Non-equilibrium condensation of supercritical carbon dioxide in a converging-diverging nozzle

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Abstract. Carbon dioxide (CO₂) is a promising alternative as a working fluid for future energy conversion and refrigeration cycles. CO₂ has low global warming potential compared to refrigerants and supercritical CO₂ Brayton cycle ought to have better efficiency than today’s counter parts. However, there are several issues concerning behaviour of supercritical CO₂ in aforementioned applications. One of these issues arises due to non-equilibrium condensation of CO₂ for some operating conditions in supercritical compressors. This paper investigates the non-equilibrium condensation of carbon dioxide in the course of an expansion from supercritical stagnation conditions in a converging-diverging nozzle. An external look-up table was implemented, using an in-house FORTRAN code, to calculate the fluid properties in supercritical, metastable and saturated regions. This look-up table is coupled with the flow solver and the non-equilibrium condensation model is introduced to the solver using user defined expressions. Numerical results are compared with the experimental measurements. In agreement with the experiment, the distribution of Mach number in the nozzle shows that the flow becomes supersonic in upstream region near the throat where speed of sound is minimum also the equilibrium reestablishment occurs at the outlet boundary condition.

NOMENCLATURE

| Symbol | Description |
|--------|-------------|
| H, h   | total and static enthalpy |
| J      | nucleation rate |
| k      | Boltzmann constant |
| Kn     | Knudsen number |
| L      | Latent heat |
| m      | molecular mass |
| N      | droplet number per unit of volume |
| p      | pressure |
| r      | droplet radius |
| S₁, S₂| source terms |
| T      | temperature |
| ΔT     | supercooling degree |
| t      | time |
| u      | velocity |
| w      | specific lost work |
| X      | Cartesian coordinate |
| Z      | compressibility factor |
| α      | volume fraction |
| ζ      | Markov loss coefficient |
| λ      | vapor thermal conductivity |
| θ      | divergence angle |
| ρ      | density |
| σ      | surface tension |
| τ      | viscous stress tensor |
| c      | critical |
| r      | reduced property |
| s      | saturation |

GREEK SYMBOLS

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|--------|-------------|
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SUBSCRIPTS

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|--------|-------------|
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| s      | saturation |
1. Introduction
Supercritical Brayton cycles have several advantages over conventional ones. For Supercritical Brayton cycles, depending on the working fluid, a higher cycle efficiency can be achieved with the relatively low temperature at the turbine inlet.

A previous study by Angelino and Invernizzi [1] indicated that the efficiency of the supercritical compressor and therefore, supercritical Brayton cycle becomes higher when the compressor inlet operation condition approaches the critical point. Previous studies showed that for low flow coefficient compressors operating in the vicinity of the critical point, due to the flow acceleration near the suction side of the main blade leading edge, the fluid state crosses the saturation curve and therefore, there is the possibility of spontaneous condensation [2-3]. Accordingly, an investigation of the non-equilibrium condensation of the supercritical carbon dioxide (SCO₂) is essential. Near the critical point, fluid has non-linear behavior and the behavior of the fluid is very sensitive to temperature and pressure. Previous studies discussed the difficulties of the compressor design and numerical calculations near the critical point [2, 4-5].

Numerical and thermophysical investigations of the formation of the dispersed phase in the rapid expansion of SCO₂ were studied in literature [6,7] and it was concluded that the most important factor which has a significant effect on the pressure and flow fields inside a supercritical nozzle is the inlet pressure. Moreover, the pressure at the inlet can alter the location at which the pressure goes below the critical pressure and consequently it changes location changes of onset of dispersed phase formation.

Furthermore, the impact of the supercritical condensation inside a centrifugal compressor was studied [8] by a non-dimensional criterion, which is related to the nucleation time and expansion rate. It was reported that condensation might not occur when the inlet boundary condition is far from the critical point. However, near the critical point, the effects related to phase transition are expected to become more significant.

The non-equilibrium condensation for high-speed flows in converging-diverging nozzles has been investigated for different fluids in many works such as [9-13]. The latent heat release due to condensation leads to a pressure drop or rise in the converging or diverging part of a nozzle, respectively. To isolate the unnecessary difficulties of modelling the condensation in supercritical fluids and focus on the essential elements of the model, the non-equilibrium condensation in a converging-diverging nozzle is selected for investigation to keep the flow complexity to a minimum. It is hoped that the current work provides a validation basis for modeling condensation in centrifugal compressors in future.

