# Analysis of Condensation Effect of Supercritical $CO_2$ Radial Compressor

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## 1. Introduction

A new concept of innovative modular reactor, which is a supercritical $CO_2$ (S-$CO_2$) cooled micro modular reactor named as KAIST micro modular reactor (KAIST MMR), was suggested [1]. The module contains an S-$CO_2$ cooled fast reactor core, an S-$CO_2$ power generation cycle, and a passive decay heat removal system for safety.

The design of an S-$CO_2$ compressor is a major challenging process to demonstrate an efficient and robust S-$CO_2$ Brayton cycle. This is because the S-$CO_2$ fluid has high pressure and density, and thus turbomachinery should be of a small size with high rotating speed to achieve the required high performance. This may cause many issues in designing seal, bearing, and leakage flow. The property of the $CO_2$ adjacent to its critical point shows substantial variation with small change of pressure and temperature.

One of the things to consider in S-$CO_2$ Brayton cycle design is the condensation effect inside the compressor because if the inlet condition of a compressor becomes too close to the critical point, there might be some regions within the rotor in which the pressure and temperature are reaching their critical values. This may lead to unexpected energy losses of the compressor in actual operation. Previous studies have been conducted to confirm the condensation effect and conclude that the effect of liquid condensation is almost negligible [2]. However, design of the compressor in SCIEL, the experimental facility for this study, is a shrouded type (closed impeller) compressor that has a relatively small size and a rapid rotating speed in comparison to impellers used in the previous experimental studies. Hence, it is crucial to evaluate the condensation effect using a computational model appropriate for the actual compressor design.

In this study, the condensation effect inside the compressor is examined numerically using CFD approach in conjunction with the implementation of metastable properties. To simulate metastable properties, extrapolated gas properties are used. Since the nucleation mechanism of an S-$CO_2$ compressor is different from the classical nucleation theory, the non-equilibrium condensation rate was adopted to estimate time constant and other indicators required to estimate the rate of condensation. The two-phase volume of fluid (VOF) technic is used to make a quantitative evaluation of the condensation rate within an already built CFD model of a real compressor geometry and operating conditions matching the ones of the experimental facility.

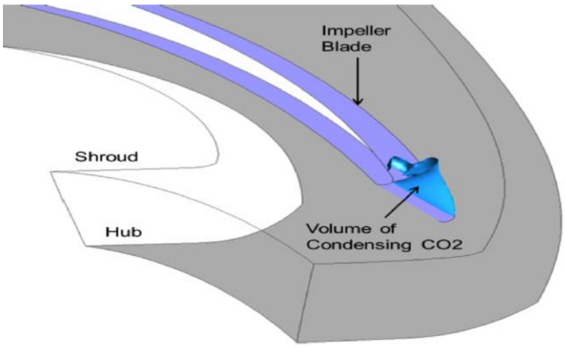

**Fig. 1.** Condensed region inside the compressor [2].

## 2. Analysis Model

The commercial CFD code, Star-CCM+ V11.06 is used for this CFD analysis. With regards to turbulence model, the high-Re type k-$\omega$ SST model is selected. This is selected as it is widely used in similar turbomachine analysis and it is known to give a good compromise between numerical stability and predictions accuracy [3]. The internal compressor geometry including ring diffuser, outlet diffuser and volute casing were used to generate the fluid domain. Hence, the fluid domain was divided into rotor and stator parts. The interfacial surfaces are connected by the mixing-plane approach. In this method, circumferential averaged flow variables on both sides are coupled at the interface.

For the property implementation of supercritical $CO_2$, the CSV table was generated using an in-house MATLAB code. The table contains properties at the given pressure, temperature columns, i.e. it contains density, dynamic viscosity, enthalpy, entropy, speed of sound, and thermal conductivity. All the properties' errors are less than 0.3% except for specific heat in constant pressure for which the error is of the order of 2%. The table used for simulation cover the ranges of 0.1-20MPa for pressure, 253-2000K for temperature with a 5,000×5,000 resolution. The wide pressure, temperature ranges were covered in order to improve numerical stability during the convergence process.

For the metastable property table, a cubic extrapolation with the 2nd order polynomial equations were used based on the NIST REFPROP 9.1 database [4].

The Grid Convergence Index (GCI) was used to access the grid independence criteria. The GCI method is a reliable method to estimate the numerical errors and the codes global discretization order [5]. The output variables such as torque acting on the impeller and total-to-total pressure ratio were considered as critical variables for the GCI analysis. After that, a fine mesh with 1,763,365 cells was chosen for the CFD analysis. The numerical uncertainty in the fine grid solutions for compressor performance was found to be less than 2.5%.

To investigate condensation effect close to the critical point, inlet conditions of 7.47MPa and 31.5℃ were used. At the inlet boundary, 5% of turbulence intensity was prescribed. Residuals of mass, momentum, energy, turbulent kinetic energy, and turbulent dissipation frequency were monitored. Furthermore, mass flow rate and temperature at the outlet were also checked for solution convergence criteria and solution accuracy.

