Numerical Simulations of CO2 Compressors: Subcritical Inlet Conditions

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Motivation

- Subcritical operation of SCO2 compressors can potentially occur in a variety of situations
  - Fluctuations in inlet conditions e.g. in air-cooled cycles and CSP applications
  - Start-up transients particularly at cold ambient conditions where the compressor initially operates like a circulator and operates in the sub-critical dome until heaters raise the temperature of CO2 to supercritical values
  - When water is present as a contaminant, the critical point of the mixture becomes large or undefined and the compressor will essentially operate at subcritical conditions *at all* operating pressures of relevance to SCO2 cycles
- Understanding performance and stability of compressors at sub-critical conditions important for design optimization and risk mitigation
- Bulk of CFD studies in literature thus far have focused on supercritical operating conditions with a few studies analyzing leading edge condensation at design conditions
  - The broader class of sub-critical and two-phase inlet conditions have not been simulated
- Focus of this work is on developing numerical framework that can analyze broad range of sub-critical operating conditions and fluid compositions
  - Phase change physics that can range from condensation to vaporization (cavitation) depending on regime
  - Framework that is versatile to allow for multiple species (e.g. CO_2, water, CO) with associated multi-phase effects

Outline

- Numerical framework for two-phase and multi-species simulations
- Phase Change Models overview
- Validation Studies for Condensation in De Laval nozzle
  - ➢ Rigorous comparisons with data published by Prof. Lettieri
- Simulations of Sandia compressor at various operating conditions
  - ➢ Supercritical inlet near design point
  - ➢ Liquid inflow at subcritical temperature of 295 K
  - ➢ Vapor Inflow at subcritical temperature of 302 K
  - ➢ 2-Phase inlet conditions at 290 K
  - ➢ Performance comparison with Sandia Test data
- Conclusions and Future Work

CRUNCH CFD® Numerical Framework

- **Generalized Preconditioned Formulation**
  - Solves for pressure and temperature instead of density and internal energy to overcome stiffness issues. Pressure and temperature are always well-defined even for stiff systems.
- **Versatile Thermodynamics**
  - Matrices retain thermodynamic derivatives in generalized form
  - Allows specification of generalized EOS routines without modifying the code numerical formulation
  - Preconditioning to robustly solve for large gradients in density and Mach number near critical point and phase change boundaries
- **Framework Extends to Multi-Species/Phases**
  - **Liquid or vapor species transport solved for separately to model finite rate phase change**
  - **Formulation is easily extendable to additional contaminant species such as water, CO, etc.**
  - **Framework applied to high pressure LNG combustors (@300 bar) and cooling channels**

$$\boxed{\begin{array}{l}\Gamma \dfrac{\partial Q_v}{\partial t} + \dfrac{\partial E}{\partial x} = S + D_v; \\ \Gamma = \dfrac{\partial Q}{\partial Q_v}; \qquad A = \Gamma^{-1} \dfrac{\partial E}{\partial Q_v}\end{array}}$$

$$Q = \begin{bmatrix} \rho \\ \rho u \\ \rho e \\ \rho Y_i \end{bmatrix}; \; Q_v = \begin{bmatrix} p - p_{ref} \\ u \\ T \\ Y_i \end{bmatrix};$$

$$\Gamma = \begin{bmatrix} \rho_p & 0 & \rho_T & \rho_{y_i} \\ u\rho_p & \rho & u\rho_T & u\rho_{y_i} \\ H\rho_p - (1 - \rho h_p) & \rho u & H\rho_T - (1 - \rho h_T) & H\rho_{y_i} + \rho h_{y_i} \\ Y_i\rho_P & 0 & Y_i\rho_T & Y_i\rho_{Y_i} + \rho\delta_{ij} \end{bmatrix}$$

$$\rho = F(P, T, Y_i),$$
$$h = G(P, T, Y_i)$$

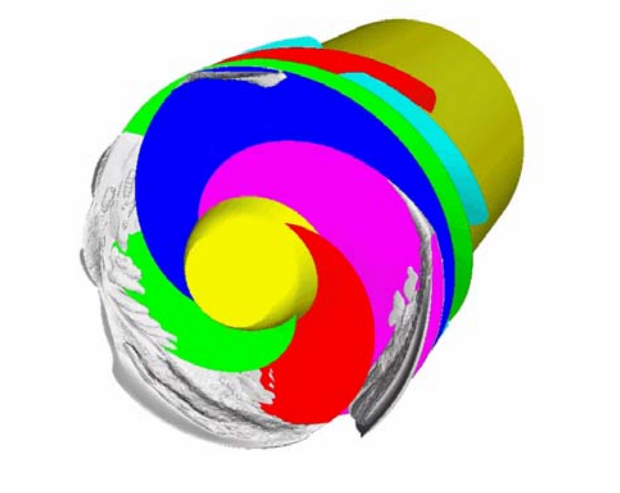
Generalized EOS property specification

EoS and Thermodynamic Property Specification

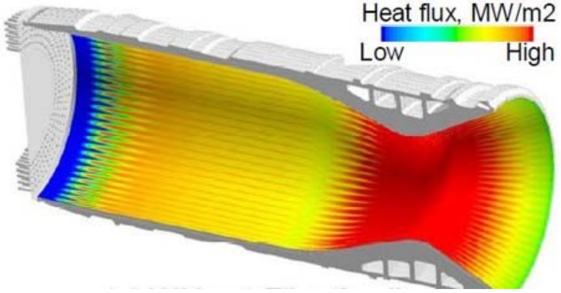
- EoS specification can either be through analytical formulations (e.g. SRK) or through NIST table look-up
  - ➢ Ability to handle real fluid properties and large “spiky” gradients near critical point for pure CO_2
- Work presented here has been using NIST table look-up: saturation bounding line curves for liquid and vapor from NIST also stored in table
  - ➢ No restriction on table resolution from numerical stability perspective
- At subcritical conditions, phase properties are bounded by these saturation curves when phasic conditions go into metastable or unphysical regime
- Finite-rate phase change terms (from liquid to vapor phase or vice-versa) drive the solution to equilibrium and alter pressure and temperature to physical saturation values
- Formulation can be extended for contaminants by solving for additional species for water (liquid and vapor)

Validation for Near Critical, High Pressure Systems

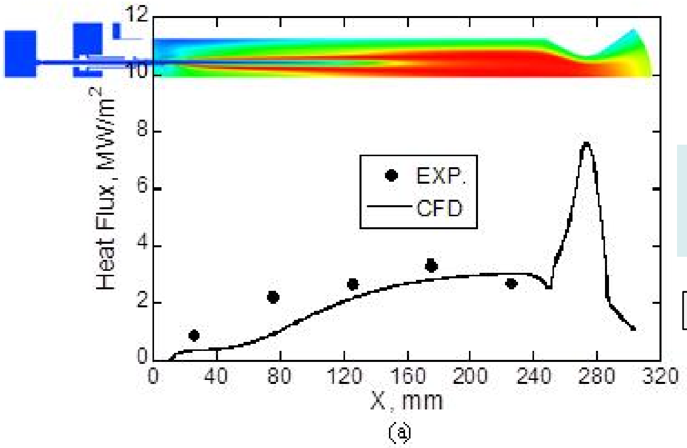
Space Shuttle Liquid Hydrogen Inducer



Combustor Wall Heat Flux



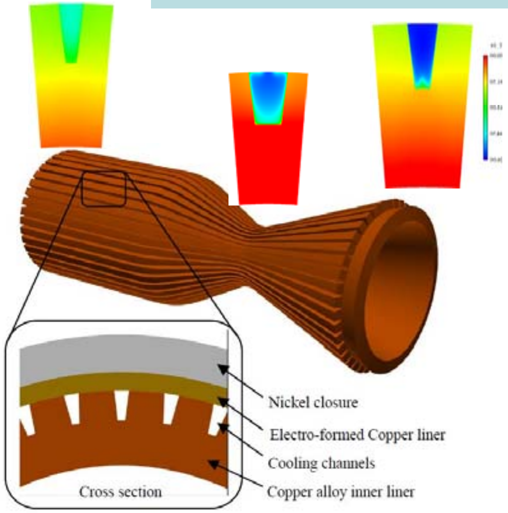
Negishi et al. (2014)



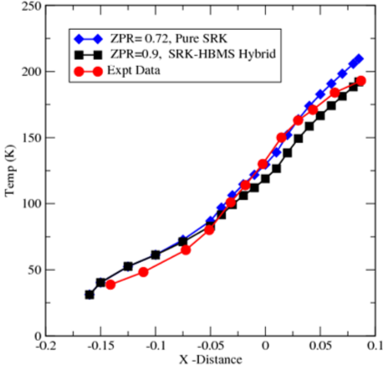
High Pressure Methane Combustion

Daimon et al. (2017)

Coupled Supercritical Combustor- Cryogenic Hydrogen Regenerative Cooling Channels with Thermal Module



Bulk Coolant Temperature



Phase Change Model Discussion

- Phase change models can range from complex non-equilibrium models to simpler equilibrium model
- Non-equilibrium models have been discussed in the context of condensation near critical point
  - Homogeneous condensation nuclei are generated based on classical nucleation theory
  - Condensation nuclei can change size from condensation on them and phase change modeled with non-equilibrium model (e.g. Hertz Knudsen)
  - Droplets solved as discrete phase with independent velocity and temperature
  - Difficulty extending to dense two-phase flows (e.g. 2-phase inlets)
- Equilibrium models are mixture based where common velocity and temperature solved for the components
  - Phase change models based on difference between local pressure and saturation pressure corresponding to local temperature with time constant
  - Cannot model slow down in condensation scales near critical point
  - But can model dense two-phase flows and in particular the phase change models can be used seamlessly for vaporization or condensation
  - Versatility useful across wide range of sub-critical dome operations for compressor
- Focus of this effort is on rigorous validation of equilibrium phase change and subsequent use for subcritical operation of compressor performance
- Non-equilibrium phase change model implementation and testing in progress

Equilibrium Phase Change Model

- Mixture transport equation is solved; velocity identical for both phases
- Finite rate phase change model based on variation of pressure relative to vapor pressure *based on local temperature of fluid*
  - Rate terms for vaporization and condensation drive the solution to pressure equilibrium as well
  - Adequate for "steady" state performance calculations where time scale of phase change is fast relative to flow time scales
  - Model has worked well for cavitating liquid rocket cryogenic pumps

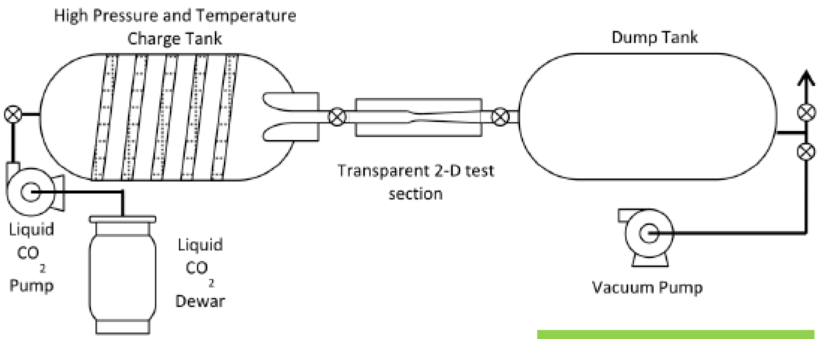
$$m_t = K_f \rho_L \phi_L + K_b \rho_g \phi_g$$

$$K_b = \begin{bmatrix} 0 & p < p_v \\ \frac{1}{\tau_b}\left(\frac{Q_\infty}{L_\infty}\right) \quad [\frac{p - p_v}{\frac{1}{2}\rho_\infty Q_\infty{}^2}] & p > p_v \end{bmatrix}; \; K_f = \begin{bmatrix} 0 & p > p_v \\ \frac{1}{\tau_f}\left(\frac{Q_\infty}{L_\infty}\right) \quad [\frac{p - p_v}{\frac{1}{2}\rho_\infty Q_\infty{}^2}] & p < p_v \end{bmatrix}$$

