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Numerical Modelling of non-equilibrium condensation of carbon dioxide (CO_2) in a converging-diverging nozzle

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Abstract. The condensing flow model is developed to predict the non-equilibrium condensation of CO_2 in a converging-diverging nozzle using computational fluid dynamics modelling, which is expected to contribute to the carbon capture and storage. The numerical result shows that the nucleation process of CO_2 occurs in the downstream of the nozzle throat where the extremely non-equilibrium state is reached, which generates the maximum value of the nucleation rate of approximately 2.5 x 10^{18} m^{-3} s^{-1}. The excessive nucleation induces the growth of the condensed droplet and the liquid fraction increase in the diverging part of the supersonic nozzle with achieving 8% of the total mass at the nozzle exit.

INTRODUCTION

The concerns of environmental pollution and climate change require the clean utilization of fossil fuels to reduce the emission of carbon dioxide (CO_2) [1]. The separation of CO_2 is one of the important steps for carbon capture and storage (CCS) technology, which provides a remarkable

measure to mitigate emissions [2]. The conventional separation technologies, such as absorption, adsorption and membranes, show good performance on CO_2 separation with some disadvantages including the large investment and the possibility of the chemicals.

The supersonic separation is introduced to remove the water vapour from wet natural gas, which is based on the non-equilibrium condensation in supersonic flows [3]. Both numerical and experimental studies have been carried out to evaluate the separation performance of water vapour inside a supersonic separator [4, 5]. In this study, we develop a condensing flow model to predict the non-equilibrium condensation of CO_2 in a converging-diverging nozzle using computational fluid dynamics modelling.

NUMERICAL MODELLING

The numerical modelling is developed based on following assumptions [6]: 1) the single-fluid model is used without considering the slip velocity between the vapour phase and liquid phase; 2) there is no temperature difference between the vapour and liquid phases; 3) the condensed droplets distributed uniformly in the vapour phase. The unsteady, compressible Navier-Stokes equations are employed to govern the fluid flow inside the converging-diverging nozzle. The governing equations are expressed as:

$$\frac{\partial(H)}{\partial t}+\frac{\partial\left(U_x\right)}{\partial x}+\frac{\partial\left(U_y\right)}{\partial y}=\frac{\partial\left(J_x\right)}{\partial x}+\frac{\partial\left(J_y\right)}{\partial y}+S \tag{1}$$

where

$$H=\begin{bmatrix}\rho\\ \rho u\\ \rho v\\ \rho E\\ \rho\zeta\\ \rho N\end{bmatrix},U_x=\begin{bmatrix}\rho u\\ \rho uu+p\\ \rho uv\\ \rho u(E+p)\\ \rho u\zeta\\ \rho uN\end{bmatrix},U_y=\begin{bmatrix}\rho v\\ \rho uv\\ \rho vv+p\\ \rho v(E+p)\\ \rho v\zeta\\ \rho vN\end{bmatrix} \tag{2}$$

$$J_x = \begin{bmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ q_x \\ 0 \\ 0 \end{bmatrix}, J_y = \begin{bmatrix} 0 \\ \tau_{xy} \\ \tau_{yy} \\ q_y \\ 0 \\ 0 \end{bmatrix}, S = \begin{bmatrix} -\dot{m} \\ -u\dot{m} \\ -v\dot{m} \\ -(h_v - h_{fg})\dot{m} \\ \dot{m} \\ \rho I \end{bmatrix} \tag{3}$$

where H represents conservation variables, U and J are inviscid and viscid fluxes, S is the source term. ζ and N are the liquid fraction and droplet numbers. ρ and p are density and pressure. E is the total energy, u and v are the velocity components. I is the nucleation rate. $\dot{m}$ is the condensation mass per unit vapour volume per unit time [7]:

$$\dot{m} = \frac{4\pi r_c^3}{3}\rho_l I + 4\pi r^2 \rho_l N \frac{dr}{dt} \tag{4}$$

