



Numerical modelling of non-equilibrium condensation of carbon dioxide (CO₂) in a converging-diverging nozzle

Wen, Chuang; Zhu, Xiaowei; Yang, Yan; Ding, Hongbing; Yan, Yuying

Published in:
AIP Conference Proceedings

Link to article, DOI:
[10.1063/5.0027863](https://doi.org/10.1063/5.0027863)

Publication date:
2020

Document Version
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

Citation (APA):
Wen, C., Zhu, X., Yang, Y., Ding, H., & Yan, Y. (2020). Numerical modelling of non-equilibrium condensation of carbon dioxide (CO₂) in a converging-diverging nozzle. *AIP Conference Proceedings*, 2293(1), Article 420077 . <https://doi.org/10.1063/5.0027863>

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Numerical modelling of non-equilibrium condensation of carbon dioxide (CO₂) in a converging-diverging nozzle

Cite as: AIP Conference Proceedings **2293**, 420077 (2020); <https://doi.org/10.1063/5.0027863>

Published Online: 25 November 2020

Chuang Wen, Xiaowei Zhu, Yan Yang, Hongbing Ding, and Yuying Yan



View Online



Export Citation



New

Your Qubits. Measured.

Meet the next generation of quantum analyzers

- Readout for up to 64 qubits
- Operation at up to 8.5 GHz, mixer-calibration-free
- Signal optimization with minimal latency

Find out more





Numerical Modelling of Non-equilibrium Condensation of Carbon Dioxide (CO₂) in a Converging-diverging Nozzle

Chuang Wen^{1, a)}, Xiaowei Zhu², Yan Yang², Hongbing Ding³ and Yuying Yan^{1, 4, b)}

¹Faculty of Engineering, University of Nottingham, University Park, Nottingham NG7 2RD, UK

²Department of Mechanical Engineering, Technical University of Denmark, Nils Koppels Allé, 2800 Kgs. Lyngby, Denmark

³Tianjin Key Laboratory of Process Measurement and Control, School of Electrical and Information Engineering, Tianjin University, Tianjin 300072, China

⁴Center for Fluids & Thermal Engineering, University of Nottingham Ningbo, China

^{b)} Corresponding author: Yuying.Yan@nottingham.ac.uk

^{a)} Chuang.Wen@nottingham.ac.uk

Abstract. The condensing flow model is developed to predict the non-equilibrium condensation of CO₂ 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 CO₂ 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 $2.5 \times 10^{18} \text{ m}^{-3} \text{ s}^{-1}$. 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 (CO₂)¹. The separation of CO₂ is one of the important steps for carbon capture and storage (CCS) technology, which provides a remarkable measure to mitigate emissions². The conventional separation technologies, such as absorption, adsorption and membranes, show good performance on CO₂ 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 flows³. 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 CO₂ in a converging-diverging nozzle using computational fluid dynamics modelling.

NUMERICAL MODELLING

The numerical modelling is developed based on following assumptions⁶: 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:

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

where

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

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

where H represents conservation variables, U and J are inviscid and viscous 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:

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

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

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

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 ν is the modelling correction coefficient.

RESULTS AND DISCUSSION

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.

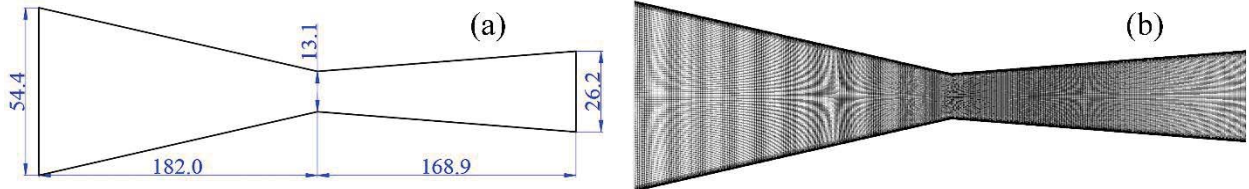


FIGURE 1. Geometry and structural mesh of the converging-diverging nozzle

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 $2.5 \times 10^{18} \text{ m}^{-3} \text{ s}^{-1}$. 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.