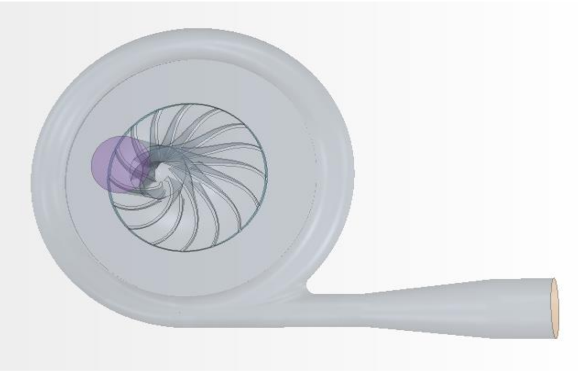

**Fig. 2.** Fluid domain of impeller and diffuser for CFD analysis model.

## 3. Results & Discussions

The time scale ratio (T) was used to investigate the quantity of liquid condensation. Two-phase volume of fluid (VOF) model is used for the CFD analysis. It is a rather simple two-phase model utilizing the volume fraction and solves a set of mass, momentum, energy, and turbulence equation.

$$T = \frac{t_r}{t_n} = \frac{residence\ time\ of\ flow}{time\ for\ droplets\ to\ form} \cdots (1)$$

Where, $t_n = \frac{1}{J_{max}V}$, $t_r = \frac{l}{C_{avg}}$,

and $l$ = length of condensed volume along the blade's camber line

The condensation effect of S-CO$_2$ compressor was investigated by N. Baltadjiev et al [2]. In this previous study, the authors performed a two-phase 3-D CFD analysis to investigate condensation effect with real gas properties. The table of metastable property of CO$_2$ was made, and implemented in the ANSYS CFX code. In their study, the authors used the classical nucleation theory (CNT) to calculate the nucleation rate directly affecting the time constant. However, one might argue that the equations for non-equilibrium heterogeneous nucleation should be more appropriate to predict the condensation of supercritical fluid at impeller's edge, because the condensation phenomena inside high-speed gas flow is totally different from CNT. Fig. 3 shows the ratio of the nucleation rates of argon and nitrogen as measured in a cryogenic pulse chamber and the predictions by CNT, as a function of the inverse of temperature [6]. The deviations in both cases range from 10 to 25 orders of magnitude.

First, the calculation results using CNT are shown in Table I. Results show that this approach returns unphysical values and it turns out that the time constant and condensation rate obtained from CNT is quite high in spite of the reasonable time scale ratio value.

### Classical nucleation theory

(i) Nucleation rate

$$\mathrm{J} = \sqrt{\frac{2\sigma}{\pi m^3}}\frac{\rho_g^2}{\rho_l}\exp\left[-\frac{\Delta G^*}{kT}\right] \cdots (2)$$

σ : Surface tension [N/m], $\Delta G^*$ : Critical Gibbs free energy [J/kg], $m$ : mass of single molecule [kg]

(ii) Critical radius

$$r^* = \frac{2\sigma}{\rho_l[g(p_g,T)-g(p_s,T)]} \cdots (3)$$

(iii) Critical Gibbs free energy

$$\Delta G^* = \frac{4}{3}\pi {r^*}^2\sigma \cdots (4)$$

**Table I:** The brief result obtained with classical nucleation theory

| Parameter | Value | Unit |
|---|---|---|
| Nucleation rate (*J*) | 4.548e-04 | m$^{-3}$s$^{-1}$ |
| **Time required to form stable droplet ($\boldsymbol{T_n}$)** | **3.424e+02** | **sec** |
| Residence time of flow ($\boldsymbol{T_r}$) | 5.836e-07 | sec |
| The time scale ratio (T=T$_r$/T$_n$) | 1.704e-09 | - |

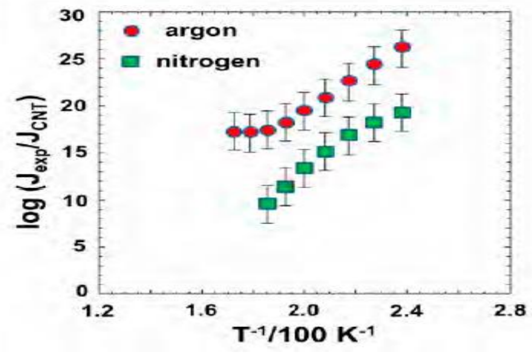

**Fig. 3.** Ratio of nucleation rates of experiment to prediction by CNT [6].

As authors then have opted to use the non-equilibrium heterogeneous condensation model due to the non-realistic aspect of the CNT shown above. Ryzhov [7] suggested a theory for the non-equilibrium condensation in high-speed gas flows. In this reference, the condensation and droplet rate in the non-equilibrium state was established. It is assumed that the Gibbs free energy of activation for surface diffusion is much lower than the critical Gibbs free energy, which is reasonable. In addition, it assumes that the impingement effects of monomers are negligible since the number of molecules of cluster structure of CO$_2$ is ranging from 20 to 533. The nucleation rate formula is as follows:

(i) Heterogeneous nucleation rate,

$$\mathrm{J} = \mathrm{Z}\frac{a_v^*\alpha_a}{\upsilon}\frac{P_g^2}{2\pi mkT}\exp\left[-\frac{\Delta G^*}{kT}\right] \cdots (5)$$

Where, Z : Zeldovich factor, $a_v^*$ : surface area of embryo $[m^2]$, $\alpha_a$ : adsorption coefficient $[m^{-1}]$, υ : vibration frequency $[m^{-1}]$, $P_g$ : Pressure of gas [Pa], $k$ : Boltzmann constant, T : Gas pressure [K],

(ii) Critical radius,

$$r^* = \frac{2\sigma V_l}{kT\ \ln(P_g\ /\ P_l)} \cdots (6)$$

σ : Surface tension [N/m], $V_l$ : Volume of single molecule [$m^3$], $P_l$ : Liquid pressure [Pa]

(iii) Critical Gibbs free energy,

$$\Delta G^* = \frac{16\pi\sigma^3}{3}\left(\frac{V_l}{kT\ln\left(\frac{P_g}{P_l}\right)}\right)^2 f\left(\frac{r^*}{R}, \cos\theta\right) \quad \cdots (7)$$

R : Radius of embryo, θ : Wetted angle

Where, $C_\theta = \left\{1 \div \left(\frac{r}{R}\right)^2 - \frac{2r}{R}\cos\theta\right\} \quad \cdots (8)$

Saturation ratio is defined to : $S = \frac{P_{gas}}{P_{sat\ liq}}$

In the marked region as shown in Fig. 4, low entropy value less than 1,550J/kg-K was observed, which is inside the spinodal limit at the given pressure. Comparing several time constants is necessary in order to conduct a quantitative analysis to determine if the fluid has enough time to change phases while flowing through the impeller. After conducting an analysis of the single-phase flow simulation but closest to the critical point, it was found that the compressor performance is almost the same to that the one obtained from VOF model.

After obtaining the above values, the residence time of flow ($t_r$), and the time required to form stable droplets ($t_n$) can be calculated to estimate the time scale ratio (T) [2]. The result of variables and time constant are listed in Table II. The results showed that the time scale ratio is 1.83e-05. It means that liquid condensation is unlikely to occur in the SCIEL compressor.

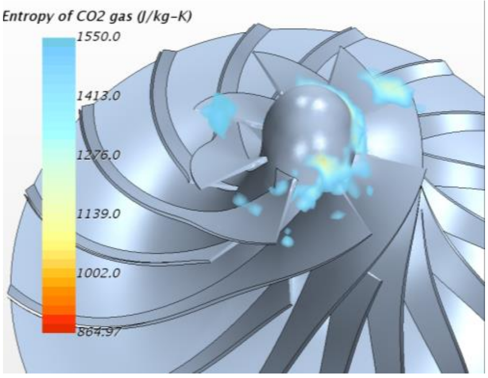

**Fig. 4.** Entropy plot of condensed region under spinodal limit.

**Table II:** The result obtained with non-equilibrium heterogeneous nucleation model.

| Parameter | Value | Unit |
|---|---|---|
| Surface tension ($\boldsymbol{\sigma}$) | 3.011e-03 | N/m |
| Condensed volume (V) | 6.221e-12 | $m^3$ |
| Critical radius (r*) | 1.396e-08 | M |
| Critical Gibbs free energy ($\Delta\boldsymbol{G}^*$) | 1.701e-19 | J/kg |
| Adsorption coefficient ($\boldsymbol{\alpha_a}$) | 2.0 | $cm^{-1}$ |
| Surface area of embryo ($\boldsymbol{a_v^*}$) [8] | 1.232e-11 | $cm^{-2}$ |
| Vibrational frequency ($\boldsymbol{\nu}$) | 2650 | $cm^{-1}$ |
| Attachment angle ($\boldsymbol{\theta}$) | 30 | degree |
| Saturation ratio (S) | 2.68 | - |
| Zeldovich Factor (Z) [9] | 0.09 | - |
| Nucleation rate (*J*) | 5.019e+12 | $m^{-3}s^{-1}$ |
| Time required to form stable droplet ($\boldsymbol{T_n}$) | 3.193e-02 | sec |
| Residence time of flow ($\boldsymbol{T_r}$) | 5.836e-07 | sec |
| **The time scale ratio ($T=T_r/T_n$)** | **1.828e-05** | - |

## 4. Conclusions

To confirm condensation effect for the S-$CO_2$ compressor case, a quantitative study using the two-phase CFD model was conducted. Metastable properties were made by extrapolations of state functions of gas and implemented to the CFD code while utilizing two-phase VOF model. Through comparison of CNT model with non-equilibrium heterogeneous model, it was confirmed that it more appropriate to use the non-equilibrium heterogeneous model as using the CNT model returns unphysical values for the time required to form a stable droplet. The present results obtained for time scale ratio further confirm the fact that the compressor has negligible amount of condensation and the associated effects are expected to be minimal during the operation. This is in good agreement with findings of previously conducted experimental studies found in the literature. The methodology developed in this study could allow designers to estimate the condensation effects from other compressor designs or MMR compressor designs.

## ACKNOWLEDGEMENT

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