

Non-Equilibrium Nucleation and Droplet Growth Near Critical Conditions

- **Objective:** Maturation of non-equilibrium condensation and droplet growth in CRUNCH CFD® as part of a coupled compressor simulation
- Non-equilibrium models for condensation require significant upgrades to current numerical framework:

1. Calculation of nucleation rate from classical nucleation theory and generation of condensation nuclei at critical radius to serve as condensation sites for droplet formation
2. Non-Equilibrium droplet growth with localized condensation and vaporization using advanced non-equilibrium phase change model

Classical Nucleation Theory

Non-Equilibrium Phase Change

$$\text{Nucleation Rate: } J = \frac{\rho_v^2}{\rho_L} \sqrt{\frac{2\sigma}{\pi m^3}} \exp\left(-\frac{\Delta G^*}{kT}\right)$$

$$\text{Nuclei Radius: } r^* = \frac{2\sigma}{\rho_L R_v T \ln(P/P_{sat})}$$

ΔG^* = Gibbs Free Energy
 σ = Surface Tension
 ρ = Vapor/Liquid Density

k = Boltzmann Constant
 m = single vapor molecule mass
 T = Vapor Phase Temperature

$$\frac{dm_v}{dt} = 4\pi r^2 \left[h_c \frac{P_{partial}}{\sqrt{2\pi RT_g}} - h_e \frac{P_{sat,eff}}{\sqrt{2\pi RT_d}} \right]$$

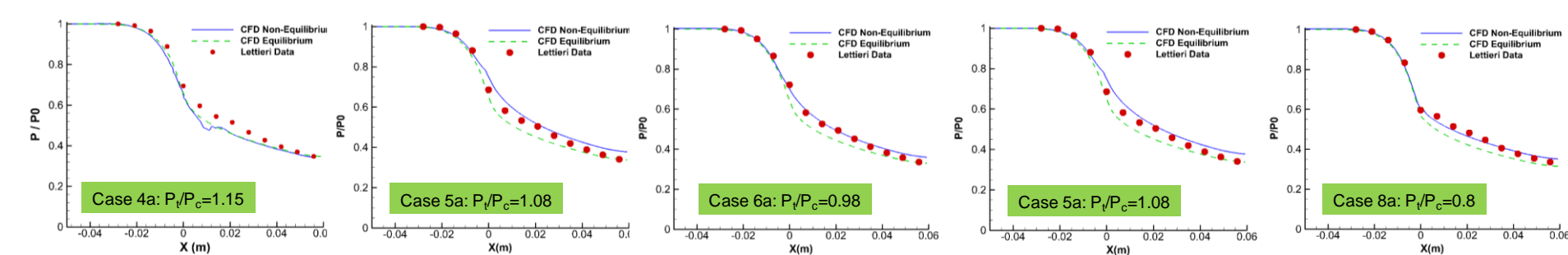
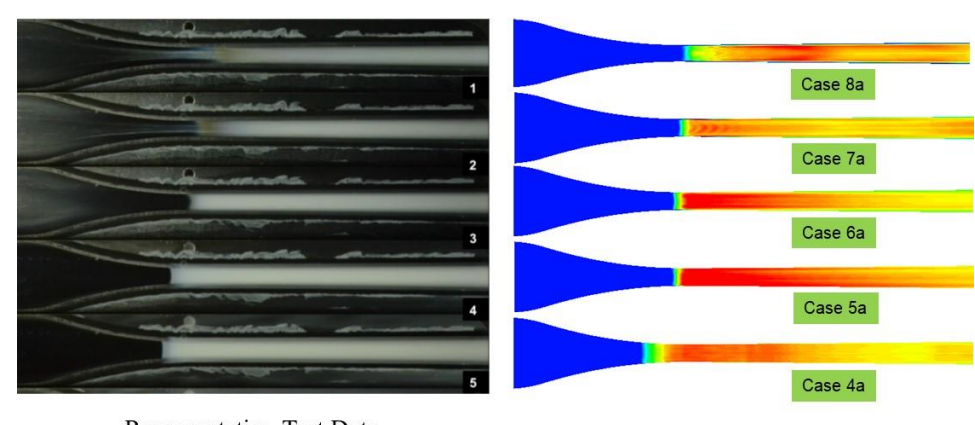
Rate of mass exchange between vapor & droplet phase