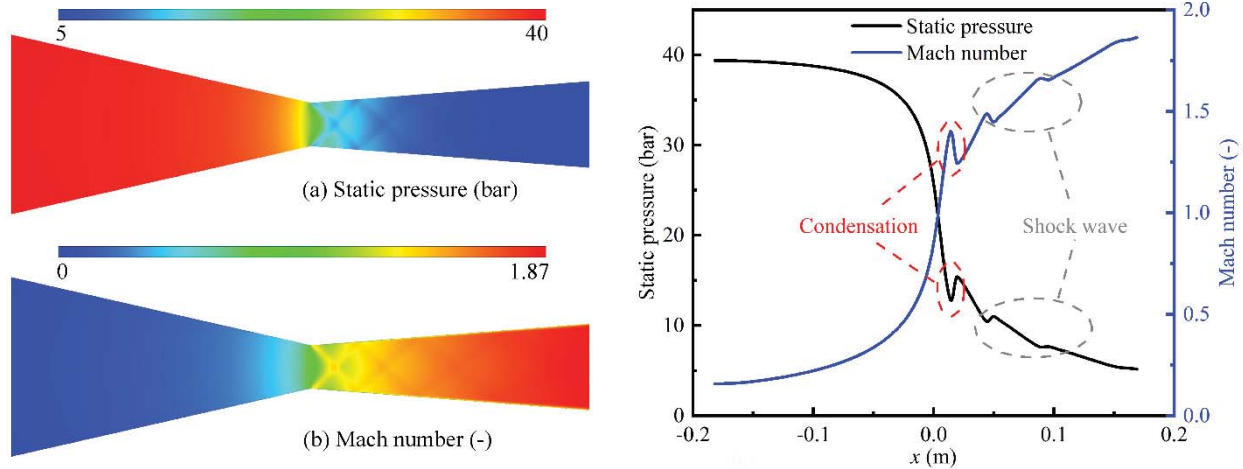


FIGURE 2. Static pressure and Mach number in the converging-diverging nozzle

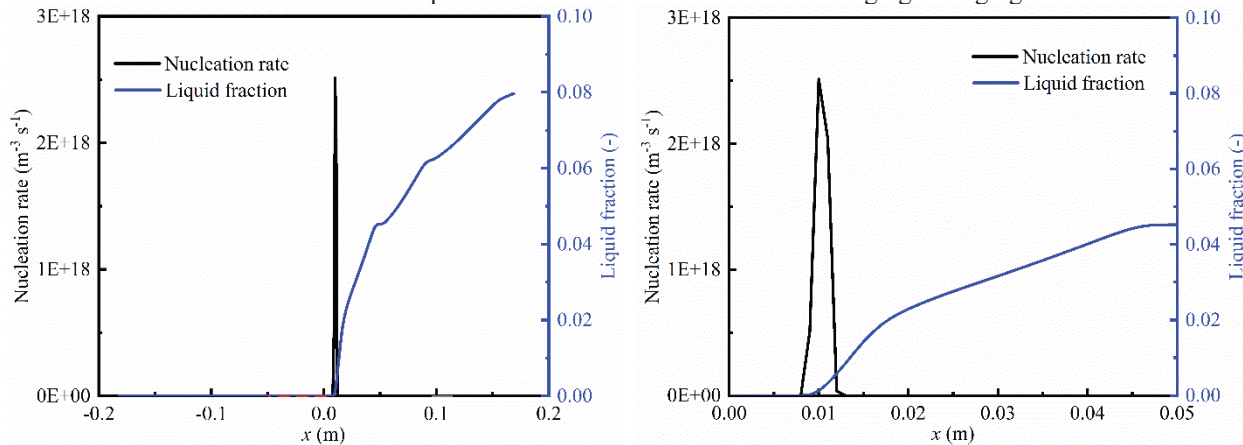


FIGURE 3. Nucleation rate and liquid fraction in the converging-diverging nozzle

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.

ACKNOWLEDGEMENTS

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 792876 and No 778104.

REFERENCES

1. S. Sgouridis, M. Carbajales-Dale, D. Csala, M. Chiesa and U. Bardi, [Nat. Energy](#) **4** (6), 456 (2019).
2. C. Wen, N. Karvounis, J. H. Walther, Y. Yan, Y. Feng and Y. Yang, [Appl. Energy](#) **238**, 311-319 (2019).
3. Y. Yang, C. Wen, S. Wang and Y. Feng, [Appl. Energy](#) **132**, 248-253 (2014).
4. S. F. Interlenghi, F. S. Raquel de Pádua, J. L. de Medeiros and O. d. Q. F. Araújo, [Energy Convers. Manage.](#) **195**, 1334-1349 (2019).
5. Y. Yang and C. Wen, [Sep. Purif. Technol.](#) **174**, 22-28 (2017).
6. Y. Yang, X. Zhu, Y. Yan, H. Ding and C. Wen, [Appl. Energy](#) **242**, 157-167 (2019).
7. Y. Yang, J. H. Walther, Y. Yan and C. Wen, [Appl. Therm. Eng.](#) **115**, 1357-1362 (2017).
8. J. Young, *Phys. Chem. Hydrodyn.* **3** (1), 57-82 (1982).