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Sensitivity Maps of Thermodynamic Properties of Carbon Dioxide Near the Critical Point for Optimization in Centrifugal Compressor Design

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ABSTRACT

The centrifugal compressor is one of the main components within the supercritical carbon dioxide Brayton power cycle, yet the one with the most critical design challenges. This cycle is normally designed so that the compressor operates at inlet conditions close to the critical point of the CO_2 to take advantage of the thermodynamic properties of the fluid. This provides an improvement in cycle efficiency, but implies a challenge in compressor design because slight variations in system conditions lead to significant changes in the physical properties of the fluid. Therefore, it is essential to perform a sensitivity analysis in the vicinity of the critical point to help identify the best behavior path and facilitate decision-making when designing the compressor. This work starts from the equation of state (Span & Wagner) that governs the behavior of carbon dioxide and which is currently reported within the REFPROP database of transport properties and thermodynamics of reference fluids. Through the concept of directional derivative, a thermodynamic sensitivity map is constructed that shows the trajectories of the gradients where the properties of carbon dioxide near the critical point vary more rapidly. The result obtained is a design methodology based on thermodynamic sensitivity maps that facilitates the identification of fluid behavior and can be used to predict compressor performance.

INTRODUCTION

The use of sCO_2 for power cycle comes from using a supercritical fluid that can increase cycle efficiency by taking advantage of the fluid properties near the critical region [1]. The centrifugal compressor is the main component within the Brayton supercritical carbon dioxide power cycle. This cycle is normally designed so that the compressor operates at inlet conditions close to the critical point to take advantage of the thermodynamic properties of the fluid such as high density and low compressibility [2]. These fluid properties greatly reduce the work of the compressor resulting in a higher proportion of work in the turbine, increased net power output, this provides an improvement in cycle efficiency, but implies a challenge in the design of the compressor because slight variations in system conditions lead to significant changes in the physical properties of the fluid. Therefore, it is essential to perform a sensitivity analysis in the vicinity of the critical point to help identify the best path of behavior and facilitate decision making when designing the compressor. For this we rely on the CO_2 equation of state developed by R. Span and W. Wagner [3], which is an empirical representation of the fundamental Helmholtz energy equation and is currently used and reported within the REFPROP database of transport properties and thermodynamics of reference fluids.

METHODOLOGY

The equation of state for CO_2 starts from the fundamental Helmholtz energy equation as a function of two independent variables, density and temperature. The dimensionless expression of the Helmholtz energy φ is commonly split into a part dependent on the ideal-gas behavior φ^o and a part which takes into account the residual behavior of the fluid φ^r.

$$\varphi(\delta,\tau) = \varphi^o(\delta,\tau) + \varphi^r(\delta,\tau) \tag{1}$$

Ideal gas behavior

$$\varphi^o(\delta,\tau) = In(\delta) + {a_1}^o + {a_2}^o\tau + {a_3}^o In(\tau) + \sum_{i=4}^{8} {a_i}^o In\left[1 - e^{(-\tau{\theta_i}^o)}\right] \tag{2}$$

Residual fluid behavior

$$\varphi^r(\delta,\tau) = \sum_{i=1}^{7} n_i\delta^{d_i}\tau^{t_i} + \sum_{i=8}^{34} n_i\delta^{d_i}\tau^{t_i}e^{-\delta^{c_i}} + \sum_{i=35}^{39} n_i\delta^{d_i}\tau^{t_i}\, e^{-\alpha_i(\delta-\epsilon_i)^2-\beta_i(\tau-\gamma_i)^2} + \sum_{i=40}^{42} n_i\Delta^{b_i}\delta\Psi \tag{3}$$

with

$$\Delta = \theta^2 + B_i[(\delta-1)^2]^{a_i}$$

$$\theta = (1-\tau) + A_i[(\delta-1)^2]^{1/(2\beta_i)}$$

$$\Psi = e^{-C_i(\delta-1)^2-D_i(\tau-1)^2}$$

Where $\delta = \rho/\rho_c$ is the reduced density and $\tau = T_c/T$ is the inverse reduced temperature. Both the density ρ and the temperature T are reduced with their critical values $\rho_c = 467.6 \pm 0.6\ kg/m^3$ and $T_c = 304.1282 \pm 0.015\ K$ respectively [3]. Since the Helmholtz energy as a function of density and temperature is one form of a fundamental equation, all the thermodynamic properties of a pure substance can be obtained by combining derivatives of Eq. (1). For this study we will focus on the sensitivity of the CO_2 pressure field behavior in the supercritical zone as a function of density and temperature.