Gas Phase Properties
 Condensation Term

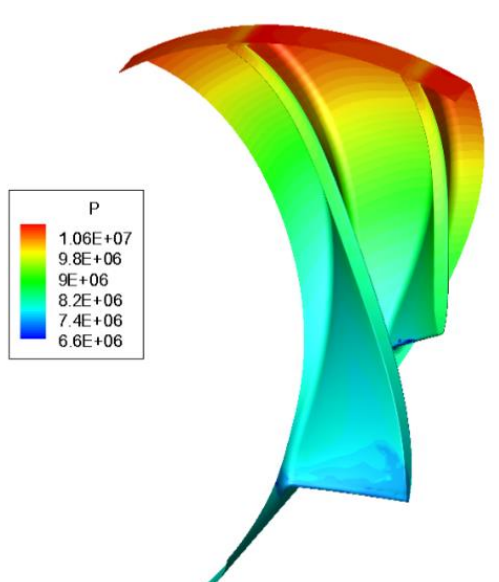
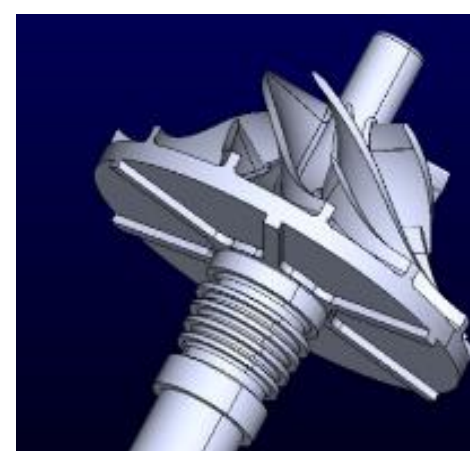
Droplet Properties
 Evaporation Term

- **Validation:** The homogeneous nucleation and non-equilibrium condensation model has been validated for CO₂ condensation predictions:

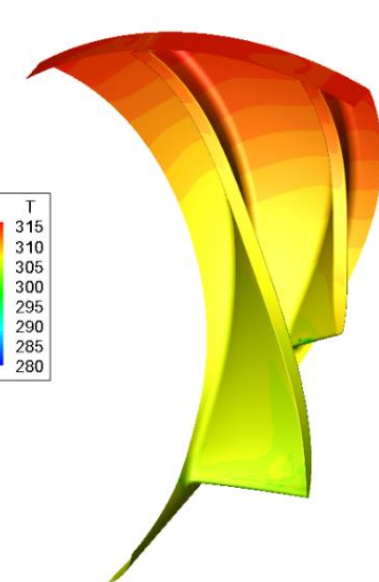
Case	P(MPa)	T(K)	P/P _c	T/T _c
8a	5.896	314.7	0.799	1.035
7a	6.535	312.0	0.886	1.026
6a	7.353	313.6	0.997	1.031
5a	7.999	313.9	1.084	1.032
4a	8.474	313.9	1.149	1.032



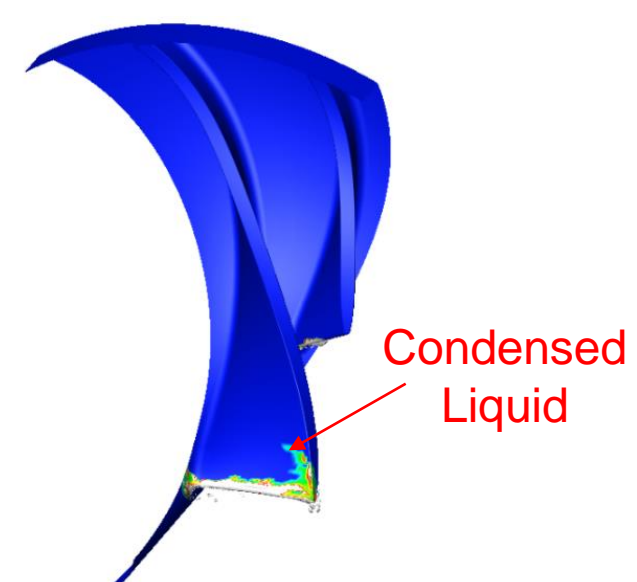
- **Analysis:** The Sandia sCO₂ compressor modeled with the non-equilibrium phase change model
- Super-critical inlet conditions (305.4 K, 78.43 bar)



Predicted Pressure (Pa)



Predicted Temperature (K)



