas density
ρ_l	particle density
τ_{ij}	viscous stress

INTRODUCTION

Supersonic gas separation is a novel technology, which has been used to remove the water vapor and higher hydrocarbons from natural gas (Okimoto and Brouwer, 2002; Alferov et al., 2005; Brouwer et al., 2004; Schinkelshoek and Epsom, 2006; Betting and Epsom, 2007; Kalikmanov et al., 2007; Wen et al., 2011a). A supersonic separator is usually composed of a Laval nozzle, a swirl device and a diffuser, as shown in Figure 1 (Wen et al, 2012a). The Laval nozzle is used to accelerate the natural gas to the supersonic velocity, resulting in a low pressure and temperature. The swirl device is employed to generate a strong swirling flow to separate and remove the condensed liquids from the gas-liquid mixture. The diffuser is designed for the purpose of the pressure recovery.

The computational fluid dynamics (CFD) modelling has been employed to study the flow behavior in a supersonic separator. Malyshkina (2008, 2010) obtained the distribution of gas dynamic parameters through a supersonic separator with a computational method, and a procedure was developed to predict the separation capability of water vapor and higher hydrocarbons from natural gas by using a supersonic separator determined by the initial parameters. Karimi and Abdi (2009) predicted the effect of the dynamic parameters of the nozzle entrance and exit on the selective dehydration of high-pressure natural gas by using the MATLAB and HYSYS packages. The generalized radial basis function artificial neural networks were used to optimize the geometry of a supersonic separator by Vaziri and Shahsavand (2013). Shooshtari and Shahsavand developed a new theoretical approach based on mass transfer rates to calculate the liquid droplet growth in supersonic conditions for binary mixtures (2013). In our previous studies, a new supersonic nozzle was designed incorporating a central body and the
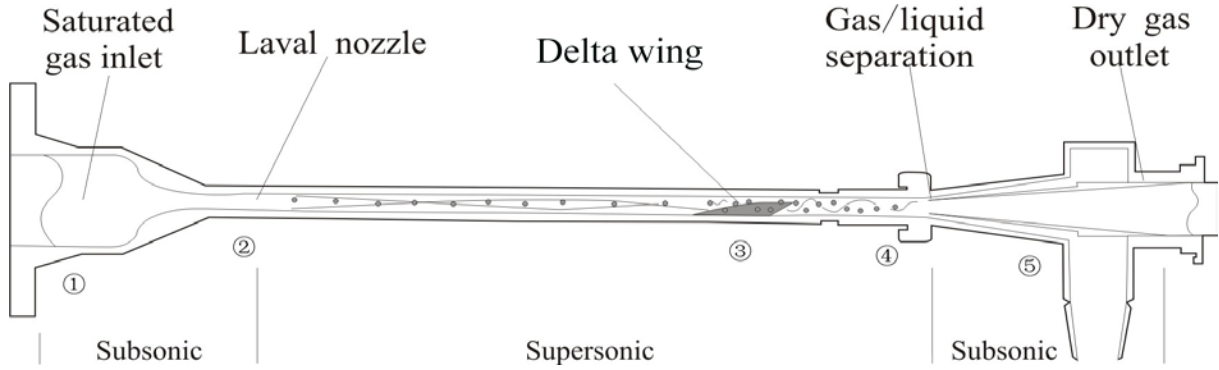
Figure 1: Schematic diagram of a supersonic separator (Wen et al, 2012a).

effect of the nozzle geometric structure on the separation characteristics was analyzed by the numerical simulation (Wen et al., 2011b). A new swirling device composed of some vanes and an ellipsoid was designed for the supersonic separator. The natural gas flows in diffusers were numerically calculated using the Navier-Stokes equations with the Reynolds Stress Model (RSM) to account for the swirling turbulence effect (Wen et al., 2011c). The results show that the shock waves appear as bifurcation structures as a result of the interaction between the shocks and the boundary layer in the diffuser (Wen et al., 2012b).

The experimental studies also have been conducted to test the dehydration performance of a supersonic separator. An indoor experiment loop was set up to test the dehydration characteristics of a designed supersonic swirling separator with the moist air by Liu et al. (2005). The dew point depression between the inlet and outlet of the separator was analyzed under various pressure loss ratios. A supersonic separator was compared to a Joule-Thomson valve with TEG and the results demonstrated the high economic performance and natural gas liquids recovery of a supersonic separator by Machado et al (2012). Wen et al. (2012c) designed a new type supersonic swirling separator based on the principle of conservation of angular momentum. An experimental loop was set up to test the dehydration characteristics of the new supersonic separator with a moist air. The effect of the pressure recovery coefficient on the dew point depression was analyzed experimentally.