$$I = \frac{q_c}{1+\phi}\frac{\rho_v^2}{\rho_l}\sqrt{\frac{2\sigma}{\pi m_v^3}}\exp\left(-\frac{4\pi\sigma}{3k_B T_v}r_c^2\right) \tag{5}$$

$$\frac{dr}{dt} = \frac{\lambda_v (T_s - T_v)}{\rho_l h_{lv} r}\frac{(1 - r_c/r)}{\left(\frac{1}{1+2\beta \mathrm{Kn}} + 3.78(1-\nu)\frac{\mathrm{Kn}}{\mathrm{Pr}}\right)} \tag{6}$$

where ρ_l is the droplet density, r is the droplet radius. dr/dt is the growth rate of droplets [8], and r_c is critical droplet radius. q_c is the condensation coefficient, σ is the liquid surface tension, m_v is the mass of a vapour molecule, k_B is the Boltzmann's constant. T_v is the vapour temperature. ϕ is a correction factor. T_s is the saturated temperature, Pr is the Prandtl number, Kn is the Knudsen number and v is the modelling correction coefficient.

RESULTS AND DISCISSION

The converging-diverging nozzle is used to model the non-equilibrium condensation of CO_2 in supersonic flows. The diameters at the inlet, throat and outlet are 54.4 mm, 13.1 mm and 26.2 mm, respectively. The structural grid is generated for the numerical simulation and 28 480 cells are

chosen based on the mesh independent test with 12 000 cells, 28 480 cells and 57 600 cells. The detailed dimension and mesh generation are shown in Fig. 1.

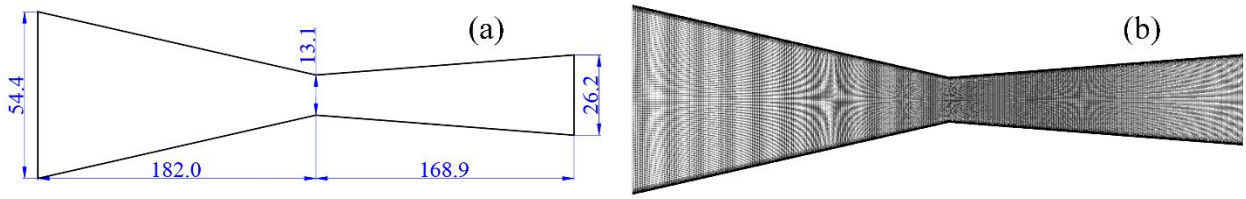

Fig. 1 Geometry and structural mesh of the converging-diverging nozzle

Figure 2 shows the static pressure and Mach number of CO_2 inside the converging-diverging nozzle during the non-equilibrium condensation process. It can be seen that CO_2 accelerates in the converging part of the nozzle and reaches the critical state at the nozzle throat with the Mach number of unity. Then the supersonic flow is achieved in the diverging part with a Mach number of 1.87 at the exit plane of the nozzle.

Figure 3 describes the distribution of the nucleation rate and liquid fraction inside the converging-diverging nozzle. It can be observed that the nucleation process occurs in the downstream of the nozzle throat with a maximum value of approximately 2.5×10^{18} m^{-3} s^{-1}. Combining with the static pressure and Mach number in Fig. 2, the profiles jump due to the release of the latent heat during the phase change in a non-equilibrium state. When looking at the details of the nucleation and liquid fraction, it can be observed that the onset of liquid fraction is in the downstream of the onset of nucleation which means that growth of the droplet follows the nucleation process. In this case, the liquid fraction can reach 8% of the total mass of the CO_2.

In addition, the shock wave appears in the diverging part of the nozzle due to the existence of the sharp point at the nozzle throat. The shock wave not only influences the flow structure but also the phase change process, which results in the energy loss. It indicates that the effect of the nozzle geometry needs to be improved for efficient energy utilization.