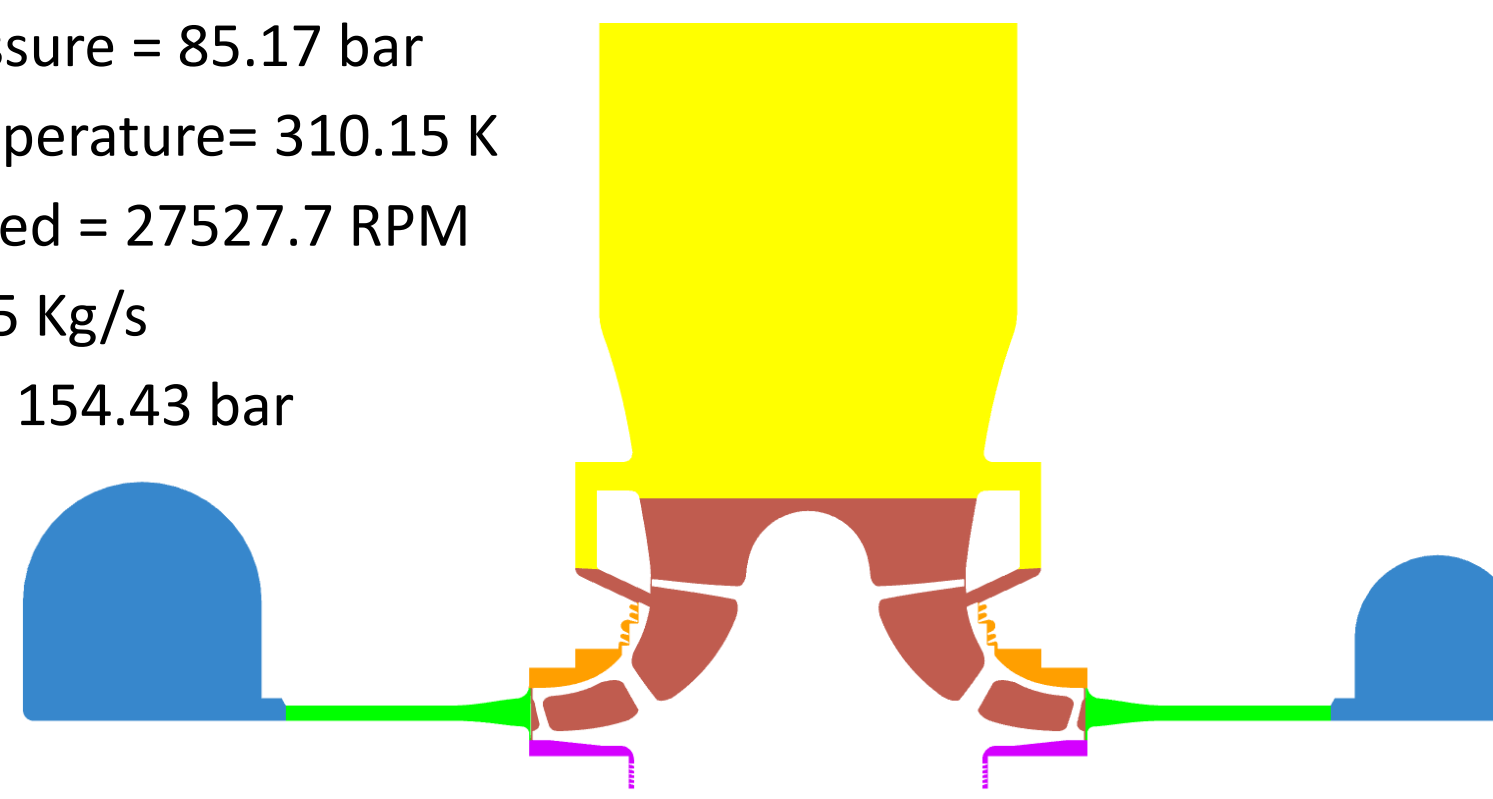
Predicted Liquid Volume Fraction

sCO₂ Power Cycle CSP Compressor Analysis

- **Objective:** To develop an integrally-gear compressor-expander in a sCO₂ recompression cycle for a 10 MWe CSP application for steady performance and unsteady dynamics
- Effort will leverage EERE funded project by SwRI and Hanwha Techwin (HTW)
- Compressor system designed for stable wide-range operation to account for inlet excursions and transients expected in an air-cooled CSP environment