This work applies the numerical model developed by Gerber [14] to predict the flow field in the course of spontaneous condensation. The focus is on the prediction of the location of condensation and its effects on the flow field.

2. Experimental, theoretical and numerical procedures
2.1. Experimental setup
In the experimental measurements (which numerical results in this paper are compared with) performed by Nakagawa et al. [11] different converging-diverging nozzles with the same divergence angles and different boundary conditions were used. The shape and dimensional parameters of the nozzle are shown in Figure 1. The nozzle was rectangular due to ease construction and the heat transfer through the walls was reported to be too small to affect the experiment. The nozzle with the closest inlet conditions to the critical point is selected for the numerical investigation in this study, which has a divergence angle θ of 0.48°.
2.2. Non-equilibrium model

The foundations for almost all non-equilibrium phase change models are laid upon the prediction of the new phase evolution in forms of two consecutive stages described by the nucleation and droplet growth theories. It is believed that initially the condensation is favored by nucleation providing the first droplets of the liquid phase. Then, the phase transition is governed by the growth of supercritical droplets, which ideally quenches the nucleation and reestablishes the equilibrium [15]. The supercritical term is referred to the droplets larger than a critical radius, $r^*$, which is calculated according to the theory developed by Gibbs and Thomson for the equilibrium between a vapor with supersaturation ratio $S$ and a liquid droplet. Here by use of Clausius-Clapeyron equation [16], critical radius $r^*$ is related to the supercooling degree, $\Delta T$, and the specific enthalpy of evaporation, $L$, as below,

$$r^* = \frac{2\sigma}{\rho_l R \ln(S)} \approx \frac{2\sigma T_s}{\rho_l L \Delta T} , \Delta T = T_s (\rho_v) - T_v$$

where $T_s$ is the saturation temperature at vapor pressure, $p_v$, $\rho_l$ is the liquid density and $\sigma$ is surface tension. The calculation of the surface tension of the liquid carbon dioxide is based on a semi-empirical formulae proposed by Brock and Bird [17] using critical pressure, temperature and volume to express the liquid’s surface tension as follows

$$\sigma = (-0.951 + 0.432 \frac{1}{Z_c}) (1 - T_r)^{11/9} (P_c^2 T_c)^{1/3}$$

where $T_r$ and $Z_c$ are reduced temperature and critical compressibility factor, respectively. These parameters are given as follow

$$T_r = \frac{T}{T_c}$$

$$Z_c = \frac{1}{R} \left( \frac{P_v}{T_c} \right)$$

where subscript c refers to the critical state of the variables. Several expressions of surface tension equation are available in the literature [18-20]. A comparison between these surface tension models and experimental data was conducted by Jianxin and Yigang [21] and it was concluded that close to the critical point and in the range of interest in this article, Brock and Bird model has the highest accuracy. Therefore, this model was implemented to the flow solver by means of a user defined CFX Expression Language (CEL).
Despite decades of research after formulating the classical nucleation theory by Becker and Döring [22] and Zeldovich [23], the classical nucleation theory is still the most popular approach to model the nucleation process. Also, here the formation rate of critical droplets per unit volume $J$ is computed by the Becker and Döring expression for the classical theory of the homogenous steady nucleation as follows

$$J = \frac{\rho_l^2}{\rho_l} \left[ \frac{2\sigma}{\pi m^3} \right]^{1/2} \exp \left( -\frac{4\pi r^*^2 \sigma}{3 k T_v} \right).$$

A growing droplet absorbs monomers of the vapor phase through molecular collisions. Simultaneously, the droplet needs to give away the latent heat released by the condensation of monomers into the droplet. Due to large amount of the latent heat, of the droplet growth is dictated by the rate of heat transfer between the droplet and the vapor [24]. As the droplet temperature is unknown, one needs to iteratively solve the heat and mass transfer equations to obtain the growth rate. Although, the iterative method can be discarded applying the following estimation for a droplet temperature $T_l$ sized $r$ [25].