τ_f = Time constant for vapor formation

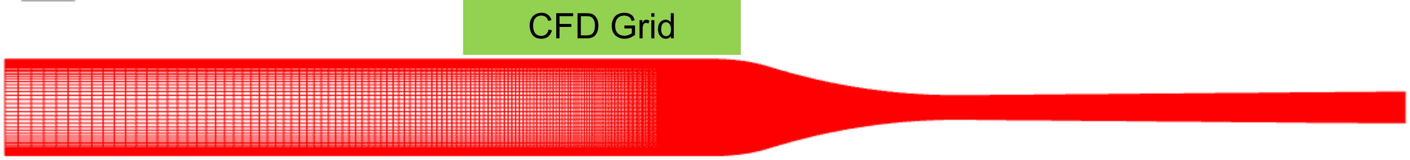
τ_b = Time constant for liquid reconversion

Condensation Validation – Supersonic Nozzle



Lettieri, C., Paxson, D., Spakovszky, Z., and Bryanston-Cross, P., " Characterization of Non-Equilibrium Condensation of Supercritical Carbon Dioxide in a DeLaval Nozzle", Journal of Engineering for Gas Turbines and Power 140 (4), 201

CFD Grid

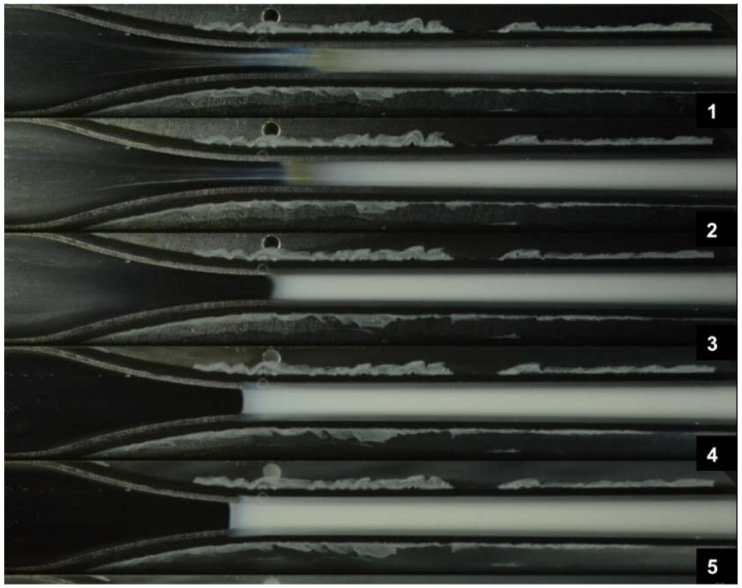


- Blowdown facility for high pressure CO2 (58 – 84 bar) at low temperatures (around 310-315 K) leads to subcooled supersonic flow in nozzle throat resulting in condensation
- Three different grid resolutions in throat region were simulated: a) 0.1 mm, b) 0.05mm, and 0.0025mm
  - As inlet pressure goes up calculation difficulty increases due to larger density ratio and more rapid condensation at onset
  - For the highest pressure cases of 84 and 80 bar the 0.05 mm grid was not adequate and the fine grid of 0.0025 m was necessary
  - All cases were calculated on fine grid for consistency
- NIST table was generated with 3001 points in temperature from 245-315K and 5001 points in pressure from 1.5-8.5 MPa
  - The increased resolution in table did not make any appreciable difference compared to table with 1001 points in temperature and 3001 points in pressure
- Present CFD calculations with CRUNCH CFD done with *equilibrium framework* where mixture conservation equations solved for a fluid that can consist of liquid and vapor

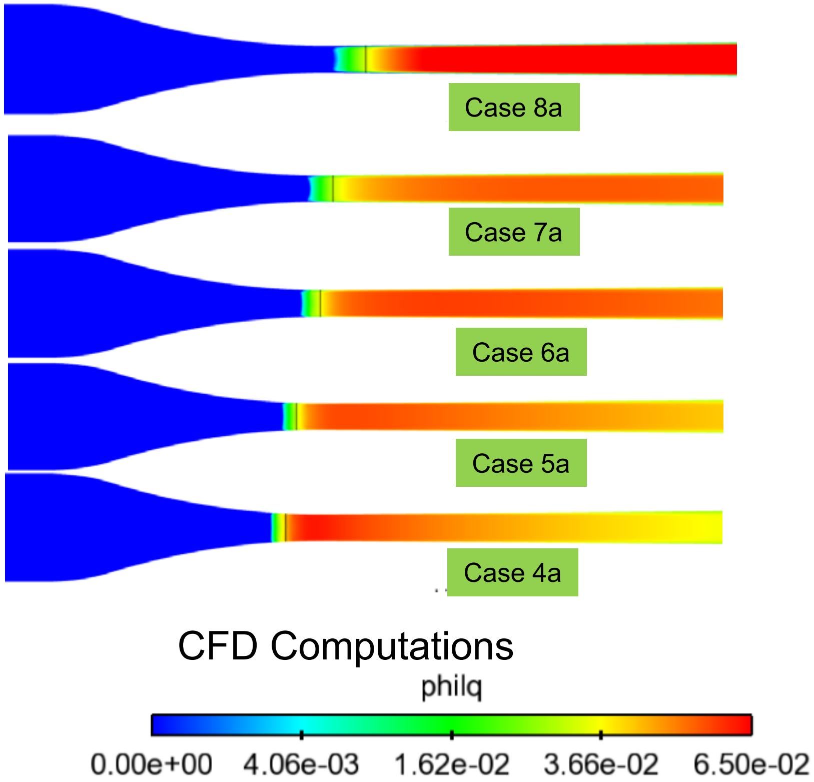
Test Data Points For Validation

Case	P_T (bar)	T_T(K)	S (J/Kg-K)	P_T/P_c	T_T/T_c	S/S_c
8a	58.96	314.67	1862.6	0.7992	1.0346	1.298
7a	65.35	311.99	1796.2	0.8858	1.0258	1.252
6a	73.53	313.60	1736.2	0.9767	1.0311	1.210
5a	79.99	313.94	1669.8	1.0842	1.0322	1.164
4a	84.74	313.88	1599.0	1.1486	1.0321	1.114

Qualitative Comparison of Condensation Pattern



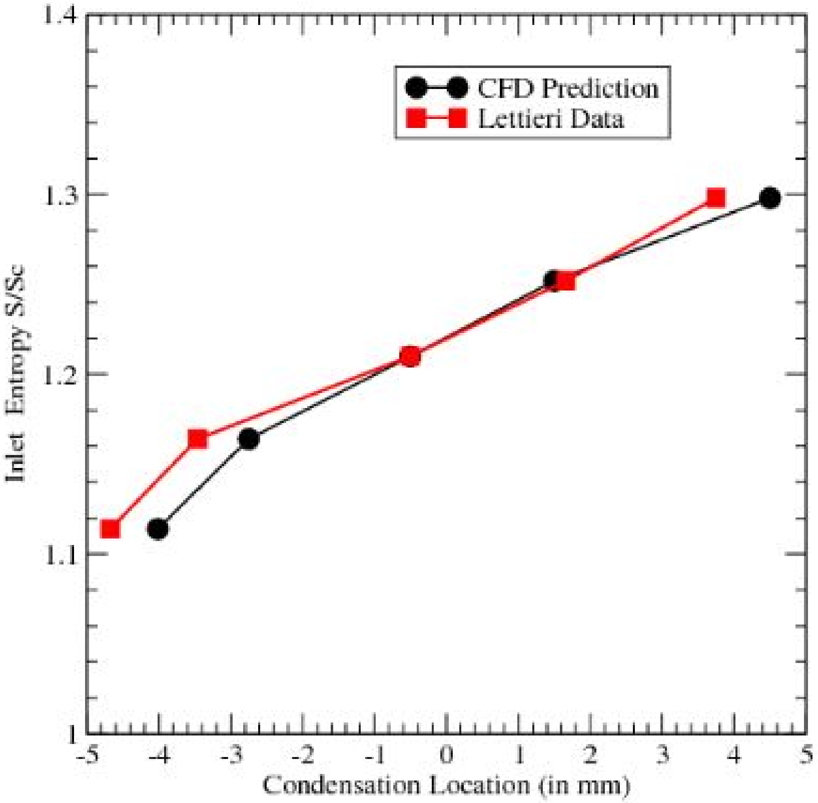
Representative Test Data



CFD Computations

Good qualitative comparison of condensation onset as inlet pressure increases; condensation onset moves upstream and into converging section at highest pressure of 84 bar

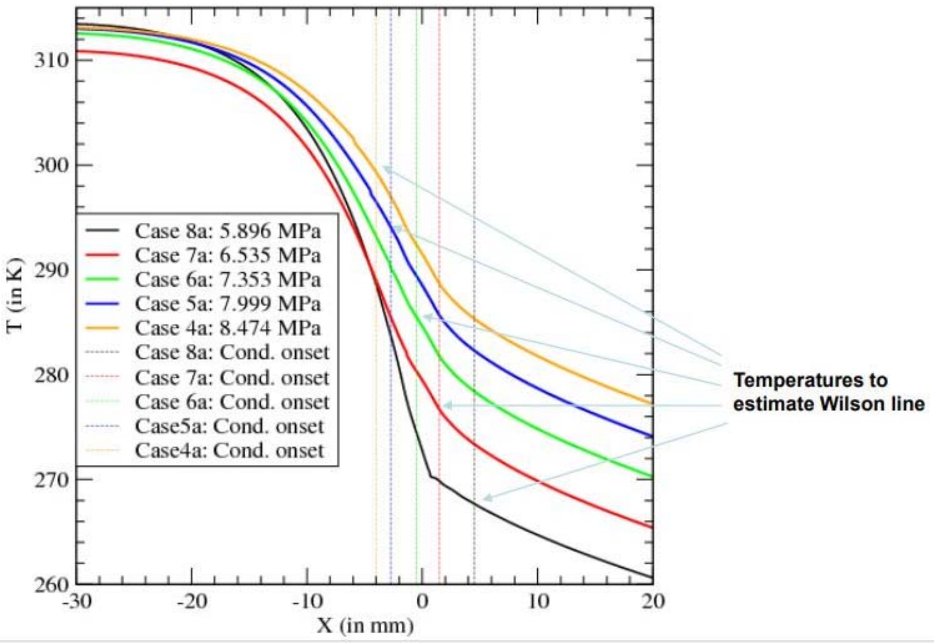
Quantitative Comparison of Condensation Onset



Quantitative comparison of condensation onset is good including change in slope at highest pressure of 84 bar (inlet entropy close to 1.1)

