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REAL GAS EFFECTS ON NON-EQUILIBRIUM CONDENSATION OF CARBON DIOXIDE CONTRIBUTING TO CARBON CAPTURE AND STORAGE

Chuang Wen [1], Yan Yang [2], Xiaowei Zhu [2], Jens Honore Walther [2, 3], Hongbing Ding [4], Yuqing Feng [5], Yuying Yan [1*]

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

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

3 Computational Science and Engineering Laboratory, ETH Zürich, Clausiusstrasse 33, CH-8092 Zürich, Switzerland

4 School of Electrical and Information Engineering, Tianjin University, Tianjin 300072, China

5 CSIRO Mineral Resources, Bayview Avenue, Clayton VIC 3168, Australia

ABSTRACT

In the present study, we propose a new concept to capture carbon dioxide (CO_2) from gas industries using a supersonic separator. We develop and validate a computational fluid dynamics model to evaluate the effect of a real gas model on the non-equilibrium condensation CO_2 in high-pressure supersonic flows. The results show that the ideal gas equation of state under-predicts the CO_2 condensation with the predicted liquid fraction of approximately 15% of the total mass. The Redlich-Kwong equation of state incorporating with the condensing flow model shifts the onset of the CO_2 nucleation process upwards to the nozzle throat, while predicting a liquid fraction up to 28% of the total mass. The study indicates that the CO_2 condensation in supersonic flows provides an efficient way to mitigate the CO_2 emissions from gas industries.

Keywords: carbon capture and storage, carbon dioxide separation, non-equilibrium condensation, real gas

NOMENCLATURE

Abbreviations	
CO_2	Carbon dioxide
Symbols	
a, b	coefficient for Redlich-Kwong equation
h_{lv}	latent heat
H	total specific enthalpy
I	nucleation rate
k_B	Boltzmann's constant
Kn	Knudsen number
m_v	mass of a vapour molecule
n	droplet number per volume
p	pressure
Pr	Prandtl number
q_c	condensation coefficient
r	droplet radius
r_c	critical droplet radius
R	gas constant
t	time
T	temperature
u	velocity
V_m	molar volume
x	Cartesian coordinates
y	liquid fraction
β	modelling parameter
λ_{eff}	effective conductivity
λ_v	vapour conductivity
λ_t	turbulent thermal conductivity
v	modelling correction coefficient
ρ	density
σ	liquid surface tension
τ	stress tensor
φ	Kantrowitz's correction factor
Ω	condensation mass
Subscript	

i, j	Cartesian tensor notation
l	liquid phase
s	saturation condition
v	vapour phase

1. INTRODUCTION

The carbon emission from fossil energy is the primary cause of global warming and climate change. CarbonBrief [1] reports that the carbon dioxide (CO_2) emission from fossil fuels and industry grew by approximately 2.7% in 2018, the largest increase in last seven years, which dashes the hope that global CO_2 emissions might be nearing a peak. Taking China as an example, the natural gas consumption grew rapidly by 17.7% in 2018 and this rapid growth pushed the growth in total CO_2 emissions. Therefore, the removal of CO_2 is crucial to reduce the emissions at the source for the natural gas industry.

The conventional technologies for gas separation include the absorption, adsorption and membrane separation. The membrane process is still not used widely in gas industries due to the high equipment cost and possible damage at high flow rates [2]. The absorption and adsorption techniques demonstrate favourable performance while remaining a challenge as a result of the utilization of chemicals during the operation [3]. The supersonic separator is an environmental-friendly technique for gas removal with a focus on the water vapour from natural gas [4, 5]. However, considering the formation of liquid droplets in supersonic flows under high-pressure conditions remains a challenge.

In the present study, a mathematical model is developed to evaluate the influence of the thermodynamic properties on the non-equilibrium condensation of CO_2 in supersonic flows based on the Redlich-Kwong equation of state. We discuss the static pressure and liquid fraction in detail due to the CO_2 phase transition under high-pressure conditions.

2. MATHEMATICAL MODEL

2.1 Governing equations

The conservation equations of continuity, momentum and energy governing the compressible fluid for non-equilibrium condensation of pure CO_2 in supersonic flows are described as follows:

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u_j)}{\partial x_j}=-\Omega \tag{1}$$

$$\frac{\partial}{\partial t}(\rho u_i)+\frac{\partial}{\partial x_j}(\rho u_j u_i)=-\frac{\partial p}{\partial x_i}+\frac{\partial \tau_{ij}}{\partial x_j}-u_i\Omega \tag{2}$$

$$\begin{aligned}&\frac{\partial}{\partial t}(\rho H)+\frac{\partial}{\partial x_j}(\rho u_j H+p)\\&=-\frac{\partial}{\partial x_j}(\lambda_{eff}\frac{\partial T}{\partial x_j})+\frac{\partial}{\partial x_j}(u_i\tau_{ij})-h_{lv}\Omega\end{aligned} \tag{3}$$

where ρ, u_i, p, T and H are the density, velocity, pressure, temperature and total specific enthalpy, respectively. h_{lv} is the latent heat. λ_{eff} is the effective conductivity, λ_{eff} = λ_v + λ_t, where λ_v and λ_t are the vapour conductivity and turbulent thermal conductivity, respectively. t is time.

