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# Atypical Fluid Behavior on the Liquid Side of the Saturation Line of CO<sub>2</sub> With Implications for Compressor Design

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### ABSTRACT

The non-linear fluid properties near the critical point have received very significant consideration in terms of their effect on  $CO_2$  compressors. Less well documented, is the potential for even more non-linear behavior when the inflow conditions to the compressor shift toward the liquid side of the saturation curve. Depending on the cycle conditions and heat sources, moderate to strong variation in inflow conditions to the compressor can be expected in many cycles and the effect on compressor performance must be considered.

Very strong variation in density and specific heat ratio come into play near the critical point which strongly impacts the compressor design. Near the liquid saturation line, the nature of the fluid properties changes and the speed of sound becomes the dominant nonlinear variation. This variation has significant potential to affect the performance of the compressor at off-design cycle conditions.

In this work, both 1D and 3D numerical and analytical methods are used to demonstrate highly unexpected behavior of the fluid crossing the liquid side of the saturation dome. These effects include choking flows at Mach numbers significantly less than unity as well as shock-like behavior at Mach numbers well below the sonic point.

#### INTRODUCTION

The two most serious issues in sCO<sub>2</sub> turbomachinery are the rapid variation of the thermodynamic properties and the potential for two-phase flow phenomena. While neither of these issues precludes the development of effective turbomachinery designs for sCO<sub>2</sub>, they greatly complicate the modeling and prediction process, since many modeling assumptions that may be perfectly reasonable for conventional designs no longer apply. There are many commercially available CFD codes today that have implementations of these advanced equations of state. Several different thermodynamic models are available to calculate the real fluid properties. Depending on the model, these calculations may be viable across different domains: liquid, gas, and solid. In general, these models carry a very significant computational overhead that can overwhelm the baseline CFD solver. Computational penalties of as much as 50 times over baseline perfect gas calculations have been reported [1-3].

Resolving the equation of state adequately in all regions of the map is critical for effective design and analysis of sCO<sub>2</sub> turbomachinery. Results of this work will show this is particularly true near the liquid side of the saturation dome, where fluid properties are particularly non-linear and flow phenomena likely to impact design viability are found.

### **RESULTS AND DISCUSSION**

The solution often used to address these concerns is a selectively refined table near the saturation line [3-5]. In this application, the table uses a predefined upper and lower limit on pressure and enthalpy, which are determined from the operating conditions input by the user. The table is then enhanced with

progressively refined cells down to the selected level. These settings are made with predetermined course table range ( $20 \times 20$ ) and level of refinement (four levels) but this can be overridden by the user if necessary. The cells near, but not touching, the saturation line, are progressively coarsened such that no more than one level of coarsening is made in neighboring cells. The baseline calculation used to populate the tables is typically taken from the NIST REFPROP program [6]. The figure below, on the left, shows an example.



Plot of selectively refined thermodynamic table now used in Concepts NREC software (left) and paths of 1D nozzle flows over the thermodynamic map

A series of one-dimensionalized nozzle studies was done at three locations: the critical point, the gas phase side, and the liquid phase side. Each of these cases started with an inflow condition close to the saturation curve, but just above the actual dome, so the flow accelerated and passed into the saturation dome. The figure above, on the right, shows the thermodynamic states on the enthalpy-entropy map of these three different flow fields.

In the course of the validation studies of the solver, some very interesting results were observed that have ramifications for future compressor design. The critical point and gas phase flows showed the more or less expected results, with some deviation from classical compressible flow theory (perfect gas). The case starting on the liquid side, however, showed a radical departure from typical flows. These departures were so significant that it was first thought to be an error in the solver, but careful examination confirmed the behavior. The figure below shows the curious results.



CFD results of a sCO<sub>2</sub> nozzle expansion from the liquid side showing atypical results

Two striking observations stand out in this case. One is the choked mass flow at the throat of the nozzle being only about Mach 0.3. This is a vastly different number than the Mach 1 in an ideal gas. The other strange result is that a clear shock wave is forming, but the maximum Mach number does not exceed 1.0, entering the shock. The source of both these effects is the result of the highly nonlinear speed of sound near the left saturation line, as seen below. The method of calculation of the speed of sound in the two-phase region is based on the model outline by Brennen [7].



Speed of sound values derived from REFPROP and Brennen

### SUB-SONIC CHOKING

The flow phenomena observed was confirmed using careful one-dimensional analysis, coupled with accurate thermodynamic calls from the REFPROP program. The figure below shows the mass flux (mass flow per unit area) as a function of Mach number for an isentropic expansion, calculated using 1D analysis and REFPROP. The results show a maximum mass flux (choking point) at a Mach number value of approximately 0.3. This closely matches the findings in the CFD solution. This maximum mass flux point corresponds to the saturation line. It seems the void fraction of gas serves as a blocking mechanism that inhibits the mass flux that can pass, thus forming a choked throat, far from the sonic point.



## Mass flux as function of Mach number for isentropic expansion through the liquid side of the saturation line

### SUB-SONIC SHOCK WAVES

The second observation of a shock wave forming at a Mach number less than one, was also confirmed with detailed 1D flow evaluations that were somewhat more involved than the choke calculation. Taking a control volume and balancing mass, momentum, and energy on both sides yields an analytical result (when coupled with REFPROP calculations). This was done by forcing both the mass and energy terms and iterating on the velocity until the momentum matched on each side. The figure below shows the process.



### Conversation equations (left) and stream thrust distribution as a function of exit velocity (right)

The results showed that a shock-like behavior is indeed possible, even though the Mach number coming into the shock is less than one. The results showed the expected pressure rise and entropy (albeit a small one), as one would expect from a typical shock.





Iterations in 1D model on velocity to match mass, momentum, and energy across the shock results of a sCO<sub>2</sub> nozzle expansion from the liquid side showing atypical results



1D and 3D results of sub-sonic shock calculation

### SUMMARY

A great deal of attention has been focused on the non-linear thermodynamic effects near the critical point, normally the design point in an sCO<sub>2</sub> cycle. Actual cycle variations have the potential to cause the inflow condition to the compressor to drift over to the liquid side of the domain, due to changes in ambient temperature or a temporary reduction in heat, added to the cycle. The highly nonlinear behavior of the fluid in this region has the potential to significantly impact compressor performance at off-design points for a cycle.

The two primary effects were observed in CFD results and confirmed in 1D analysis. 1) The choking condition can occur at Mach numbers far below the sonic point. This poses the significant risk of severe premature choking in the compressor in this region. 2) Shock structures and the characteristic losses they produce can occur again with Mach numbers well below the sonic point. These two effects have the potential to seriously limit both the range and performance of sCO<sub>2</sub> compressors, when cycle conditions drift toward the liquid side of the saturation dome.

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