$$T_l = T_s - \Delta T - \frac{r^*}{r}$$

The details of the non-equilibrium model were provided by Gerber, in [26]. Here only a general description about the model in accordance with choices and assumptions made in this work are given. For the continuous and dispersed phases, the discretized transport equations are solved in an Eulerian reference frame. The model can also benefit from the so-called Source Specific capability to divide the liquid phase into separated groups based on their locations of nucleation/introduction. The mass and energy transfer between the dispersed phases and the continuous one are handled through source terms. Similar to the continuous phase, the dispersed phases are also evolving in the form of volume fractions. Thus, the conservation equations for the continuous and the dispersed phases are expressed using their volume fractions respectively denoted by $\alpha_v$ and $\alpha_l$, along with the constraint $\alpha_v + \sum_{l=1}^{n_l} \alpha_l = 1$

$$\frac{\partial (\alpha \rho)}{\partial t} + \frac{\partial (\alpha \rho u_j)}{\partial x_j} = -\sum_{l=1}^{n_l} S_{1,l} - \sum_{l=1}^{n_l} S_{2,l}$$

$$\frac{\partial (\alpha_l \rho)}{\partial t} + \frac{\partial (\alpha_l \rho u_j)}{\partial x_j} = S_{1,l} + S_{2,l}.$$  

Above equations define the mass conservation for each phase and they are connected by means of source terms $S_{1,l}$ and $S_{2,l}$. The mass transfer from the continuous phase to the dispersed one, induced by nucleation is computed by $S_{1,l}$, and $S_{2,l}$ accounts for the growth/decay of a dispersed phase as follows

$$S_{1,l} = m^* \alpha_v J$$

$$S_{2,l} = \left( \frac{3 \rho \alpha}{r} \frac{dr}{dt} \right)_l, r_l = \left( \frac{3 \alpha_l}{4 \pi N_l} \right)^{1/3}$$

where $m^*$ is the mass of a critical droplet, $\alpha$ is the volume fraction. Moreover, the droplet number $N_l$ of each dispersed phase must be conserved,
\[
\frac{\partial(\alpha N)}{\partial t} + \frac{\partial(\alpha Nu_j)}{\partial x_j} = S_{1,l}
\]

In the same manner as with the mass conservation equations, by neglecting the relative acceleration between phases and discarding energy equations for dispersed phase, the conservation of momentum and energy for the continuous phase yield as below

\[
\frac{\partial(\alpha \rho u_i)}{\partial t} + \frac{\partial (\alpha \rho u_i u_j)}{\partial x_j} = -\alpha \frac{\partial p}{\partial x_j} + \frac{\partial (\alpha \tau_{ij})}{\partial x_j} - \sum_{l=1}^{n_l} u_l S_{2,l}
\]

(12)

\[
\frac{\partial(\alpha \rho H)}{\partial t} + \frac{\partial (\alpha \rho u_j H)}{\partial x_j} = -\alpha \frac{\partial p}{\partial t} + \frac{\partial (\alpha \nu T)}{\partial x_j} + \frac{\partial (\alpha u_j \nu T)}{\partial x_j} - \sum_{l=1}^{n_l} L S_{2,l}
\]

(13)

2.3. Numerical procedure

Commercial Navier-Stokes flow solver ANSYS CFX 17.0 [27] was used for the steady states simulations in this article. Furthermore, RANS equations were closed through the two-equation \(k - \omega\) SST turbulence model of Menter [28]. Convergence criteria of the simulation were based on the reduction of Root Mean Square (RMS) momentum, mass and energy residuals below \(10^{-4}\), reduction and stability of the imbalance (difference between inlet and outlet) of mass, volume, energy and momentum below \(10^{-3}\%\), and constant volume fractions for both phases and droplet numbers at the outlet. Turbulence Intensity of \(5\%\) was prescribed at the inlet and reference pressure was set to zero. Total energy model, including the viscous work term was defined and all walls were assumed as non-slip. Total pressure and temperature were defined as the inlet boundary conditions and the static pressure was set as the outlet boundary condition. According to the different experimental measurements at the different boundary conditions, the closest inlet boundary condition to the critical point was selected to investigate the difficulty of the simulation and have a similar inlet boundary condition as one could have in a supercritical centrifugal compressor. Pressure and temperature at the inlet are 9 MPa and 40\(^\circ\)C, respectively. Static pressure 3.89 MPa was set as the outlet boundary condition.