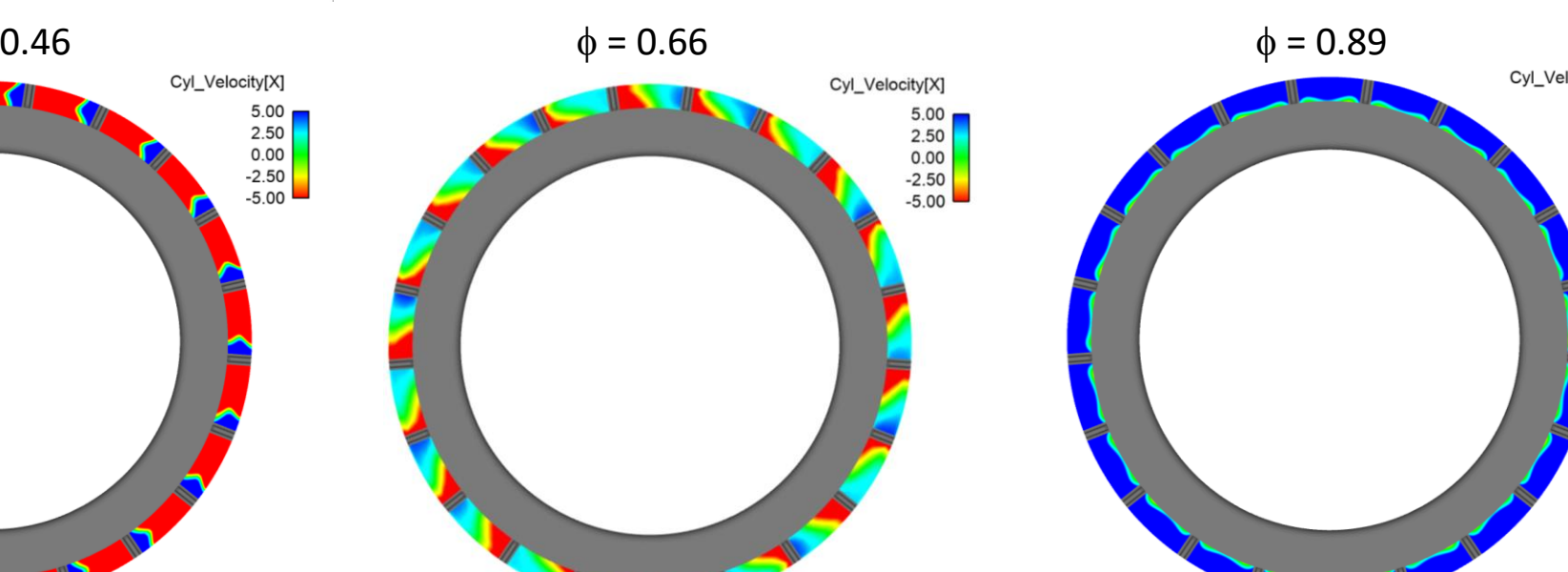
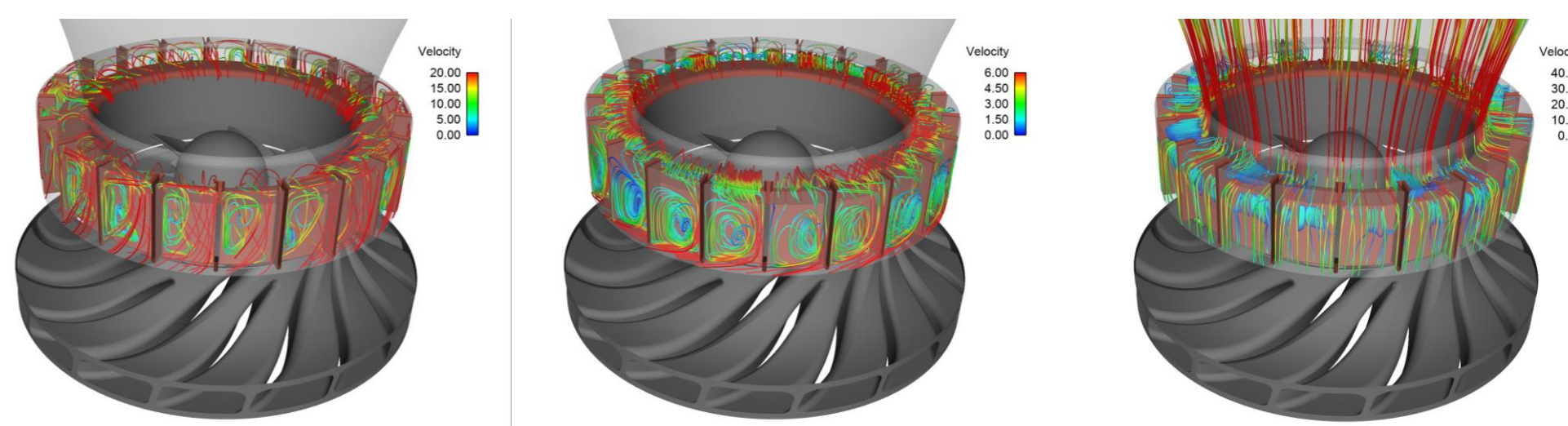