The thermodynamic definition for pressure p in relation to the reduced Helmholtz energy φ is

$$p(\delta,\tau) = (1 + \delta\varphi_\delta{}^r)\,\delta\rho_c R\frac{T_c}{\tau} \tag{4}$$

where

$$R = 0.000188924\frac{MJ}{kg\ K}$$

$$\varphi_\delta{}^r = \sum_{i=1}^{7} n_i d_i \delta^{d_i-1}\tau^{t_i} + \sum_{i=8}^{34} n_i e^{-\delta^{c_i}}[\delta^{d_i-1}\tau^{t_i}(d_i - c_i\delta^{c_i})] + \sum_{i=35}^{39} n_i \delta^{d_i}\tau^{t_i} e^{-\alpha_i(\delta-\epsilon_i)^2-\beta_i(\tau-\gamma_i)^2}\left[\frac{d_i}{\delta} - 2\alpha_i(\delta-\epsilon_i)\right] + \sum_{i=40}^{42} n_i\left[\Delta^{b_i}\left(\Psi + \delta\frac{\partial\Psi}{\partial\delta}\right) + \frac{\partial\Delta^{b_i}}{\partial\delta}\delta\Psi\right]$$

All constants are in [3]. Having identified the pressure function in relation to the reduced Helmhotz energy, the concept of directional derivative was applied to identify the trajectories of maximum change within the pressure scalar field. The directional derivative $D_u f$ enables determining the rate of change of a function of two or more variables in any direction and is defined as:

$$D_u f(x,y) = \nabla f(x,y)\cdot \boldsymbol{u} \tag{5}$$

This expresses the directional derivative in the direction of a unit vector $\boldsymbol{u}$ as the scalar projection of the gradient vector ∇f onto $\boldsymbol{u}$ [4]. The maximum value of the directional derivative $D_u f(x,y)$ is $|\nabla f(x,y)|$ and it occurs when $\boldsymbol{u}$ has the same direction as the gradient vector $\nabla f(x,y)$.

Finally, the pressure function in terms of the reduced Helmholtz energy was programmed in Wolfram Mathematica to plot the scalar field of the pressures on contour lines and then apply the gradient concept of the function to obtain a vector field that would indicate the ratios of change.

RESULTS AND DISCUSSION

Fig 1 shows the sensitivity map of the CO_2 pressure p field as a function of reduced inverse temperature τ and reduced density δ. The continuous black lines represent the isobar curves of the field in MPa, the red and blue lines the vapor and liquid saturated curves respectively and the colored arrows the vector field of the rate of change. The CO_2 critical point is located at coordinates $(1,1)$ for $T = T_c$ and $\rho = \rho_c$ .The selected range for this map goes from $200K - 450K$ for temperature and $100\ kg/m^3 - 700\ kg/m^3$ for density focusing on the supercritical zone.

To perform an analysis of the rate of change in pressure, a practical example of the estimated operating conditions for a compression process on which the authors have been working was assumed for the design of an sCO_2 compressor. Fig. 2 shows the paths of different compression processes starting from a point close to the critical point, where the paths vary as a function of their isentropic efficiency. The rate of change was calculated for five paths from a compressor inlet state defined at 304.15 K and 614.17 kg/m^3 starting from a pressure of 7.5 MPa to 11.5 MPa. The gradient vector path is shown as the red arrow.

To calculate the value of the gradient for the point defined at the entrance of the compression process, the coordinate $(304.15, 614.17)$ as a function of temperature T and density ρ is passed to its reduced form as a function of δ and τ $(1.313\ , 0.999)$. Applying the gradient to the function $p(\delta,\tau)$:

$$\nabla p(\delta,\tau) = 1.7143, -75.487$$

Where the maximum variation is given by $|\nabla p(\delta,\tau)| = 75.50\ [MPa/s]$.