The above mentioned studies focused on the single gas flow or condensation flow in a supersonic separator, and very little attention was paid to the droplet flows. The purpose of this paper is to study the droplet motion in the newly designed supersonic separator by employing the Discrete Particle Method (DPM), as well as the collection behavior of droplets at different region of the device.

COMPUTATIONAL APPROACH

Continuous Phase

The natural gas can be accelerated to supersonic velocities within a supersonic separator, and accordingly lower pressure and temperature conditions are achieved for water vapor condensation. The fluid structure of natural gas flows can be described by the conservation equations of mass, momentum and energy. Without considering a condensation flow, a gas phase is simulated as a steady state, described as Eqs. (1) - (3).

$$\frac{\partial}{\partial x_i}(\rho_g u_{gi}) = 0 \qquad (1)$$

$$\frac{\partial}{\partial x_j}(\rho_g u_{gi} u_{gj} + p\delta_{ij} - \tau_{ji}) = 0 \qquad (2)$$

$$\frac{\partial}{\partial x_j}(\rho_g u_{gj} E + u_{gj} p + q_j - u_i \tau_{ij}) = 0 \qquad (3)$$

where ρ_g, u_g, p are the gas density, velocity, and pressure, respectively. τ_{ij} is the viscous stress; δ_{ij} is the Kronecker delta; E is the total energy; q_j is the heat flux.

An equation of state must be developed to calculate the physical property of fluids in supersonic flows. In this simulation, the Redlich-Kwong real gas equation of state model, derived from the van der Waals equation (Redlich and Kwong, 1949), was employed to predict gas dynamic parameters.

Discrete Phase

A particle motion in a supersonic separator can be described as translation and rotation, which are completely determined by Newton's second law of motion. During the movement, the particle may collide with the walls at the contact points and interact with the surrounding fluid, through which the momentum and energy are exchanged.

Assume that the force on a particle can be determined exclusively from its interaction with the vicinal liquid by choosing a reasonable time step, the governing equation for a discrete liquid particle is:

$$m_l \frac{du_l}{dt} = m_l g - \rho_g g V_l + F \qquad (4)$$

where m_l, u_l and V_l are, respectively, the mass, velocity and volume of the liquid particle. g is the acceleration of gravity. t is the time. F is the gas-particle interaction force.

In a supersonic separator, the centrifugal force plays a much more significant role than the gravity force, therefore, the gravity force can be neglected. Because the density of the liquid particle is usually much larger than the gas density, the buoyancy force acting on a particle has been ignored in Eq. (4) as well.

The gas-particle interaction force F includes the drag force F_d and the additional force F_a. That is:

$$\boldsymbol{F} = \boldsymbol{F_D} + \boldsymbol{F_a} \tag{5}$$

The F_d is given by Ounis et al. (1991):

$$\boldsymbol{F_D} = \frac{18\mu_g}{\rho_l d_l^2} \frac{C_D R_e}{24} (\boldsymbol{u_g} - \boldsymbol{u_l}) \tag{6}$$

where ρ_l and d_l are the density and diameter of the liquid particle, respectively. U_g is the fluid phase velocity, μ_g is the molecular viscosity of the fluid, C_D is the drag coefficient. Re is the relative Reynolds number, which is defined as:

$$Re = \frac{\rho_g d_l |u_l - u_g|}{\mu_g} \tag{7}$$

The additional force F_d refers to the virtual mass force, pressure gradient force, thermophoretic force, and Saffman's lift force. In the supersonic separator, the virtual mass and pressure gradient forces can be ignored, because the density of the fluid (natural gas) is much lower than the density of the particles (water droplet). Therefore, these two kinds of additional forces were not considered in the simulation of the particle behavior.