The structured 3D mesh was generated using a sufficiently fine grid for one fourth of the whole geometry. Grids were denser near the walls to ensure the values of \(y^+\) close to unity. The quality of the structured grid was tested by Jacobian and skewness factors and most of the cells had skewness below 0.11. Grid dependency test was carried out and it was seen that a number of grids around 300000 cells is sufficient to ensure the grid-independent pressure trend and drag coefficient on the walls.

Fluid near its critical point has non-linear behavior and properties change rapidly. Figure 2 shows the specific heat in constant pressure at different pressure and temperature near the critical point. Sharp variation of the fluid properties causes high instabilities in the simulation. In order to calculate with high accuracy, an external look-up table of properties is coupled with the flow solver. Real Gas Properties (RGP) table includes nine main properties of fluid such as entropy, enthalpy, speed of sound, specific heat in constant pressure and volume and their derivatives. Properties of both vapor and liquid components were defined in a single RGP table.
Among different real gas Equation of States (EOS) equations, Span and Wagner (SW) [29] has been proposed especially for CO₂. This EOS was previously tested for simulations near the critical point and shown to be more accurate compared to other EOSs [2, 30]. SW EOS is formed in terms of Helmholtz energy and covers thermodynamic properties of CO₂ from the triple point up to 1100 K and 800 MPa for temperature and pressure, respectively. Full details on SW EOS and its derivatives can be found in the Ref. [31]. The fluid properties for the external look-up tables were calculated using the multipurpose NIST REFPROP 9 [31] database. These data were stored in the separate tables includes, liquid, vapor, metastable and saturated regions. Range of the RGP table is from 0.7 MPa and 230 K to 50 MPa and 730 K for pressure and temperature, respectively. Range of the table was chosen wider than the operating condition to prevent extrapolating or clipping methods by the solver, which decreases the accuracy of the numerical simulation. RGP resolution dependency test was done previously by authors [3] and it was concluded that intervals of 0.26 K and 0.05 MPa for temperature and pressure, respectively, are sufficient to have a stable and accurate simulation.

The vapor properties in the metastable region, i.e. between the saturation and the upper spinodal curves in the Figure 3, are given from a bilinear cubic extrapolation of the saturation properties to the spinodal curve. The extrapolation procedure is done by an in-house FORTRAN code.

2.4. Numerical difficulties

In the non-equilibrium condensation model in Ansys CFX, critical radius is calculated according to the following equation [32],
\[ r^* = \frac{2\sigma}{\rho \Delta G_v} \]  

(14)

where, \( \Delta G_v \) is Gibbs free energy change of the vapor. Therefore, by comparing the equation (14) with equation (1) it can be deduced that \( \Delta G_v \) in Ansys CFX must be calculated as

\[ \Delta G_v = \frac{L \Delta T}{T_s}. \]  

(15)

The Gibbs free energy change of the vapor near the critical point is very small which leads the equation to have an infinite value and causes error in the solver. In order to prevent this numerical instability, the solver clips the critical radius to a certain amount, as a default 1 mm. This extremely large default clipping value decreases the accuracy of the simulation and results in non-realistic droplet sizes. The problem is that it is not possible to change or modify the formula in the Ansys CFX by the user. To sidestep this problem, the critical radius was calculated according to the equation (1) in the post processing stage. It was observed that the critical radius, see Figure 4, changes very moderately also in the nucleation zone. Therefore, the radius of one nano meter has been estimated to be realistic for the critical droplet size in this study and in the calculations the critical radius is clipped, by a CEL, to one nano meter.

![Figure 4. Critical radius distribution over the nozzle centerline.](image)

3. Results and discussion

In order to prevent shock waves inside the nozzle, shorter length (8.38 mm) of the diverging part of the nozzle was assumed in experimental pressure measurements [11]. Thermocouple channels were implemented into the drilled holes along the nozzle wall to measure the temperature profile. Through the nozzle, saturated pressures where obtained according to the measured temperature. In figure 5, experimental saturation pressure were connected using dash lines.
Saturation pressure in numerical calculation is in a good agreement with the experimental data in most of the locations, although near the outlet of the nozzle due to the droplet condensation, slight deviation has been observed. This is mostly because of lack of accuracy of the classical nucleation theory in supercritical region, experimental uncertainties and numerical errors.