The transport equations of the liquid fraction (y) and droplet number per volume (n) are employed to account the phase transition of CO_2:

$$\frac{\partial(\rho y)}{\partial t}+\frac{\partial}{\partial x_j}(\rho y u_j)=\Omega \tag{4}$$

$$\frac{\partial(\rho n)}{\partial t}+\frac{\partial}{\partial x_j}(\rho n u_j)=\rho I \tag{5}$$

where I is the nucleation rate. Ω is the condensation mass per unit vapour volume per unit time:

$$\Omega=\frac{4\pi r_c^3}{3}\rho_l I+4\pi r^2\rho_l n\frac{dr}{dt} \tag{6}$$

where ρ_l is the droplet density, r is the droplet radius. dr/dt is the growth rate of droplets, and r_c is the Kelvin-Helmholtz critical droplet radius.

The nucleation rate, I, is calculated by the modified classical nucleation theory, which uses the non-isothermal correction of Kantrowitz [6] as follows:

$$I=\frac{q_c}{1+\varphi}\frac{\rho_v^2}{\rho_l}\sqrt{\frac{2\sigma}{\pi m_v^3}}\exp\left(-\frac{4\pi\sigma}{3k_B T_v}r_c^2\right) \tag{7}$$

where q_c is the condensation coefficient (q_c = 1.0 in this study), 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, which is obtained from Eqs (3). φ is a correction factor proposed by Kantrowitz [6].

The growth rate of droplets due to evaporation and condensation, dr/dt, is calculated by Young's model [7].

$$\frac{dr}{dt}=\frac{\lambda_v(T_s-T_v)}{\rho_l h_{lv} r}\frac{(1-r_c/r)}{\left(\frac{1}{1+2\beta \mathrm{Kn}}+3.78(1-\nu)\frac{\mathrm{Kn}}{\mathrm{Pr}}\right)} \tag{8}$$

where T_s is the saturation temperature, Pr is the Prandtl number, Kn is the Knudsen number and ν is the modelling correction coefficient. β is a modelling parameter (β = 0.0 in this study).

2.2 Real gas model

The Redlich-Kwong [8] equation of state is used to calculate the thermodynamic properties of CO_2 during the phase transition in supersonic flows:

$$p = \frac{RT}{V_m - b} - \frac{a}{\sqrt{T} V_m (V_m + b)} \tag{9}$$

where V_m is the molar volume, R is the gas constant. The coefficients a and b are functions of the critical temperature and critical pressure.

2.3 Numerical implementation

The numerical simulation is performed based on the commercial platform ANSYS FLUENT 18.2 [9]. Eqs. (4-8) are incorporated to the solver via using the User-Defined-Scalar (UDS) and User-Defined-Function (UDF) interfaces. The pressure inlet and pressure outlet conditions are adopted for the entrance and exit of the supersonic nozzle, while no-slip and adiabatic conditions are assumed for the wall boundaries [10]. The *k-ω* shear stress transport (SST) turbulence model [11] is used due to the good accuracy both for the supersonic flow [12] and the non-equilibrium condensation [13].

3. RESULTS AND DISCUSSION

3.1 Model validation

The numerical model is validated against experimental data in a half-Laval nozzle performed by Dykas et al. [14]. The operating condition of the total pressure and temperature at the nozzle inlet are 98000 Pa and 105 °C, respectively. The back pressure at the nozzle exit is 35000 Pa. The comparison in Fig. 1 demonstrates the validity of the developed model in predicting the non-equilibrium condensation in supersonic flows. In particular, the pressure jump downstream the nozzle throat indicate the formation of condensation shock due to the release of the latent heat [15].

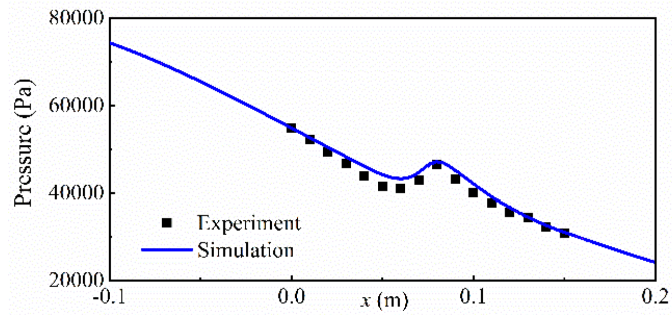

Fig. 1. Validation of the CFD model by comparing predicted static pressure with experimental data measured in a supersonic nozzle [14].