In the supersonic swirling separator, small liquid particle suspended in the gas which had a great temperature gradient, which caused a force in the direction opposite to that of the gradient. Therefore, the thermophoretic force F_t was used to consider the sharp temperature gradient effect, which was given as:

$$\boldsymbol{F_t} = -D_{T_g,l} \frac{1}{m_l T_g} \frac{\partial T_g}{\partial x} \tag{8}$$

where T_g is the local fluid temperature, $D_{T_g,l}$ is the thermophoretic force coefficient, which can be given as (Talbot et al., 1980):

$$D_{T_g,l} = \frac{6\pi d_l \mu_g^2 C_s (K + C_t Kn)}{\rho_g (1 + 3C_m Kn)(1 + 2K + 2C_t Kn)} \tag{9}$$

where K_n is Knudsen number; K is the conductivity ratio between the fluid thermal conductivity and particle thermal conductivity; C_s, C_t, and C_m are the constant, with values of 1.17, 2.18 and 1.14 respectively.

Due to the strong shear and swirling flow in the separator, the Saffman's lift force was included to account for the swirling flow effect on particle motions. The Saffman's lift force can be described as (Saffman, 1965):

$$\boldsymbol{F_S} = \frac{2K_s \sqrt{v_g} \rho_g d_{ij}}{\rho_l d_l (d_{lk} d_{kl})^{0.25}} (\boldsymbol{u_g} - \boldsymbol{u_l}) \tag{10}$$

where $\boldsymbol{F_S}$ is the Saffman's lift force, $K_s = 2.594$, v_g is the gas dynamic viscosity, d_{ij} is the deformation tensor.

Computational Method

Numerical solution of the above equations was achieved with ANSYS/Fluent. In this case, we adopted the finite volume method to solve the governing equations, while the SIMPLE algorithm (Patankar, 1980) was employed to couple the velocity field and pressure. The Reynolds stress model (RSM) (Pope, 2000) was employed to predict the strong swirling flow. The Reynolds stress model is able to capture the characteristics of anisotropic turbulence and requires the solution of transport equations for each of the Reynolds stress components as well as for dissipation transport. The Speziale-Sarkar-Gatski Reynolds stress model was employed to appropriately model turbulent flow with a significant amount of swirl in the supersonic separator.

A structured grid was generated for the Laval nozzle, the cyclonic separation section and the diffuser, while the delta wing section was meshed using a tetrahedral grid due to its complexity, as shown in Fig. 2. The grid independence was tested before the case studies were conducted. In this simulation, the Mach number at the Laval nozzle exit was selected for grid independence. When the Mach numbers are consistent with different grid numbers, the grid independence could be verified. The grid independence was investigated with the mesh cells of 192 523, 386 876 and 813 836, respectively. Even 192 523 grids provided a sufficient grid independence. However, for judging the shock wave position exactly, the simulations were performed using the 386 876 cells in the case studies.

The pressure boundary conditions were assigned for the inlet and outlet of the supersonic separator. Non-slip and adiabatic boundary conditions are specified for the walls. In addition, for the discrete phase, the escape boundary conditions are assigned for the inlet and dry gas outlet. The trap boundary conditions are used for the walls of the cyclone separation section and the liquid-collection space. We appoint the reflect boundary conditions for all other walls.

RESULTS AND DISCUSSION

The flow characteristics of a natural gas were numerically simulated in our newly designed supersonic separator based on the above mentioned mathematical methods. The multi-components gas mixture in a Baimiao gas well of the Zhongyuan Oil Field was selected for the calculation. The composition of the natural gas in mole fraction is shown in Table 1.

Natural gas composition	Mole fraction (%)
CH_4	91.36
C_2H_6	3.63
C_3H_8	1.44
i-C_4H_{10}	0.26
n-C_4H_{10}	0.46
i-C_5H_{12}	0.17
n-C_5H_{12}	0.16
H_2O	0.03
CO_2	0.45
N_2	2.04