Figure 6 shows liquid mass fraction, supercooling, surface tension and Mach number inside the nozzle. Maximum mass fraction of the liquid carbon dioxide is observed near the outlet of the nozzle. As mentioned in the experimental procedure, near the outlet, shock has been occurred which is in agreement with the numerical results. Furthermore, by investigating the Mach number inside the converging-diverging nozzle, it can be noticed that the onset of phase transition occurs near the outlet, but the flow becomes supersonic in the upstream region near the throat where the speed of sound is minimum in that region.

4. Conclusion
In this paper, non-equilibrium condensation of supercritical CO$_2$ has been modelled. An external look-up table of properties was coupled with the solver to accurately and efficiently calculate thermodynamic properties near the critical point. Bilinear cubic extrapolation of the saturation properties to the spinodal curves was done by an in-house FORTRAN code to calculate the fluid properties at the metastable region. In order to prevent clipping near the critical point, an external function was defined to estimate more accurate critical radius for CO$_2$. Shock was seen near the outlet of the nozzle in a same
location as mentioned in the experimental data. Around 5.7% mass fraction of the liquid was observed near the outlet and the flow becomes supersonic in upstream region near the throat where the speed of sound is minimum. Further investigations will be conducted by the authors to implement the same approach in turbomachines especially in the centrifugal compressors to predict the effect of the condensation on the blade loading and compressor performance. Also, more studies will be done in order to increase the accuracy of non-equilibrium condensation near the critical point by modifying the nucleation and droplet growth theories.

Acknowledgement
Authors gratefully acknowledge the financial contribution of the Graduate School of Lappeenranta University of Technology.

References

[1] G. Angelino and C. Invernizzi, "Real gas Brayton cycles for organic working fluids," Proceedings of the Institution of Mechanical Engineers, Part A: Journal of Power and Energy, vol. 215, no. 1, pp. 27-38, February 1, 2001.

[2] N. D. Baltadjiev, An Investigation of Real Gas Effects in Supercritical CO2 Compressors, Master Thesis, Massachusetts Institute of Technology, 2012.

[3] A. Alireza, T.-S. Teemu and B. Jari, "Numerical Investigation of the Flow Behavior inside a Supercritical CO2 Centrifugal Compressor," in ASME Turbo Expo, Seoul, 2016.

[4] Y. Wang, G. Guenette, P. Hejzlar and M. J. Driscoll, "Compressor Design for the Supercritical CO2 Brayton Cycle," in 2nd International Energy Conversion Engineering Conference, no. 5722 in AIAA, pp. 1599-1611, 2004.

[5] G. K. Seong, L. Jekyoung, A. Yoonhan, I. L. Jeong, A. Yacine and K. Bockseong, "CFD Investigation of a Centrifugal Compressor Derived from Pump Technology for Supercritical Carbon Dioxide as a Working Fluid," The Journal of Supercritical Fluids, vol. 86, pp. 160-171, 2014.

[6] J. Liu, G. Amberg and M. Do-Quang, "Numerical Simulation of Particle Formation in the Rapid Expansion of Supercritical Solution Process," The Journal of Supercritical Fluids, vol. 95, pp. 572-587, 2014.

[7] S. Yamamoto and T. Furusawa, "Thermophysical Flow Simulations of Rapid Expansion of Supercritical Solutions (RESS)," The Journal of Supercritical Fluids, vol. 97, pp. 192-201, 2015.

[8] C. Lettieri, D. Yang and Z. Spakovszky, "An Investigation of Condensation Effects in Supercritical Carbon Dioxide Compressors," in The 4th International Symposium - Supercritical CO2 Power Cycles, Pittsburgh, Pennsylvania, 2014.

[9] A. Guha, "Thermal Choking Due to Nonequilibrium Condensation," Journal of Fluids Engineering, vol. 116, no. 3, pp. 599-604, 1994.

[10] N. Masafumi, S. B. Menandro and K. Akinori, "Supersonic Two-phase Flow of CO2 through Converging-diverging Nozzles for the Ejector Refrigeration Cycle," International Journal of Refrigeration, vol. 32, no. 11, pp. 1195-1202, 2009.

[11] M. Nakagawa, M. S. Berena and A. Harada, "Shock Waves in Supersonic Two-Phase Flow of CO2 in Converging-Diverging Nozzles," in International Refrigeration and Air Conditioning Conference, Purdue, 2008.