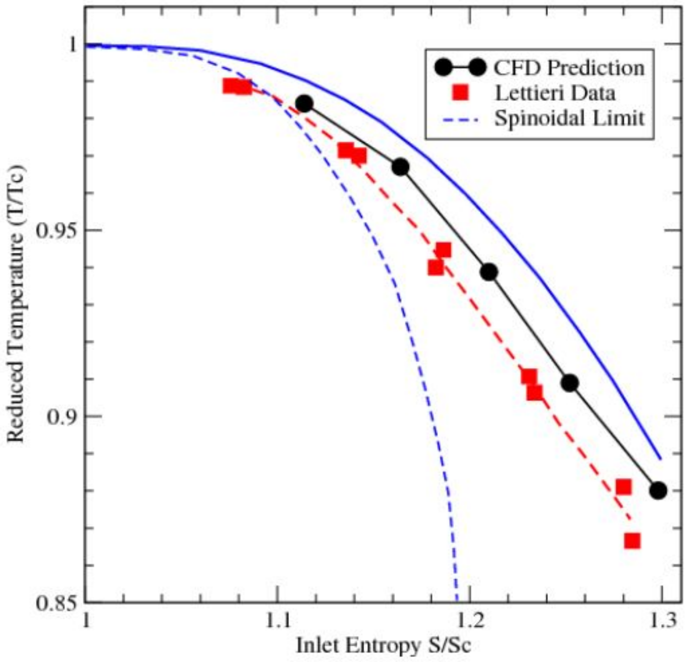
Wilson Line Comparisons

Temperature at Onset



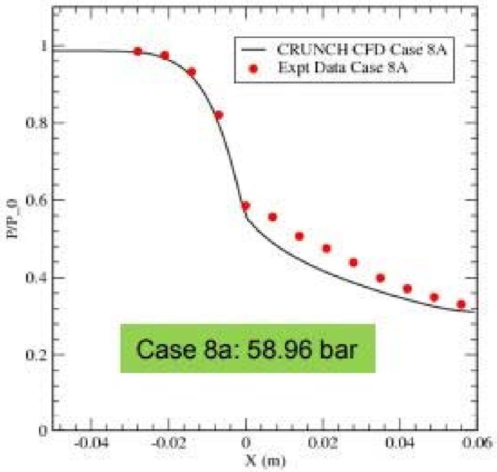
Temperatures to estimate Wilson line

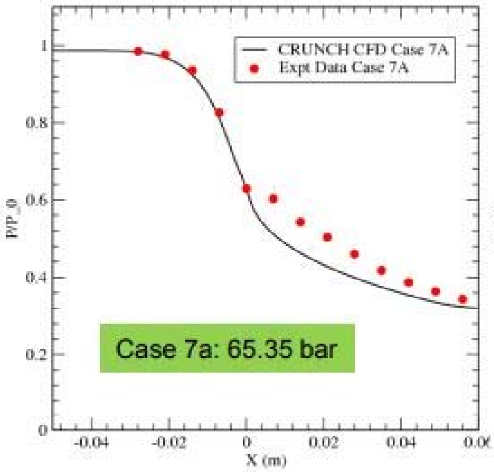
Reduced Temperature vs Inlet Entropy

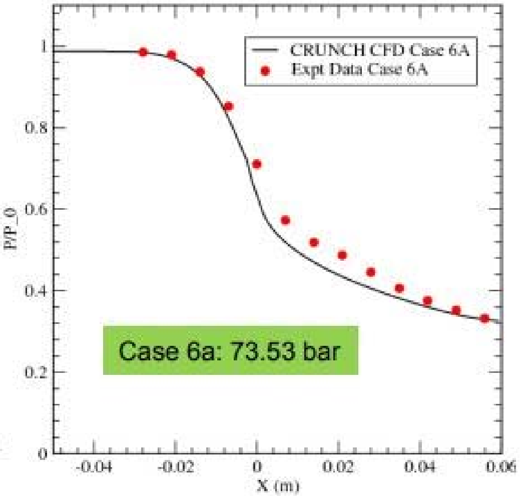


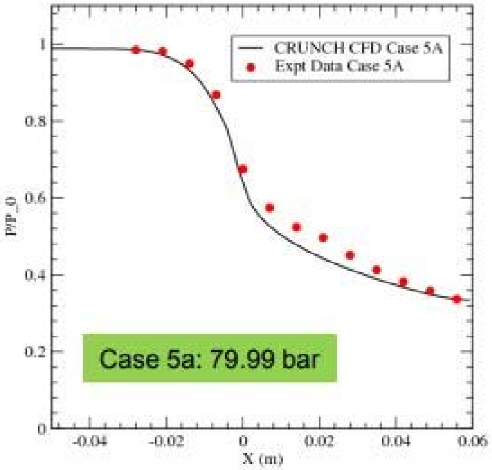
Computed Wilson line match improves at higher pressure as condensation becomes more rapid and equilibrium is attained faster

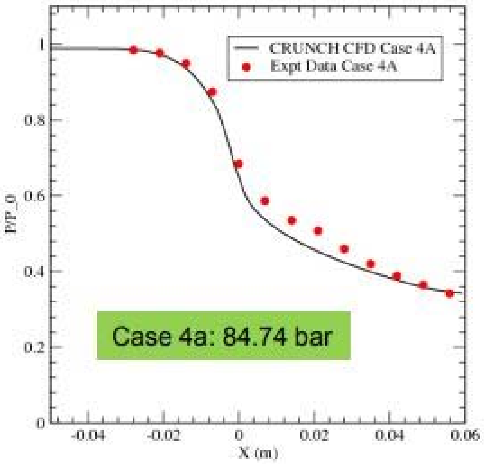
Pressure Comparisons


Case 8a: 58.96 bar


Case 7a: 65.35 bar

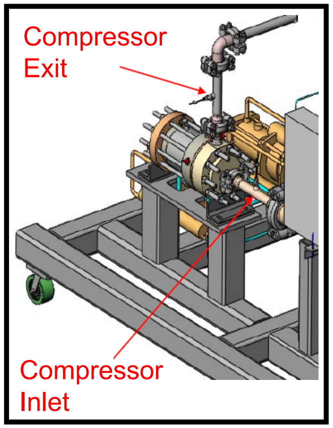

Case 6a: 73.53 bar


Case 5a: 79.99 bar

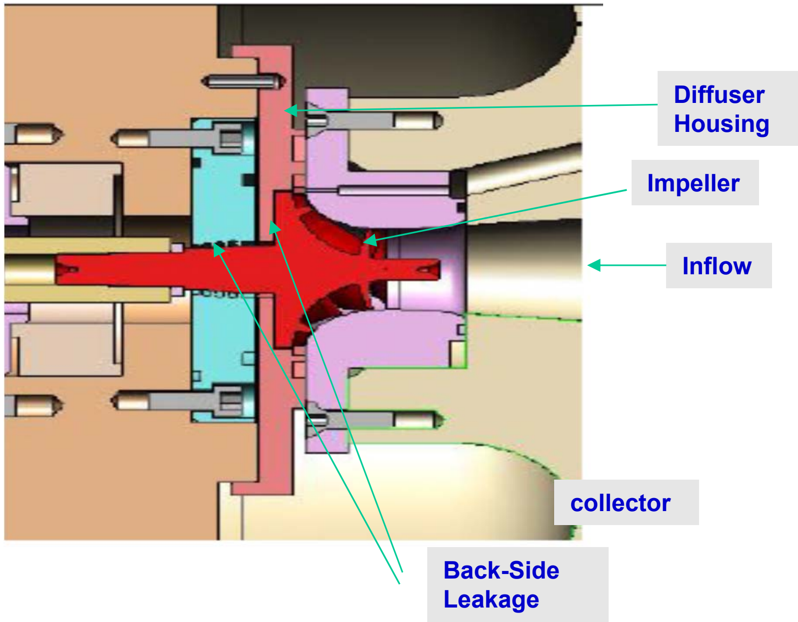

Case 4a: 84.74 bar

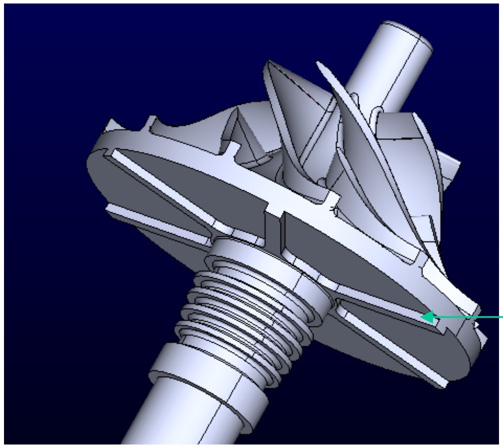
Sandia Test Loop and Hardware

Test Configuration



Compressor Configuration

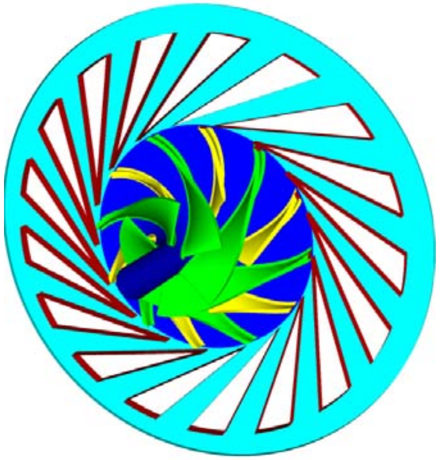




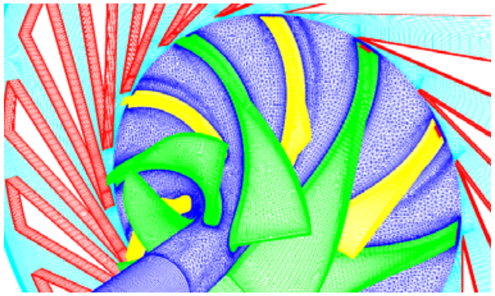
Pump-Out vanes on back-side leakage. This is not modeled in CFD and therefore shaft horse power for CFD calculations have to be corrected for these losses

CFD Model Details

- Simulated as-tested hardware. Impeller and diffuser geometry
  - Obtained impeller/diffuser geometry from Barber-Nichols Inc
- High quality grid for single passage of impeller and diffuser generated along with an axial inflow pipe section
  - Inflow pipe: 69 K cells
  - Impeller : 1.18 M cells
  - Diffuser : 65 K cells
- CFD data at the diffuser exit and impeller exit (did not have volute/pipe design information)
  - Test data at compressor exit
  - Losses in collector and exit pipe not modeled but expected to be small
  - Losses in back-side leakage not modeled. This will have a significant affect on efficiency
  - Tip gap modeled at design value
- Due to tremendous impact of inlet conditions on performance, all data and calculations are corrected to a reference (i.e., design) set of inlet condition



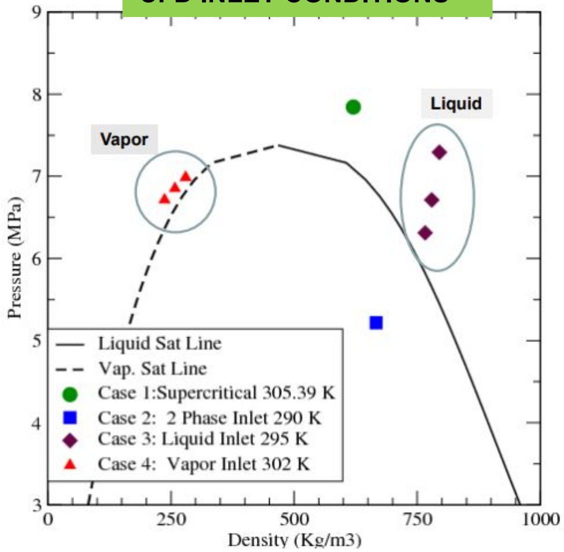
CFD CONFIGURATION:
Exit boundary at diffuser exit