Table 1: Mole composition of the natural gas.
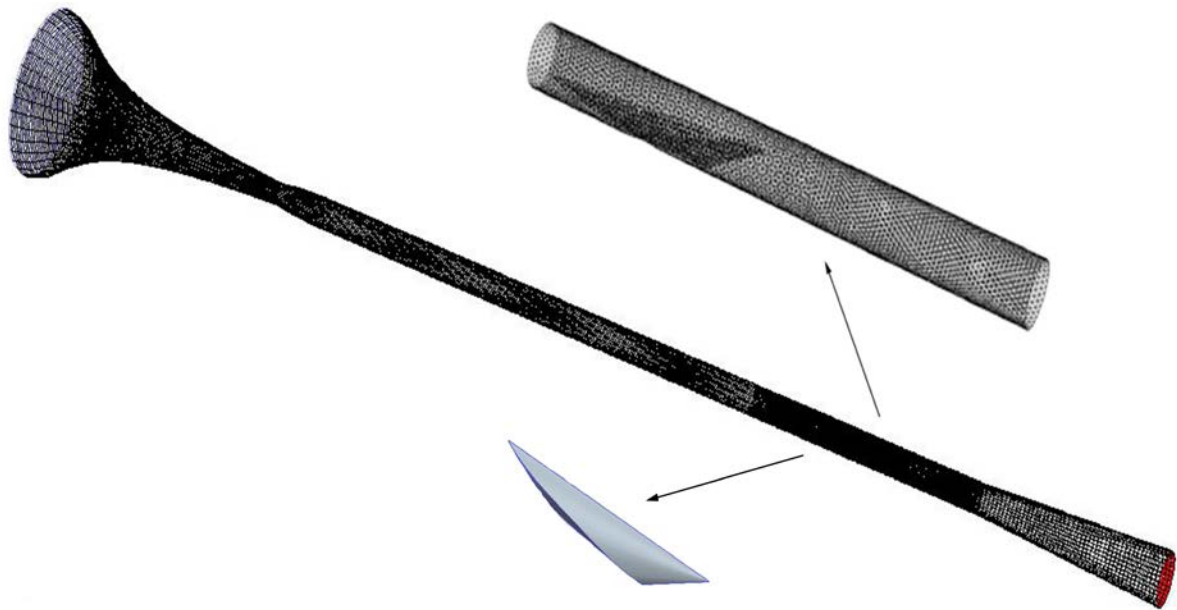
Figure 2: Grid system of the newly designed supersonic separator (Wen et al, 2012a).
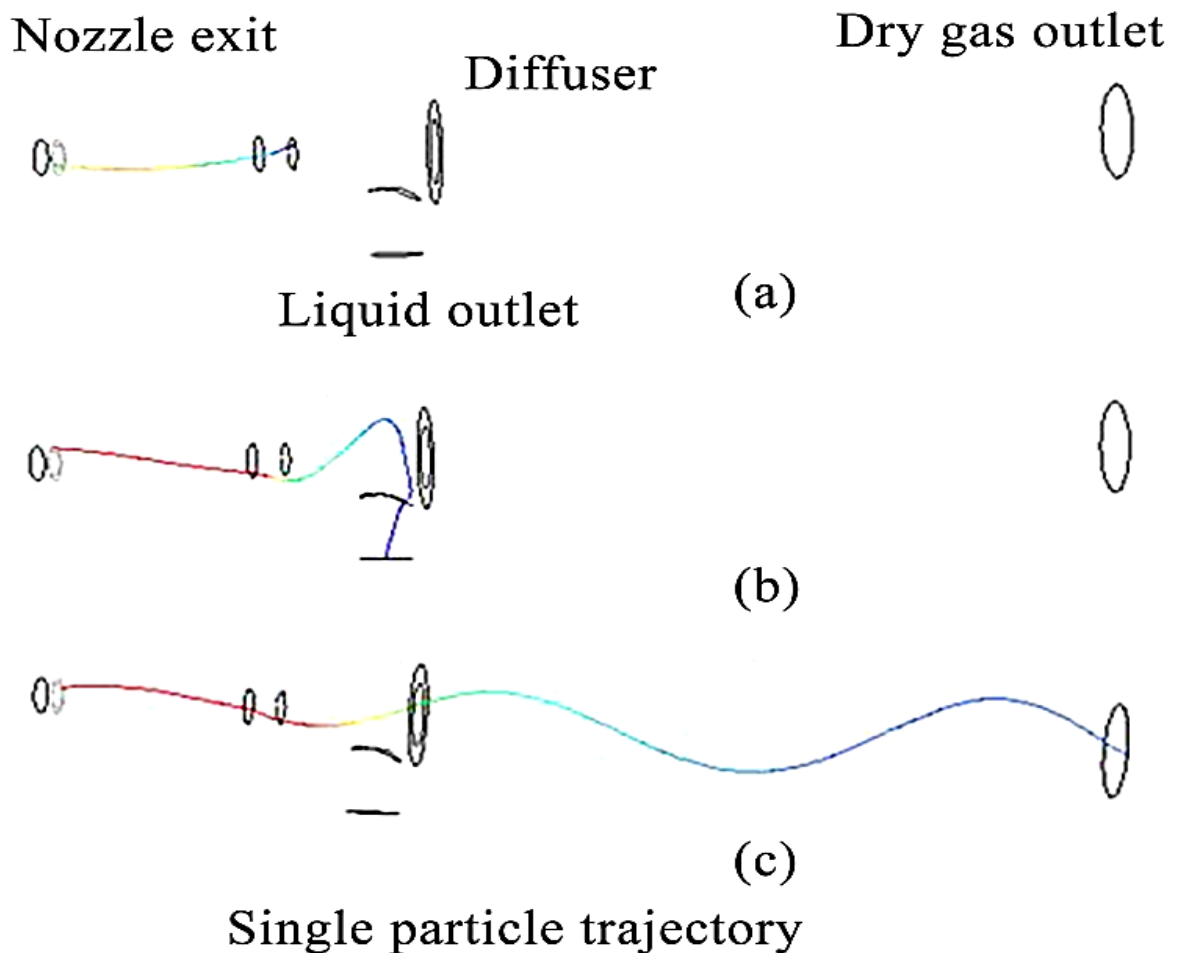
Figure 3: Trajectories of three representative particles in the supersonic separator.
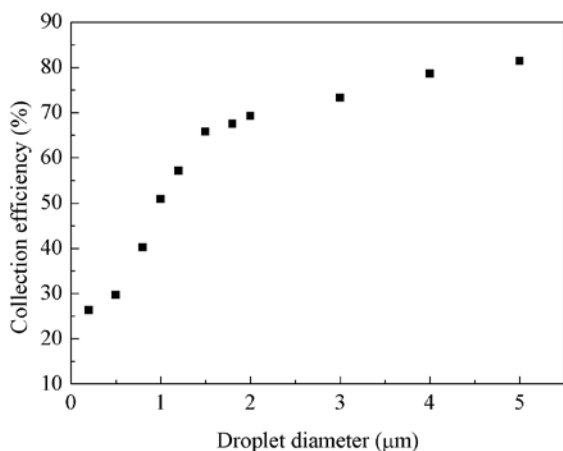
Particle Trajectories