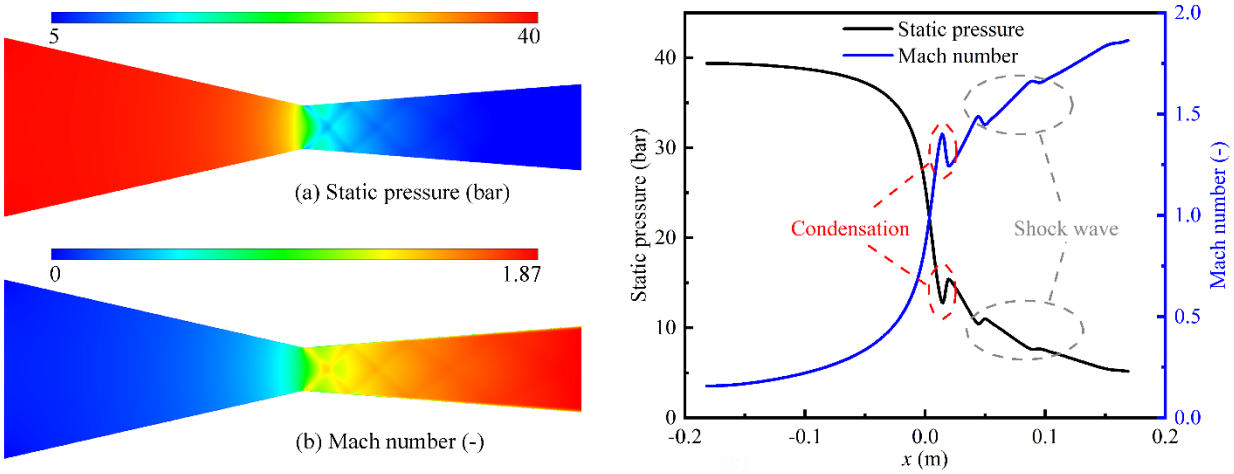

Fig. 2 Static pressure and Mach number in the converging-diverging nozzle

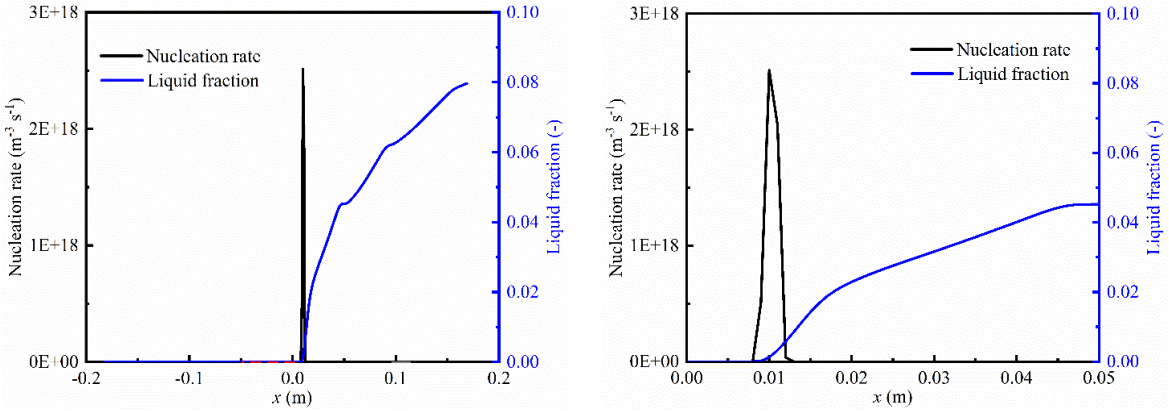

Fig. 3 Nucleation rate and liquid fraction in the converging-diverging nozzle

CONCLUSIONS

The converging-diverging nozzle is used to study the non-equilibrium condensation of CO_2 in supersonic flows, which can be used to reduce the carbon emission and contribute to the carbon capture and storage. The numerical simulation demonstrates that the nucleation occurs in the downstream of the nozzle throat and liquid fraction can achieve 8% of the total mass in this simulation case.

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