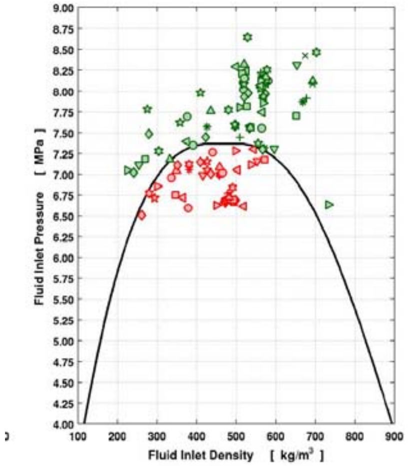


Sandia Test Compressor: Computations With Phase Change

- Four sets of calculations performed
- Case 1: Supercritical inlet conditions.
  - 7.843 MPa, 305.39 K
  - RPM 55872, Mass flow: 2.24 Kg/s (5 lbm/s)
- Case 3: Subcritical compressed liquid
  - 295 K, 100% liquid (Vapor Press: 5.982 MPa)
  - Pressure: 6.31 MPa, 6.71 MPa, and 7.29 MPa
  - RPM: 53240, Mass Flow: 2.6 Kg/s (5.37 lbm/s)
- Case 4: Subcritical vapor inlet
  - 302 K, 100% Vapor (Vapor Pressure 7.02 MPa)
  - Pressure: 6.71 MPa, 6.85 MPa, and 6.98 MPa
  - RMP: 55872, Mass Flow: 0.89 Kg/s
  - *Keep Flow Coefficient roughly same as Liquid case*
- Case 2: Subcritical 2-Phase inlet
  - 5.21 MPa, 290 K, 80% Liquid/20% Vapor Volume
  - RPM: 53240 RPM, Mass Flow: 2.6 Kg/s (5.37 lbm/s)
- Phase change modeled with equilibrium model validated for De Laval nozzle
- Validation for supercritical performance over a range of mass flow rates performed earlier

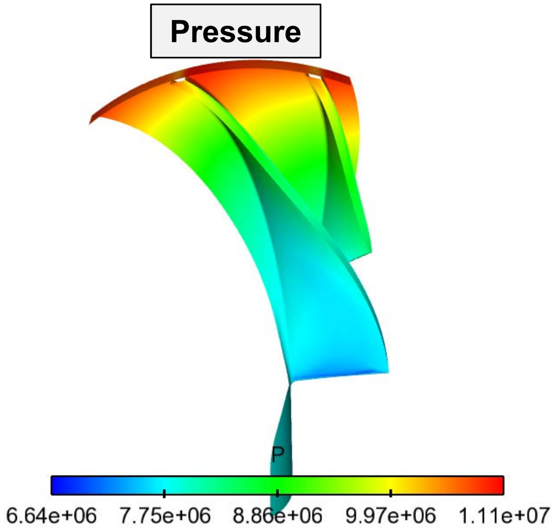
CFD INLET CONDITIONS

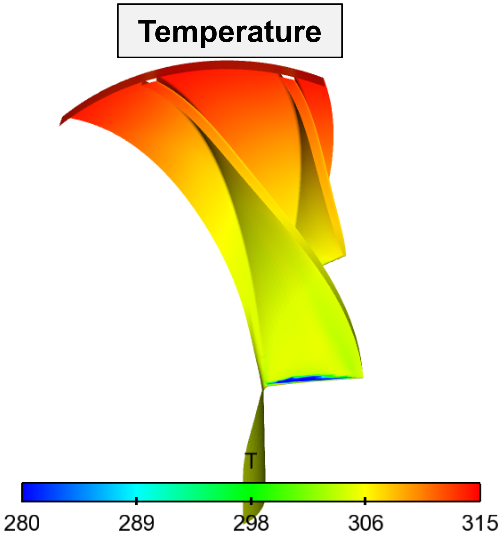


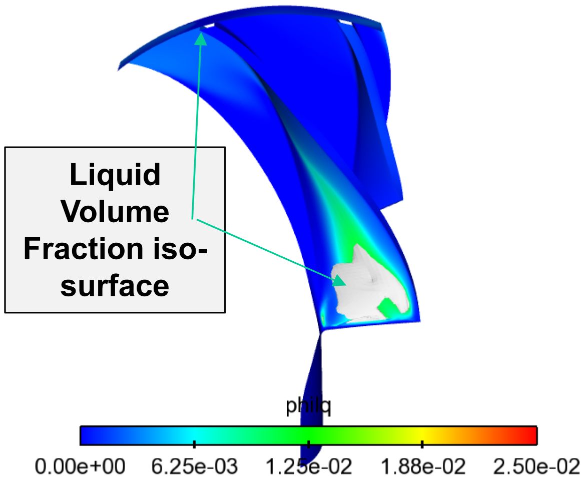


Sandia Test results (Noall and Pasch)

Condensation Supercritical Inlet Temp (305.4 K): 5 lbm/s


Pressure

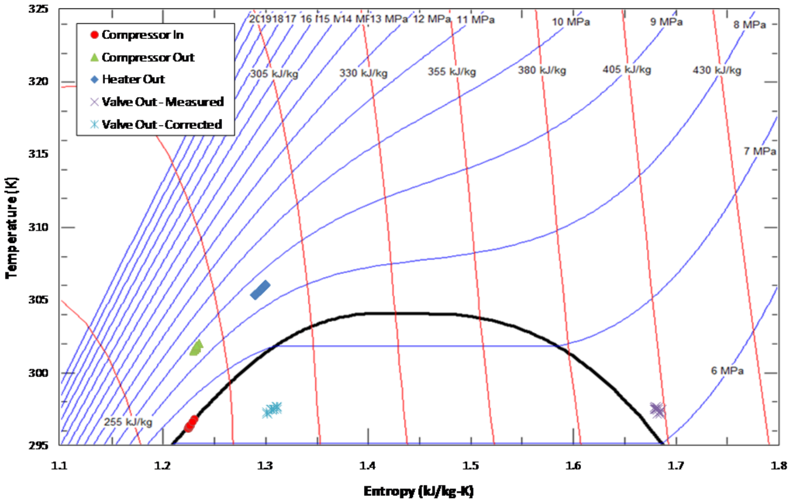

Temperature


Liquid Volume Fraction iso-surface

Very small of liquid condenses near the leading edge (max volume fraction 2.5%). The condensation zone is localized around the blade as shown by isosurface (1% volume fraction of liquid).
Issue of condensation near critical point still a point of contention in the literature

Liquid Inlet Calculation at 295K

Case	Inlet Pressure (MPa)	Inlet Temp. (K)	Exit Pressure (Mpa)	Exit Temp. (K)
Case 3a	7.292	295	11.4	303.29
Case 3b	6.711	295	11.9	302.94
Case 3c	6.311	295	12.6	302.55



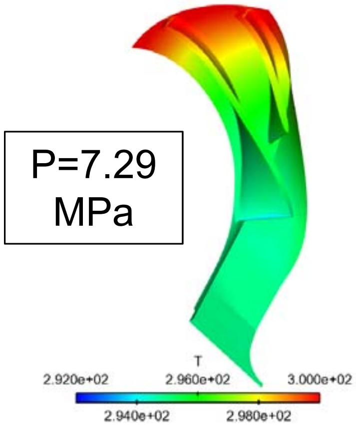
Sandia Test results:
Liquid Inlet at 296 K
(Wright et al. Sandia Report: 8840)