3.2 Assessment of ideal and real gas models

Fig. 2 shows the CFD results of the static pressure and liquid fraction during the CO_2 phase transition in the supersonic nozzle. Both the ideal gas and real gas models predict the abrupt rise of the static pressure in the process of the stream expansion in the transonic flow. However, the ideal gas law and Redlich-Kwong equation of state compute the different onsets of non-equilibrium condensation of CO_2. The real gas model predicts earlier onset of the CO_2 condensation compared to the ideal gas assumption, as shown in Fig. 2 (b). Furthermore, Fig. 2(b) and 2(c) indicate that the condensation rate of CO_2 is strongly dependent on the thermodynamic model. The ideal gas model under-predicts the CO_2 condensation with a calculated liquid fraction of approximately 15% of the total mass, while the Redlich-Kwong equation predicts a liquid fraction up to 28% of the total mass. The results from the Redlich-Kwong equation are expected to be more realistic than the idea gas model because the property of CO_2 in supersonic flow is essentially not an idea gas.

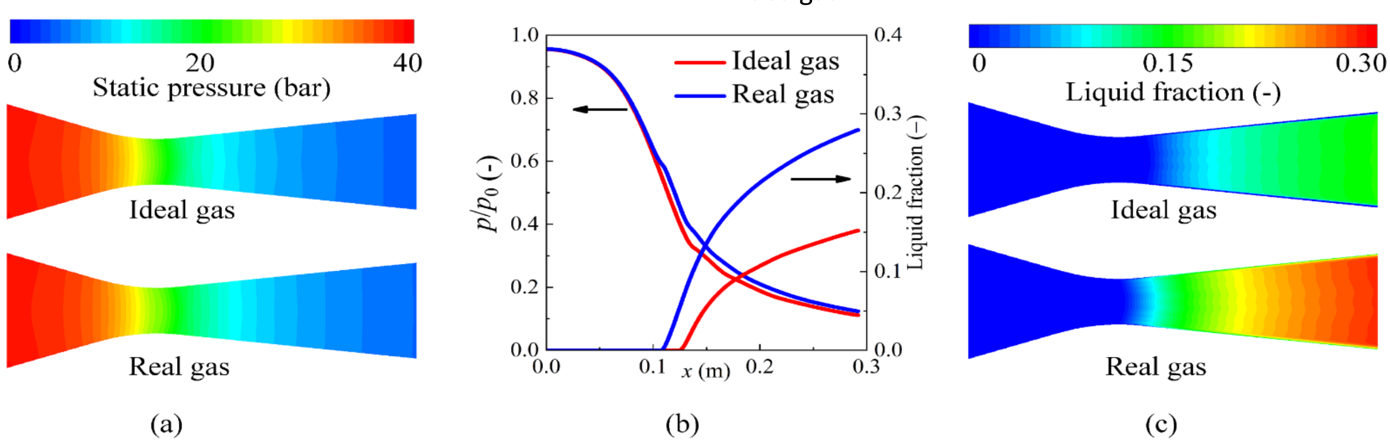

Fig. 2. Effect of ideal gas and real gas models on the CO_2 condensation in high-pressure flows. (a) and (c) show the contour of static pressure and liquid CO_2 fraction, repsectively, while (b) is a qualtative plot of the variation of the two varibles along the streamwise direction.

The difference can be further explained by the compressibility factor, which is usually considered as an indicator of the deviation from the ideal gas assumption. Fig. 3 represents that the compressibility factor varies from 0.75 at the nozzle inlet to 0.95 at the nozzle exit. As expected, the deviation from the ideal gas law results in inaccurate predictions of the heat and fluid flow inside high-pressure supersonic flows.

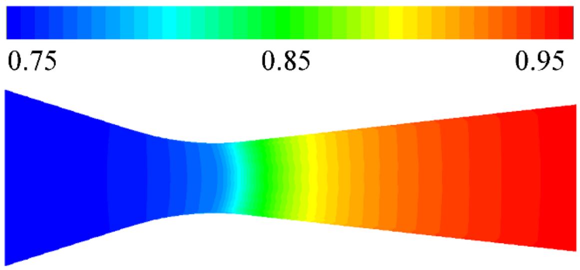

Fig. 3. Compressibility factor

4. CONCLUSIONS

We develop and validate a condensing flow model to estimate the feasibility of non-equilibrium condensation of CO_2 in high-pressure supersonic flows. By using the idea gas model and the real gas model (Redlich-Kwong equation of state), the condensed liquid CO_2 in the supersonic nozzle are 15% and 28% of the total flow mass, respectively. Therefore, the idea gas model significantly underpredicts the CO_2 condensation.

The results highlight the significance of choosing appropriate thermodynamic model to simulate CO_2 condensation in supersonic flows. Moreover, the study demonstrates the potential of applying supersonic condensation techniques to mitigate the CO_2 emission.

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