In the present model, the liquid particle formation process was not considered. Thus, the liquid particles were simply injected from the nozzle outlet. Figure 3 showed the trajectories of three particles representing some typical particle moving states: a) the particle colliding with the wall, b) the particle entering into the liquid-collection space, and c) the particle passing through the diffuser. For the first kind particle (Fig.3 (a)), the particle was

centrifuged and collided with the walls, creating a thin liquid film, which would flow into the liquid-collection space along the wall. Some particles entered into the liquid-collection space directly without colliding with the wall (Fig.3 (b)). These particles would either collide with the walls in the liquid collection region or flowed out through the liquid outlet. For a few particles, the drag force played a much more significant role than other forces. Therefore, these particles passed through the diffuser together with the dry gas flow, which caused the gas phase entraining some liquids (Fig. 3 (c)).

Collection Efficiency

The collection efficiency is one of the most important technical parameters in assessing a supersonic separator's performance. In this work, the discrete particle model was employed to track the droplet motion and analyze the effect of the droplet size on the collection efficiency at different particle diameters. We assumed that the droplets were trapped directly, when they reached the wall of the cyclone separation section. As shown in Figure 4, the collection efficiency increased with the droplet size. When the droplet diameters were less than 1μm, the collection efficiency was lower than 50%. It indicated that the smaller size droplets were easier to follow the flow of dry gas and escape with gas phase rather than to be separated. The collection efficiency was more than 70% with the droplet diameter of about 2 μm, which demonstrated a good separation performance of our designed supersonic separator.

Figure 4: Collection efficiency in a supersonic separator.

CONCLUSIONS

The Discrete Particle Method (DPM) was employed to predict the particle trajectories and separation efficiency in a supersonic separator for natural gas dehydration. It was found that the particles would mainly have three types of trajectories, namely colliding with the surrounding wall, entering into the liquid-collection space and passing through the diffuser. The separation efficiency was strongly affected by the droplet size, which increased as the particle size increases. The separation efficiency can be over 70% when the droplet diameter was more than 2μm, demonstrating a good performance of the newly designed separator.

The simulation results demonstrated that the present CFD model provided a reasonable estimation of droplet collection in the newly designed separator. Further model refinement will be conducted to consider the detailed condensation process for a quantitative validation of the developed model.

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