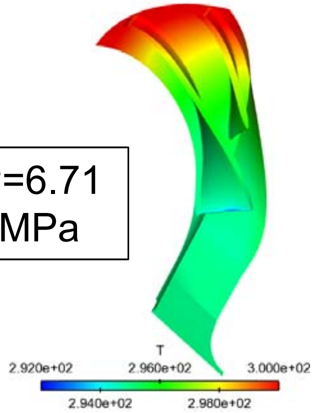
Liquid Inlet Calculation at 295K

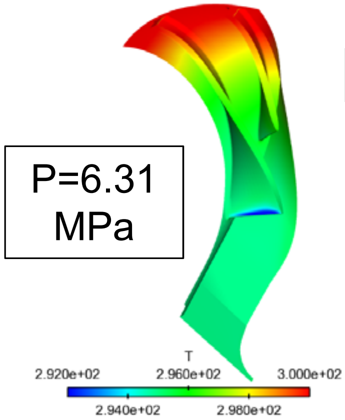
P=7.29 MPa

P=6.71 MPa

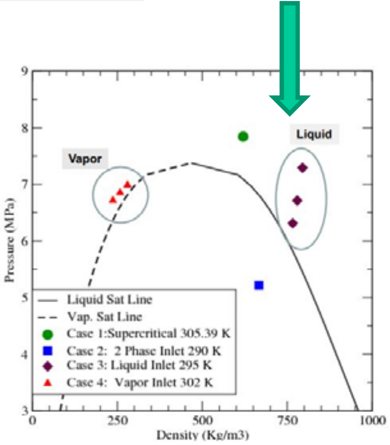
P=6.31 MPa



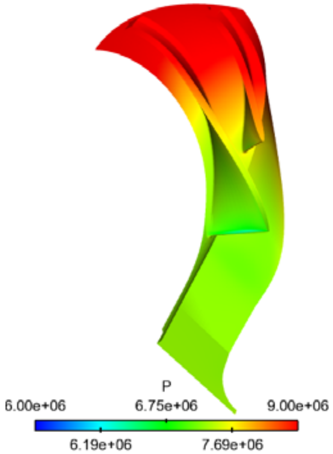


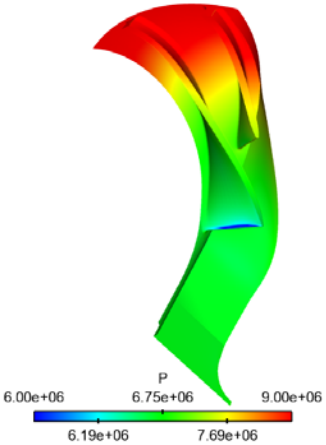


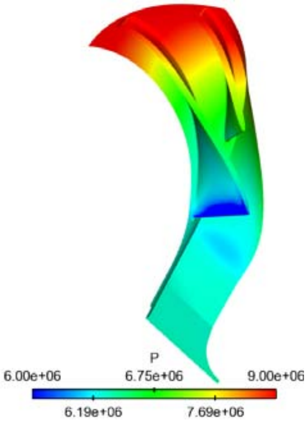
Temperature



Pressure

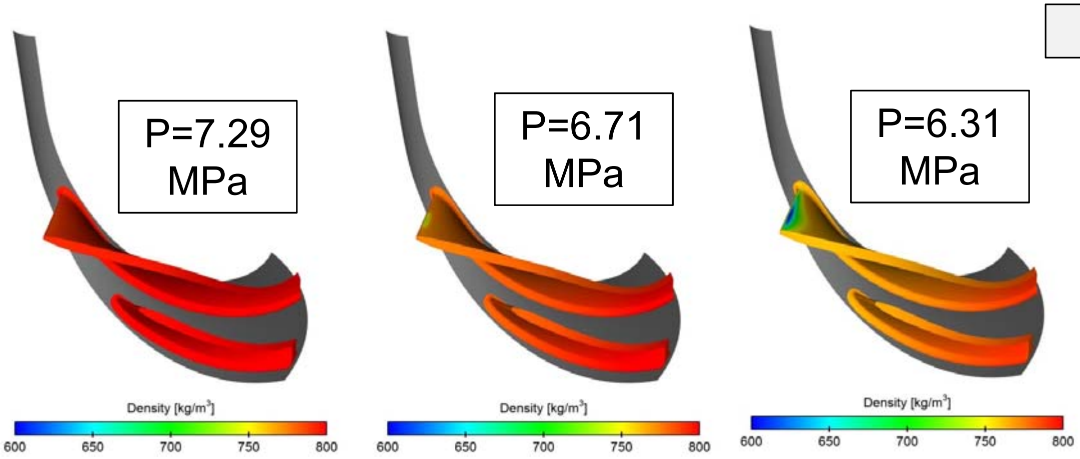






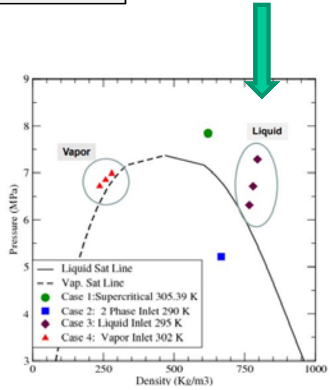
Liquid Inlet Calculation at 295K

Density

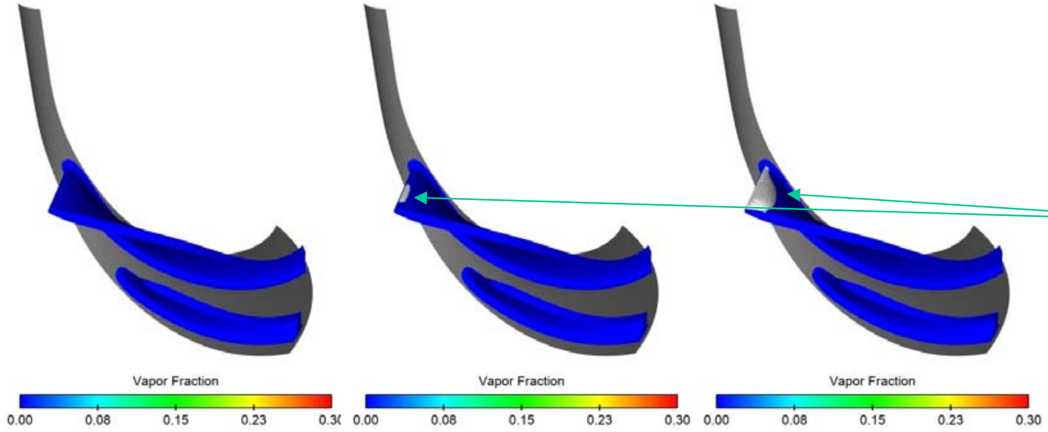

P=7.29 MPa

P=6.71 MPa

P=6.31 MPa



Vapor Volume Fraction

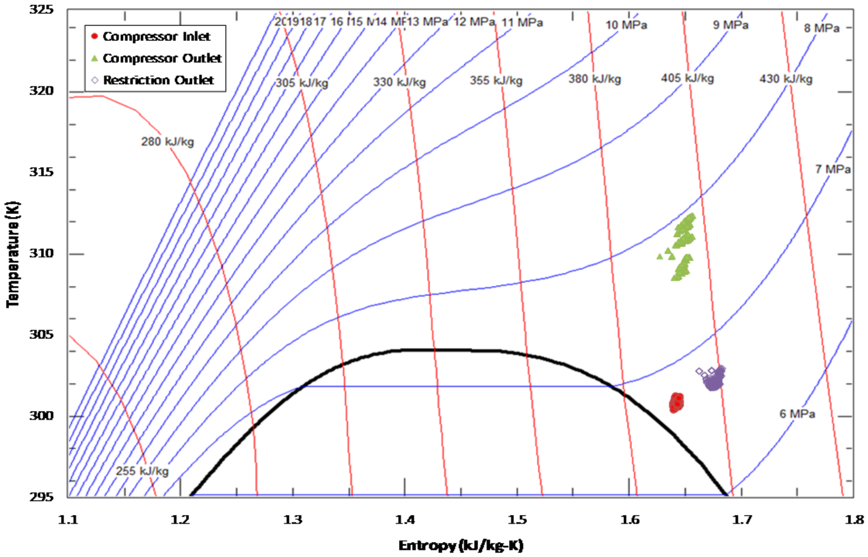


Vapor formation at leading edge as pressure drop is greater than saturation pressure drop from temperature decrease

Vapor Inlet Calculation at 302 K

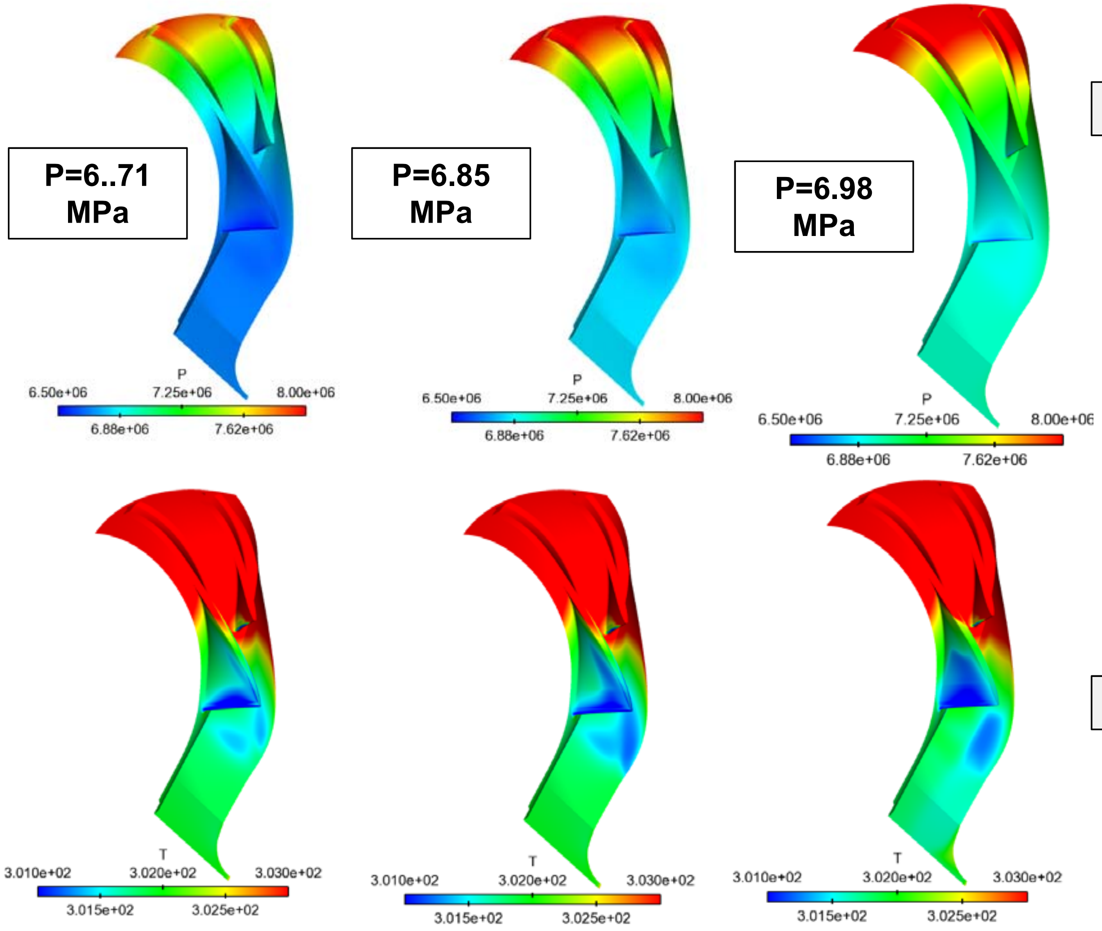
Case	Inlet Pressure (MPa)	Inlet Temp. (K)	Exit Pressure (Mpa)	Exit Temp. (K)
Case 4a	6.712	302	8.501	318.67
Case 4b	6.850	302	8.85	319.25
Case 4c	6.979	302	9.17	319.98

Mass flow rate had to be reduced to 0.89 kg/s from 2.67 kg/s for liquid since density is lower by a factor of 3. Implications for unsteady or transient conditions?



Sandia Test results:
Vapor Inlet at 300 K
(Wright et al. Sandia Report: 8840)