[12] G. Gyarmathy, "Nucleation of Steam in High-Pressure Nozzle Experiments," Proceedings of the Institution of Mechanical Engineers, Part A: Journal of Power and Energy, vol. 219, pp. 511-521, 2005.
[13] M. Yazdani, A. A. Alahyari and T. D. Radcliff, "Numerical Modeling and Validation of Supersonic Two-Phase Flow of CO2 in Converging-Diverging Nozzles," Journal of Fluids Engineering, vol. 136, p. 014503, 2014.

[14] A. G. Gerber, "Inhomogeneous Multifluid Model for Prediction of Nonequilibrium Phase Transition and Droplet Dynamics," Journal of Fluids Engineering, vol. 130, no. 3, p. 031402, 2008.

[15] K. Arthur, "Nucleation in Very Rapid Vapor Expansions," The Journal of Chemical Physics, vol. 19, no. 9, pp. 1097-1100, 1951.

[16] J. B. Young, "Two-Dimensional, Nonequilibrium, Wet-Steam Calculations for Nozzles and Turbine Cascades," Journal of Turbomachinery, vol. 114, no. 3, pp. 569-579, 1992.

[17] J. R. Brock and R. B. Bird, "Surface tension and the principle of corresponding states," AIChE Journal, vol. 1, no. 2, pp. 174-177, 1955.

[18] K. S. Pitzer, Thermodynamics, vol. 43, New York: McGraw-Hill, 1995, p. 285 pages.

[19] L. Riedel, "Kompressibilität, Oberflächenspannung und Wärmeleitfähigkeit im flüssigen Zustand. Untersuchungen über eine Erweiterung des Theorems der übereinstimmenden Zustände. Teil IV.," Chemie Ingenieur Technik, vol. 27, no. 4, pp. 209-213, 1955.

[20] D. I. Hakim, D. Steinberg and L. I. Stiel, "Generalized Relationship for the Surface Tension of Polar Fluids," Ind. Eng. Chem. Fundam., vol. 10, no. 1, pp. 174-175, 1971.

[21] J. Peng and Y. Lu, "Estimation of the surface tension of liquid carbon dioxide," Physics and Chemistry of Liquids: An International Journal, vol. 47, no. 3, pp. 267-273, 2009.

[22] R. Becker and W. Döring, "Kinetische Behandlung der Keimbildung in übersättigten Dämpfen," Annalen der physik, vol. 416, no. 8, pp. 719-752, 1935.

[23] J. Zeldovich, "Theory of the Formation of a New Phase," Zh Eksp Theor Fiz, vol. 12, pp. 525-538, 1942.

[24] J. B. Young, "Spontaneous Condensation of Steam in Supersonic Nozzles," Physicochemical Hydrodynamics, vol. 3, pp. 57-82, 1982.

[25] G. Gyarmathy, Grundlagen einer Theorie der Nassdampfturbine, ETH Zürich, Juris-Verlag Zürich. English Translation: USAF-FTD-TT-63-785, 1962.

[26] A. G. Gerber, "Inhomogeneous Multifluid Model for Prediction of Nonequilibrium Phase Transition and Droplet Dynamics," Journal of Fluids Engineering, vol. 130, no. 3, p. 031402, 2008.

[27] ANSYS® Academic Research, ANSYS CFX User Guide, Release 17.0, ANSYS, Inc, 2015.

[28] F. R. Menter, "Two-Equation Eddy-Viscosity Turbulence Model for Engineering Applications," AIAA Journal, vol. 32, no. 8, pp. 1598-1605, 1994.

[29] R. Span and W. Wagner, "A New Equation of States for Carbon Dioxide Covering the Region from the Triple-Point Temperature to 1100 K at Pressure up to 800 MPa," J. Phys. Chem, vol. 25, no. 6, pp. 1509-1596, 1996.

[30] N. D. Baltadjiev, C. Lettieri and S. Z. Spakovszky, "An Investigation of Real Gas Effects in Supercritical CO2 Centrifugal Compressors," Journal of Turbomachinery, vol. 137, no. 9, p. 091003 (13 pages), 2015.

[31] E. Lemmon, M. Huber and M. McLinden, "NIST Standard Reference Database 23: Reference Fluid Thermodynamic and Transport Properties-REFPROP, Version 9.0," National Institute of Standards and Technology, Standard Reference Data Program, Gaithersburg, 2012.

[32] ANSYS, "Private communication," 27.05.2016.