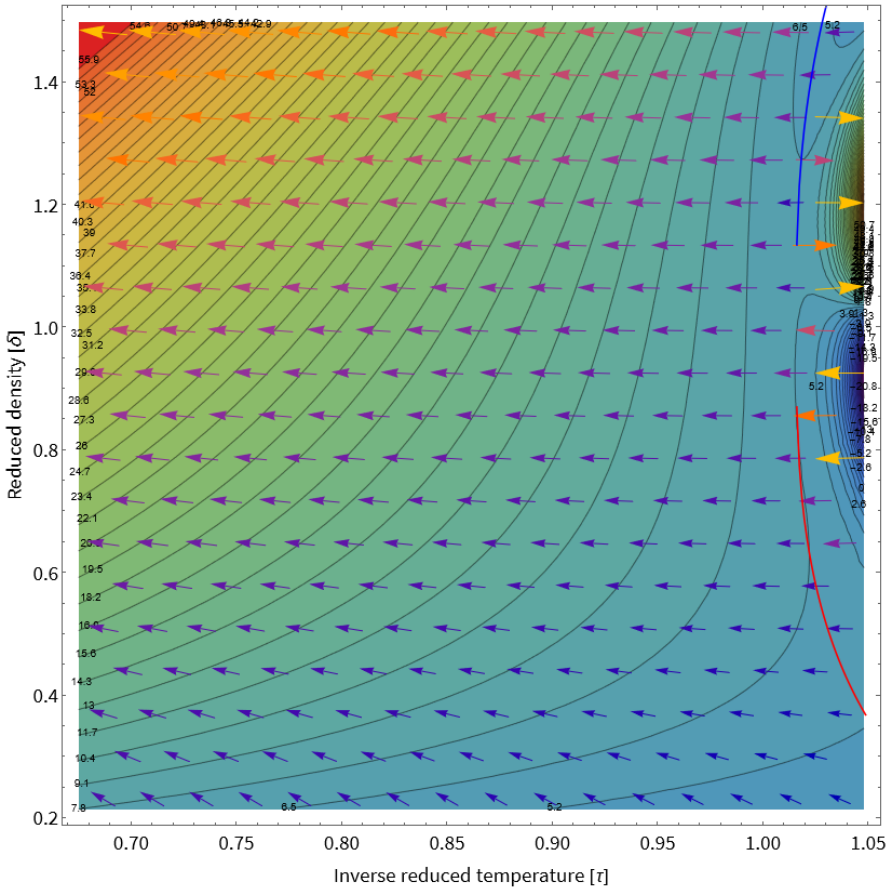

Fig. 1 Pressure gradient in inverse reduced temperature vs reduced density map.

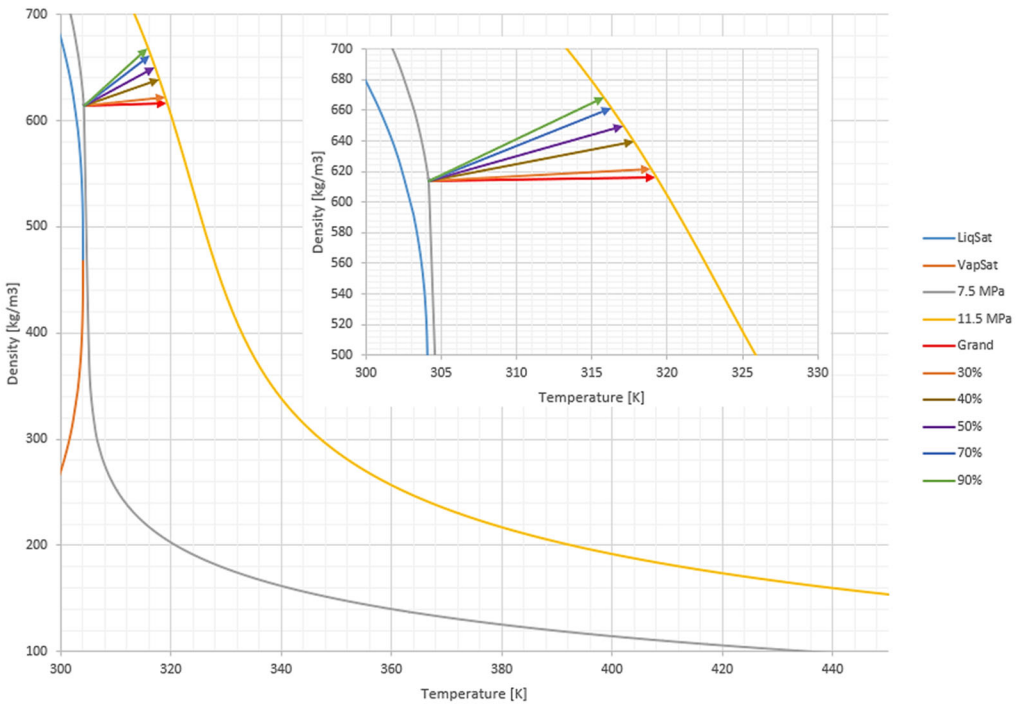

Fig. 2 Compression paths in temperature vs density graph.

Table 1 shows the comparison of paths implementing the concept of directional derivative for the output state of the compression process. The initial coordinates are changed as a function of δ and τ to obtain their unit vectors $\boldsymbol{u}$ in order to obtain the rate of change in each path.

Table 1. Comparison of paths in the compression process.

Efficiency η[%]	Output state (T, ρ)	Paths (δ, τ)	Unit vector (δ, τ)	Rate of change $[MPa/s]$
30	(318,93, 621.53)	(0.0157, -0.0463)	(0.3217, -0.9468)	72.02
40	(317.79, 639.23)	(0.0535, -0.0429)	(0.7805, -0.6250)	48.52
50	(317.08, 649.79)	(0.0761, -0.0408)	(0.8815, -0.4721)	37.15
70	(316.25, 661.78)	(0.1018, -0.0382)	(0.9360, -0.3517)	28.15
90	(315.77, 668.41)	(0.1160, -0.0368)	(0.9531, -0.3024)	24.46

As can be seen in Table 1, the rates of change for paths with high efficiencies do not change that much, the process of a path at 70% efficiency is very similar to one at 90%. However, the rates of change increase rapidly for efficiencies below 50%.

CONCLUSIONS

The rates of change within the compression paths depend on the efficiencies in the process. The lower the efficiency, the more it approximates the direction of the gradient vector. For the example used, the rate of change in paths above 70% efficiency does not increase as much until efficiencies of 90%, below 50% the rate of change increases rapidly.

The foundations were laid for the development of a methodology to help create better design models in sCO_2 compressors, taking as a criterion the thermodynamic sensitivity of their properties depending on the path to be chosen. As future work will be implemented in detail the concept of the directional derivative within the design process to identify the best trajectories and areas within the supercritical zone where the variation of the properties does not change too much and can help the understanding of the behavior of supercritical CO_2 in turbomachines.

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