Vapor Inlet Calculation at 302 K

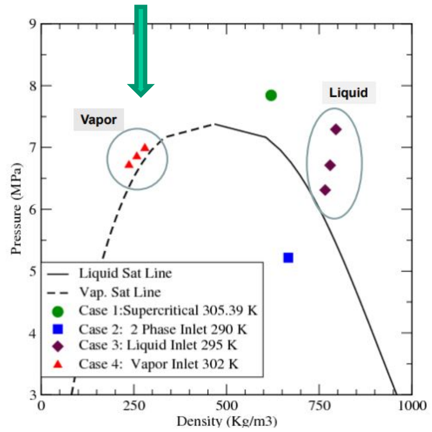


P=6..71 MPa

P=6.85 MPa

P=6.98 MPa

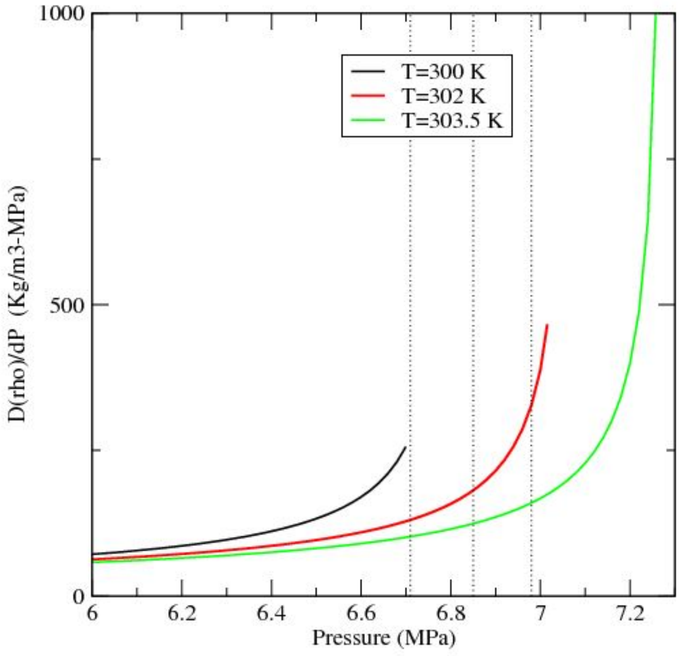
Pressure



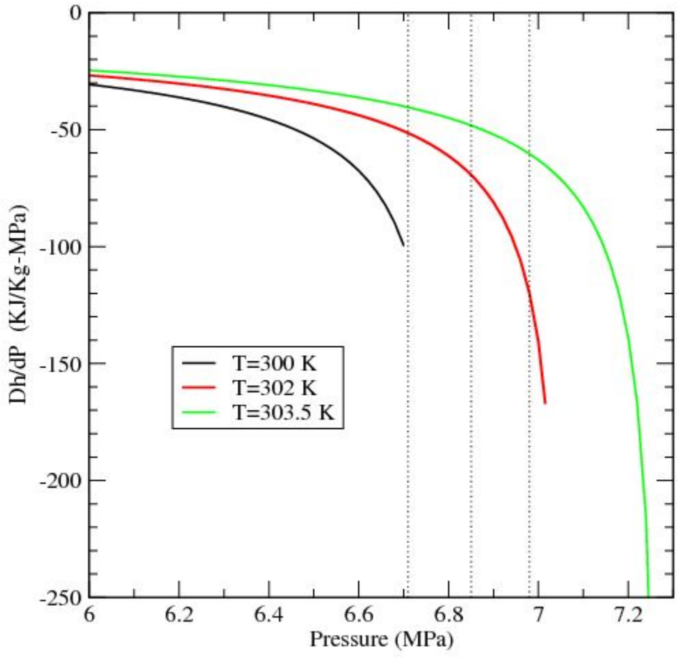
Temperature

Real Fluid Effects Near Saturation Point

Compressibility In Vapor: Isotherms



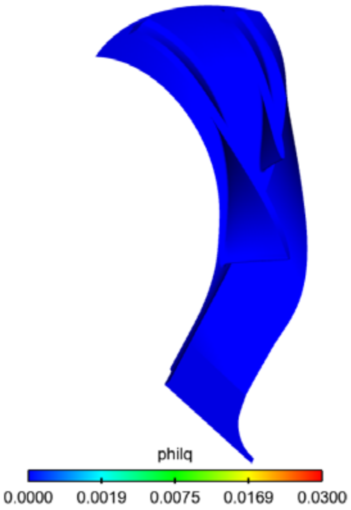
Non-ideal Enthalpy In Vapor: Isotherms



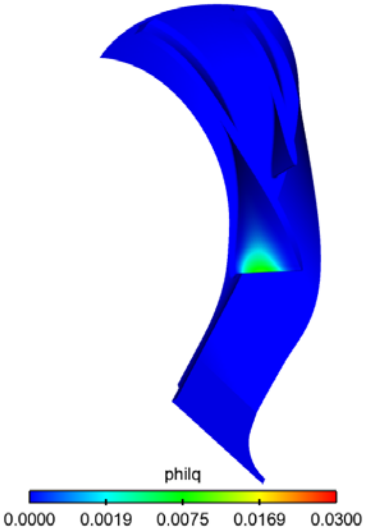
Vapor Inlet Calculation at 302 K

Condensation for Vapor Inlet Conditions

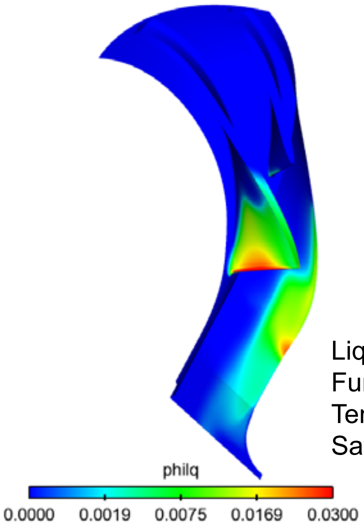
P=6.71 MPa
Temp=302 K

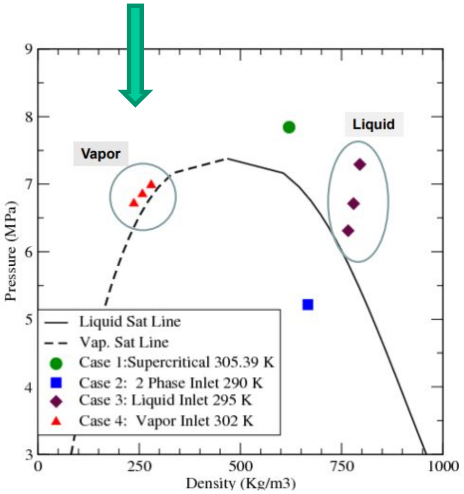


P=6.85 MPa
Temp=302 K



P=6.98 MPa
Temp=302 K





Liquid Condensation Volume Fraction as a Function of Inlet Pressure for an Inlet Temperature of 302 K.
Saturation Pressure at 302 K= 7.02 MPa

- At elevated temperatures (close to critical temperature) at pressures close to saturation value condensation will increase substantially presumably due to real fluid effects
- Condensation will likely occur in suction inflow due to flow accelerations and nonuniformity from pipe bends, area constrictions, etc.
- Inflow to impeller will be two-phase with condensate; effects are mitigated by lower density ratios as we get closer to critical temperature

2-Phase Inlet Calculation

- 2-Phase Inlet at 290 K and 5.21 MPA (close to saturation pressure at 290K) computed with 20% vapor by volume and 80% liquid by volume
  - RPM 53240
  - Mass Flow Rate: 5.736 lbm/s
- Phase change as pressure rises in compressor accounted for
- Enthalpy rise is substantial and comparable to single phase calculation
- However temperature rise is lower and the fluid exits diffuser at subcritical temperature

	Inlet	**Impeller Exit**	**Diffuser Exit**
Temperature (K)	290 K	295.43	297.83
Pressure (MPA)	5.217	8.08	9.64
Total Pressure (MPA)	5.23	10.10	9.877

$$\Delta h_{impeller} = 2.14\ Btu / lbm$$

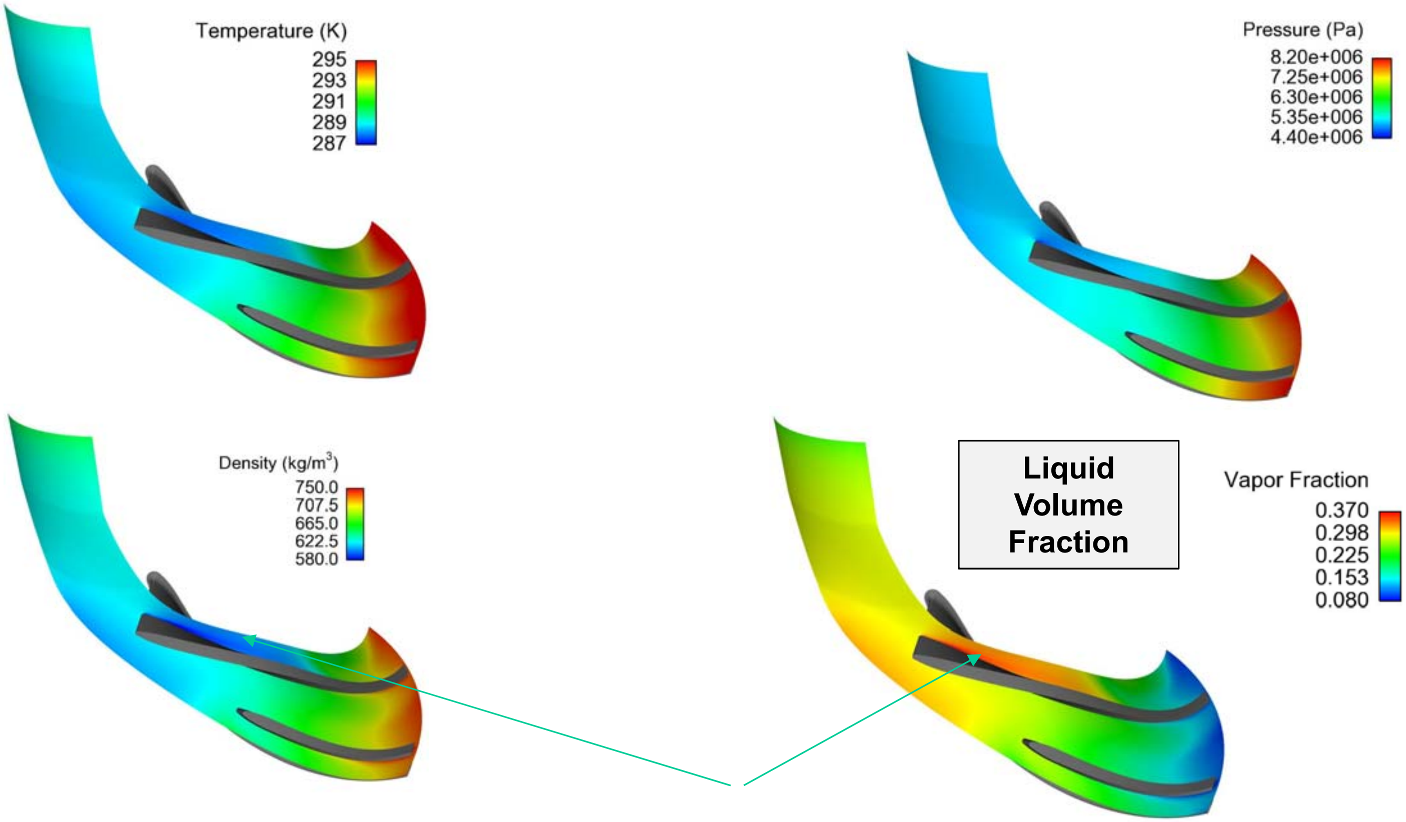
$$\Delta h_{diffuser} = 3.13\ Btu / lbm$$

2-Phase Inlet Calculation at 290K

Temperature

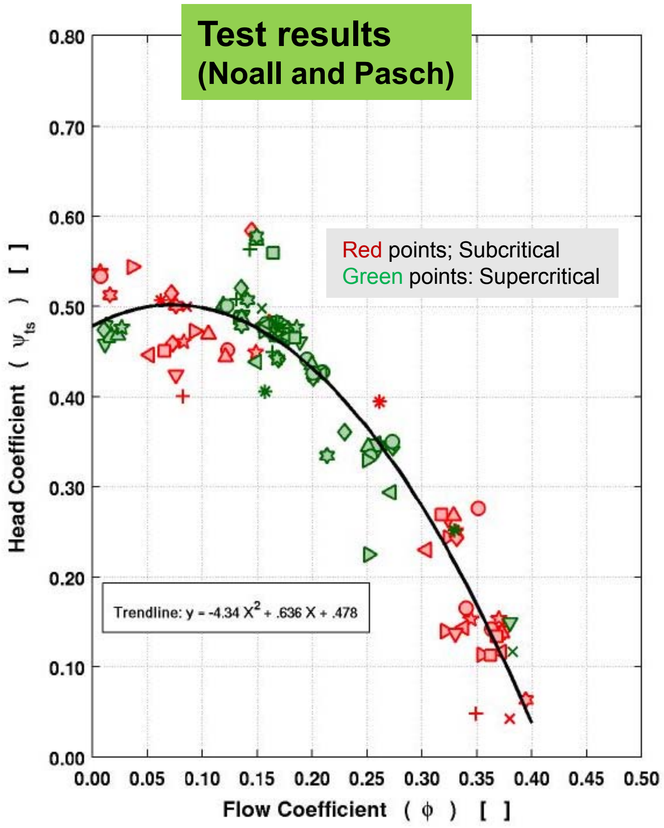
Pressure

Liquid Volume Fraction

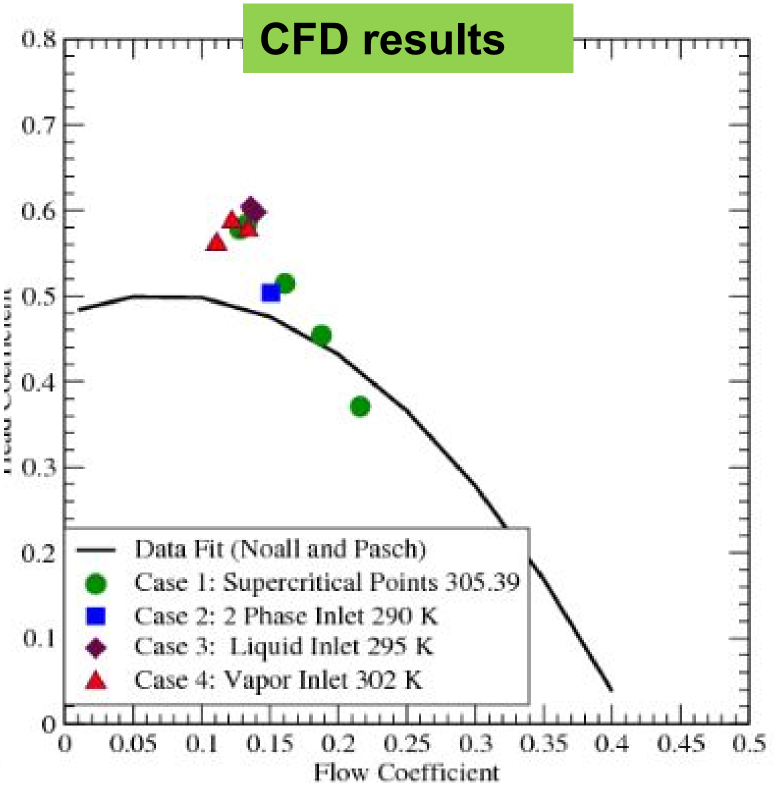


The temperature and pressure around leading edge vary in a manner to cause vaporization at the leading edge before condensation eventually occurs due to pressure rise. The situation may reverse for a different inlet composition with majority of vapor and smaller fraction of liquid

Comparison with Test Data: Head Rise vs Flow Coefficient


Test results (Noall and Pasch)

Red points; Subcritical
Green points: Supercritical


CFD results

Conclusions and Future Work

- Advanced numerical framework for CO2 compressors operating near critical point has been demonstrated in the CRUNCH CFD® code
  - Framework can model both sub-critical and supercritical conditions including 2-phase inlet
  - It permits extensions to solving CO2 with contaminants such as water for example
  - Current equilibrium phase change model has been validated and applied to two-phase compressor flowfield computations
- Rigorous validation for condensation of CO_2 in De Laval nozzle over a range of high pressures by comparing with test data from Lettieri
  - Location of condensation onset and its trend with inlet pressures compares well with data both qualitatively and quantitatively
  - Temperature values at onset location show sub-cooling is underpredicted but Wilson line from CFD is parallel to test data
  - Pressure comparisons show pressure underpredicted at condensation onset location but gets closer to test data downstream

Conclusions and Future Work (Contd…)

- Calculations of Sandia compressor with phase change performed over a range of conditions
  - At supercritical near design inlet conditions: small levels of condensation near leading edge and trailing edge of impeller observed. Issue of slow down in condensation time scales near critical point cannot be addressed with current equilibrium model
  - Liquid inlet conditions: Impeller behaves like pump with cavitation near leading edge as pressure drops near saturation values. Density variations are small and stability concerns lower.
  - Vapor inlet conditions; Large changes density and inlet mass flows have to drop to maintain floe coefficient. Significant condensation including in suction inlet as pressure rises to near saturation values. Concern for instability high for unsteady inlet conditions.
  - 2-Phase Inlet: For 80% liquid and 20% vapor (at 290K) shows cavitation in impeller. Situation may reverse if inlet composition is mainly vapor
- Future Studies:
  - Implement non-equilibrium framework with condensation nuclei and phase change driven by a non-equilibrium source term such as Hertz-Knudsen formulation. Repeat condensation validation for DeLaval nozzle.
  - Detailed validation for a integrally-geared compressor-expander in a SCO2 recompression cycle for a 10 MWe CSP application; Compressor-expander designed by Hanwha Techwin (HTW) and test to be conducted at SwRI under an EERE funded project
  - Model water contamination effects

Acknowledgements

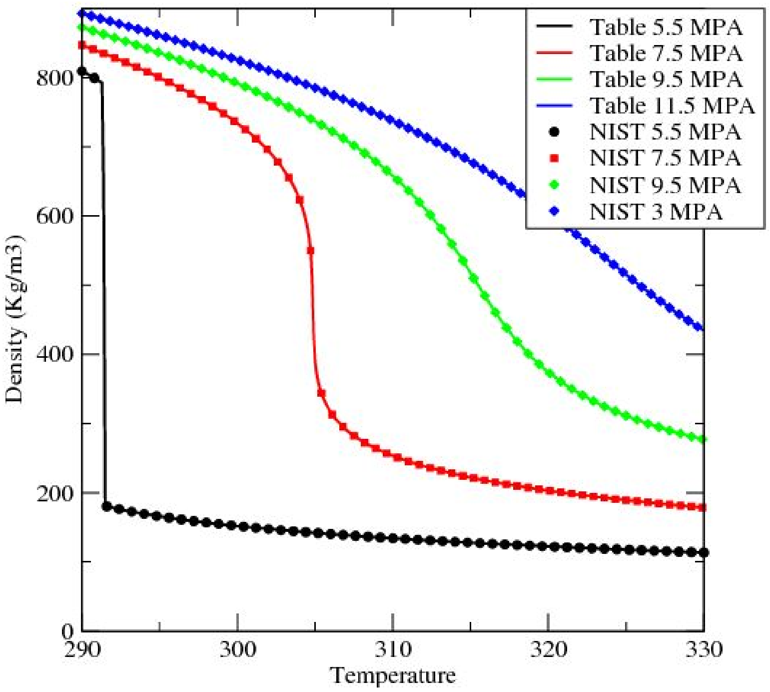
This work is being performed under an ongoing DoE Phase II SBIR grant with Mr. Parrish Galusky as the program monitor. We gratefully acknowledge support for this program from NETL, Morgantown as well as the technical guidance from Drs. Steve Zitney and Eric Liese at NETL.

We would also like to thank Mr. Bob Fuller from Barber Nichols Inc. for providing us with the geometry for the compressor as well as the raw data obtained by BNI as part of their test program. This effort would not have been possible without his help. We also gratefully acknowledge the support provided by Dr. Judy Busby from JB Design and Consulting LLC for helping us analyze and compare compressor performance data.

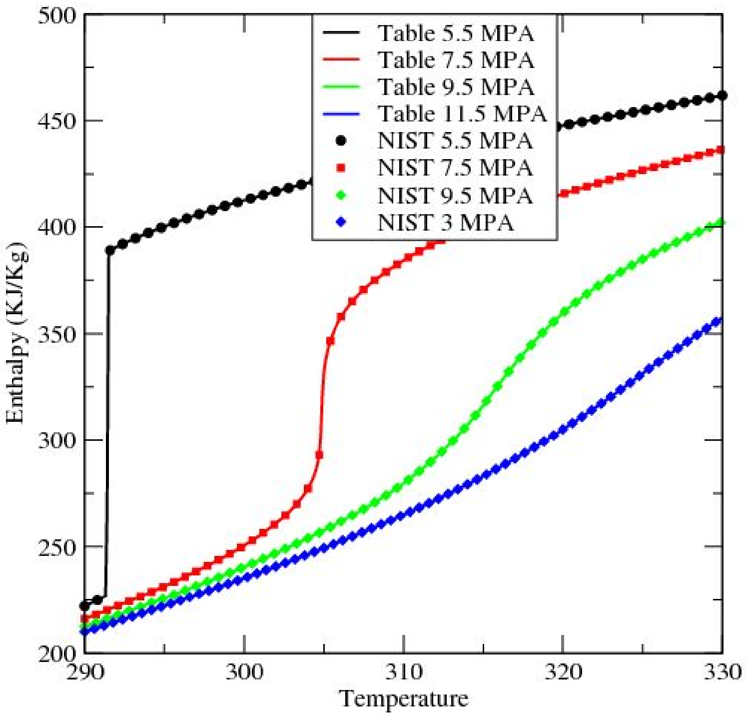
Last, but not least, we would like to thank Prof. Lettieri for providing us his test data on the De Laval nozzle and giving us his feedback on the CFD comparisons.

BACK-UP

Table Look-up Comparison with NIST



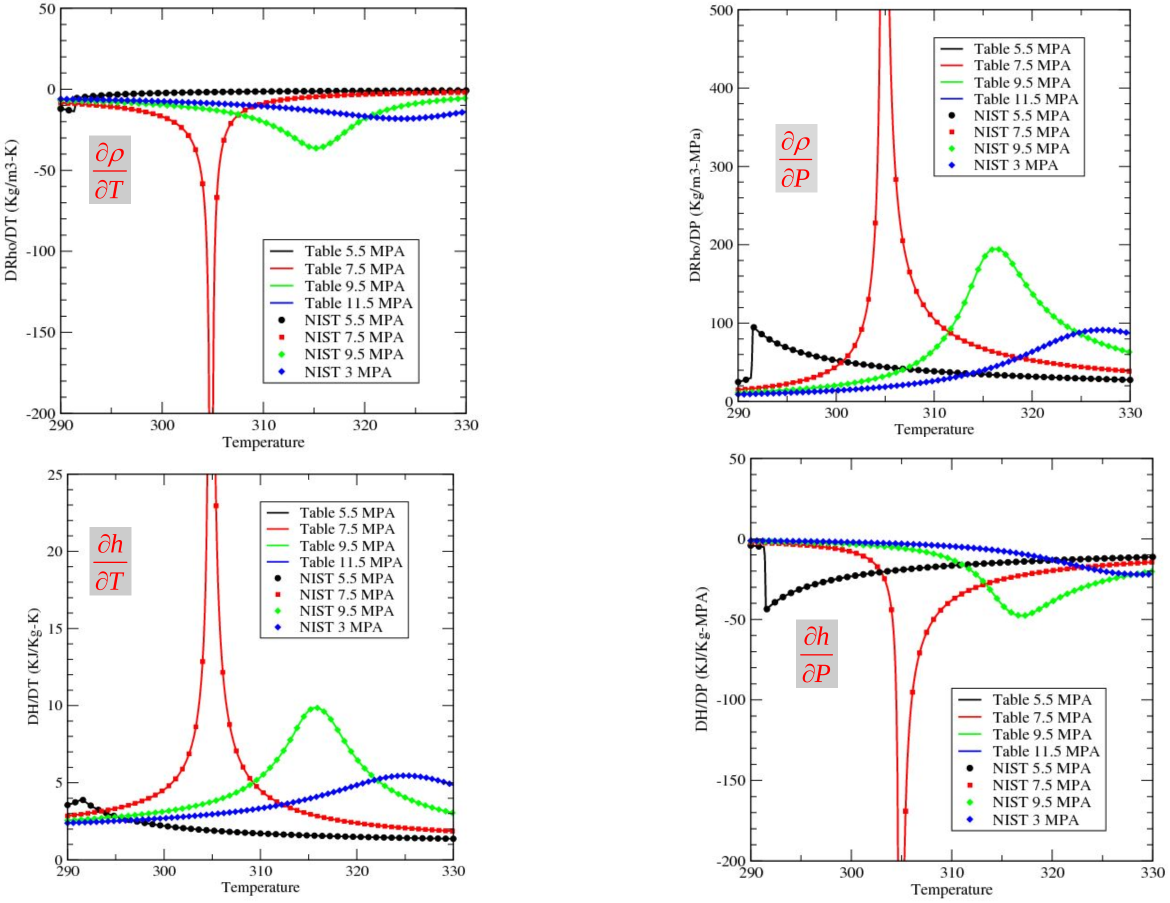
Density



Enthalpy

Verifies that table-lookup and interpolation procedure is working correctly within CRUNCH CFD®

Table Look-up Comparison with NIST: Derivatives

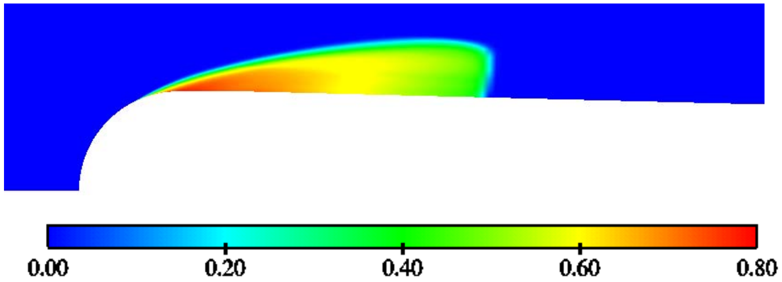


Large derivatives at critical temperature as well as pseudo-critical temperatures at higher pressure resolved accurately by table resolution

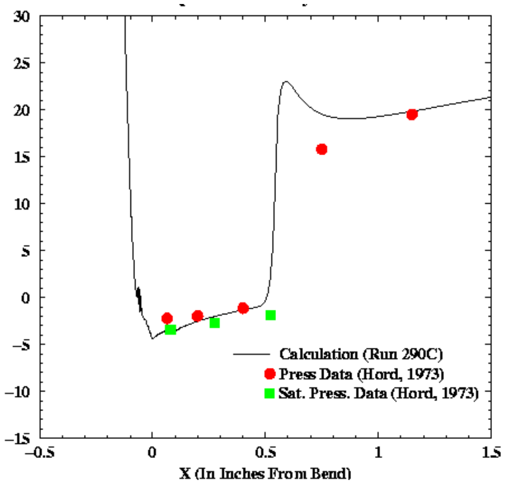
Cavitating Hydrofoil: Liquid Nitrogen

Hosangadi, A. and Ahuja, V., "Numerical Study Of Cavitation In Cryogenic Fluids," *Journal of Fluids Engineering*, Vol. 127, pp. 267-281, March 2005.

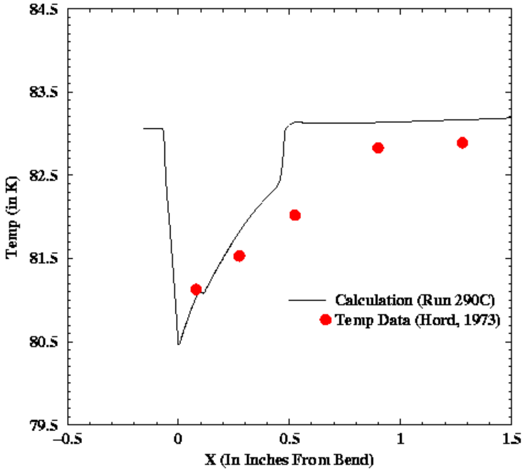
Vapor Volume Fraction



Pressure Depression



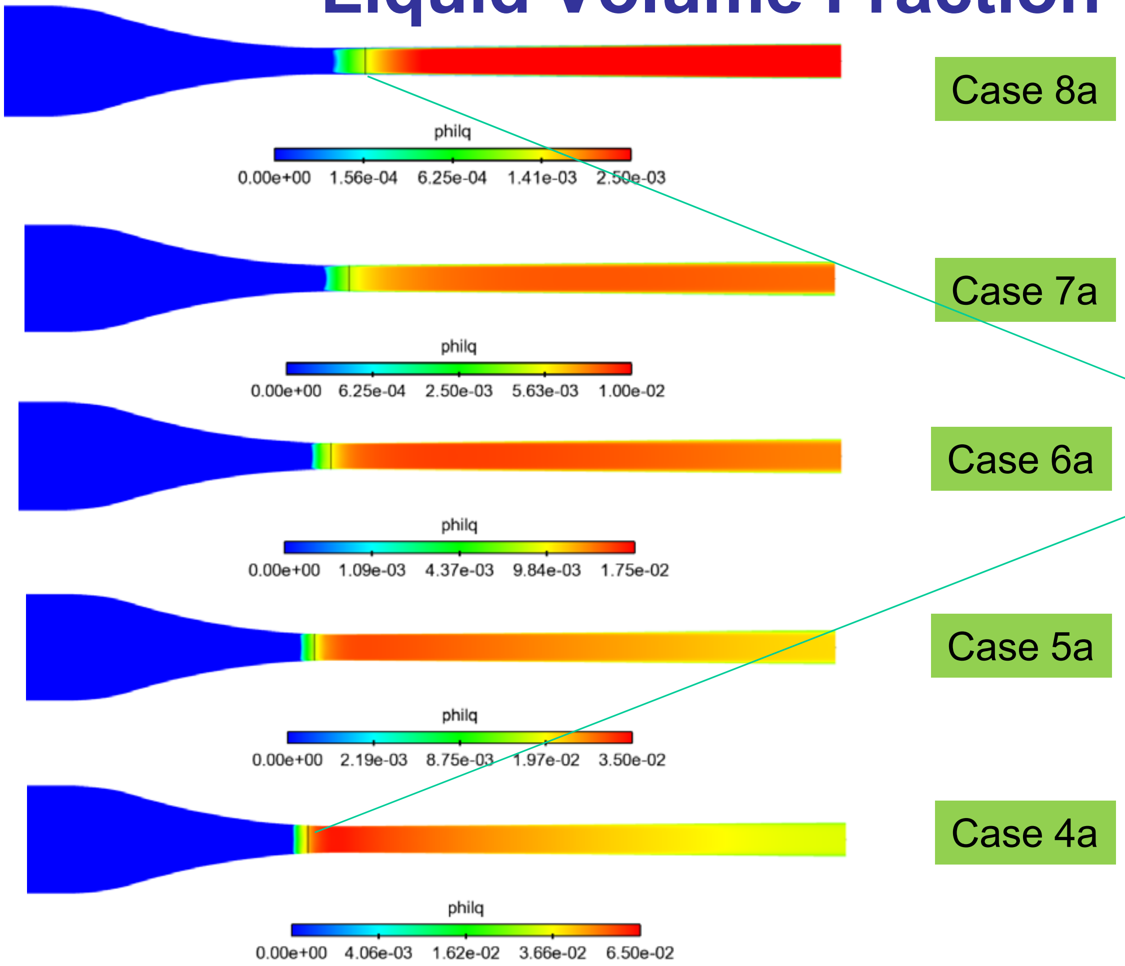
Temperature Depression



Condensation Validation – Supersonic Nozzle

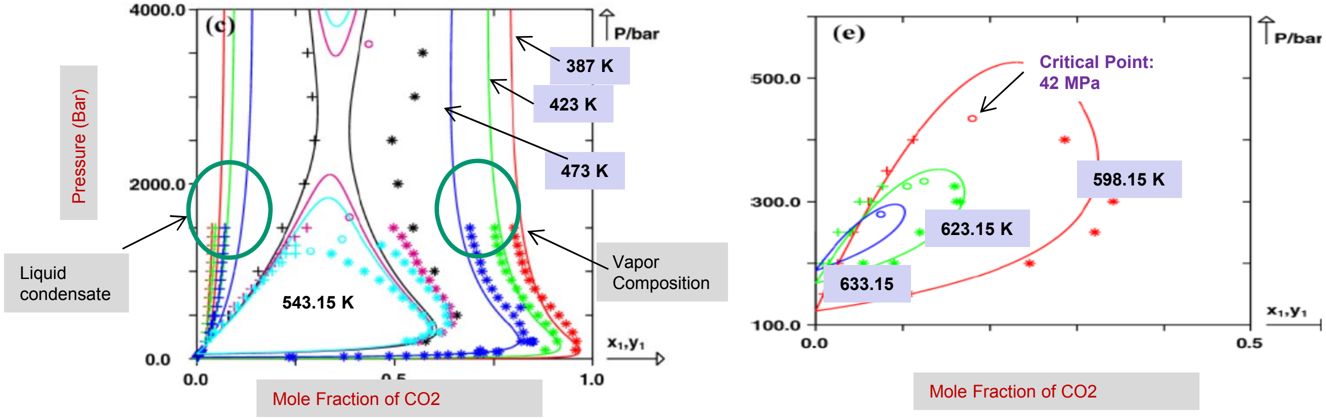
- High quality data from Prof. Lettieri for CO2 condensation in DeLaval nozzle is used for CFD validation
  - ➢ Lettieri, C., Paxson, D., Spakovszky, Z., and Bryanston-Cross, P., " Characterization of Non-Equilibrium Condensation of Supercritical Carbon Dioxide in a DeLaval Nozzle", Journal of Engineering for Gas Turbines and Power 140 (4), 2018
  - ➢ Blowdown facility for high pressure CO2 (58 – 84 bar) at low temperatures (around 310-315 K) leads to subcooled supersonic flow in nozzle throat resulting in condensation
- CFD calculation done for five cases ranging from 58.96 bar to 84.74 bar
- Present CFD calculations with CRUNCH CFD done with *equilibrium framework* where mixture conservation equations solved for a fluid that can consist of liquid and vapor
- For subcritical conditions, properties of each phase restricted to saturation values for metastable or otherwise unphysical conditions for a phase. Properties obtained from NIST table look-up covering both supercritical and subcritical conditions
  - ➢ Phase change model based on difference between local saturation pressure and fluid pressure
  - ➢ Local enthalpy differences between phases accounted for in phase change process
  - ➢ Phase change drives the fluid conditions to equilibrium as it alters the local temperature and pressure
  - ➢ The faster the flow reaches equilibrium spatially this formulation becomes more accurate

Computed Condensation Field and Onset: Contours of Liquid Volume Fraction



Black line shows estimate of condensation onset from liquid volume field

Status for CO_2-H_2O Mixtures



Phase equilibrium calculations (solid line) with modified form of Peng-Robinson PR78-EOS. Data is symbols

- As temperature drops mixture critical pressure goes up dramatically
- At temperatures below 538 K the vapor-liquid equilibrium (VLE) curve is not closed; Solubility appears invariant to pressure level (i.e. critical value undefined)
- Composition of “liquid” mixture and “vapor” mixture very different
  - At low temperatures condensate is almost pure water while vapor becomes primarily CO2 with more variation in composition
- **Implication for compressor operating between 305 K inlet and 320-340 K outlet with water as contaminant:** Water will condense out and a two-fluid liquid-vapor mixture will exist all the way through the compressor exit even at significantly elevated pressures. Impact on compressor performance / blade material damage?