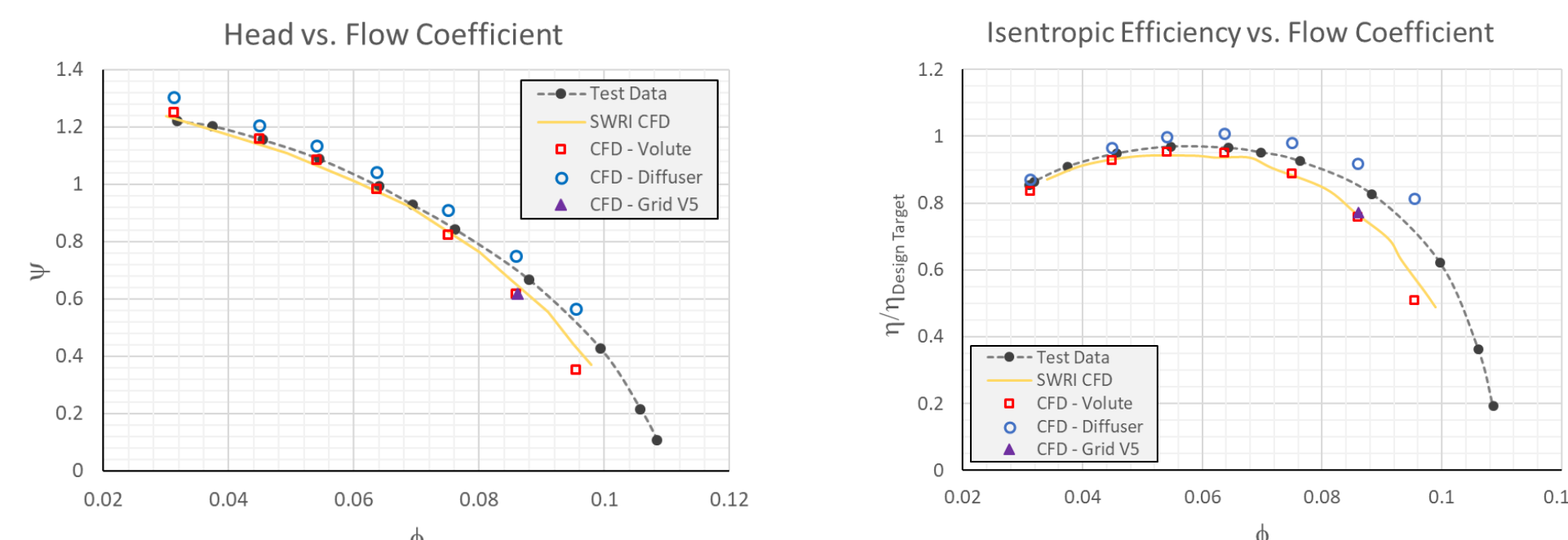
- Design Operating Conditions:

- Inlet Total Pressure = 85.17 bar
- Inlet Total Temperature = 310.15 K
- Rotational Speed = 27527.7 RPM
- Mass Flow = 55 Kg/s
- Exit Pressure = 154.43 bar



- **Validation:** Operation in air has been validated by comparison with existing data

- **Analysis:** CFD simulations for sCO₂ case are currently underway



Axial velocity contour at axial plane inside casing treatment
 Negative velocity denotes flow going toward the inlet

EoS Model Extensions for CO₂/Water

- **Objective:** To develop thermodynamic models and equation of state for VLE and density for CO₂ mixtures contaminated with water
- Reliable data will be compiled for temperature and pressure in the window of operation (290 < T < 340 K and 70 bar < P < 200 bar)
- Composition of "liquid" mixture and "vapor" mixture very different
 - At lower temperatures condensate is almost pure water while vapor becomes primarily CO₂ with more variation in composition

- Activity Coefficient Equation of State ($\gamma - \phi$) thermodynamic model developed to predict the compositions of the saturated liquid and vapor phases within the window of operation:

$$y_1 P \hat{\phi}_1^G(T, P, y_1) = x_1 H_{1,2}(T, P)$$

$$y_2 P \hat{\phi}_2^G(T, P, y_2) = x_2 f_2^L(T, P)$$

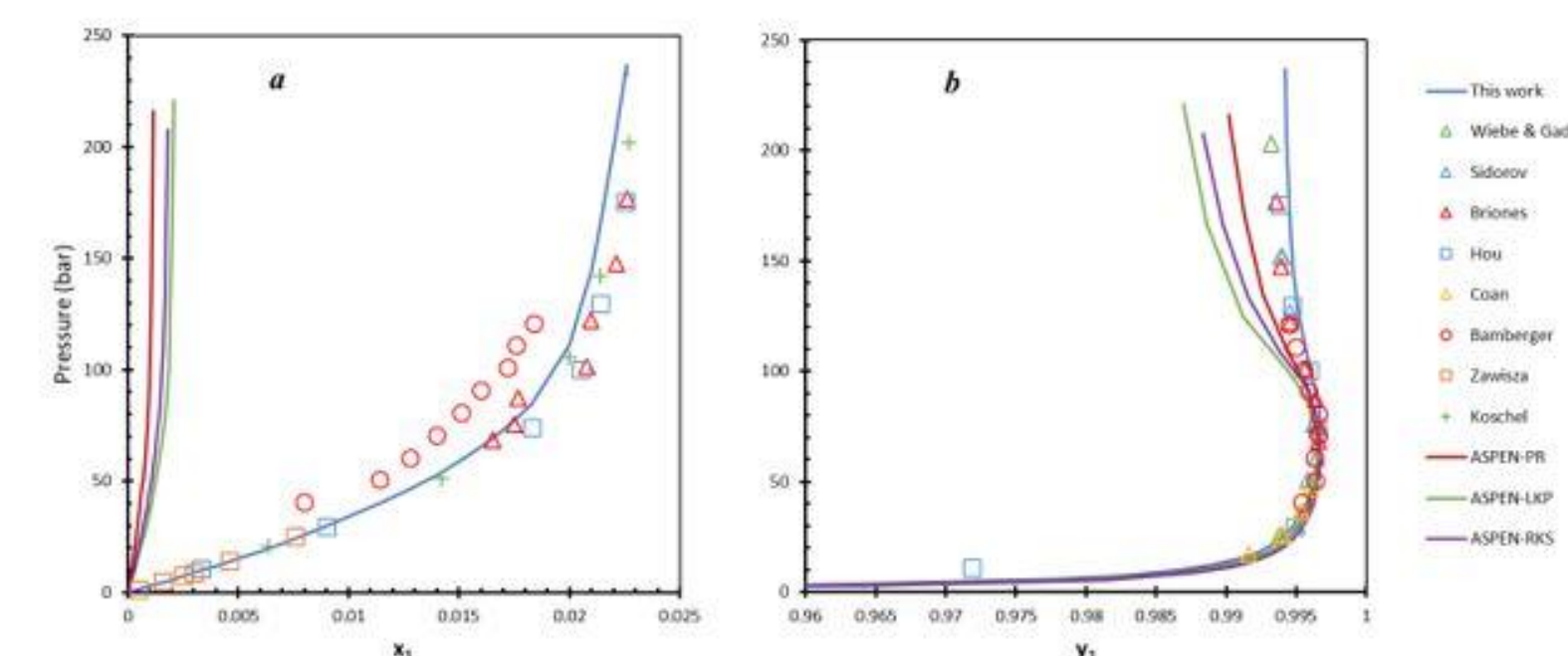
- $\hat{\phi}_i^G(T, P, y_i)$ of species i can be modeled by the Peng-Robinson equation of state

- $H_{1,2}(T, P)$ is the Henry's constant of solute CO₂ in solvent water

- $f_2^L(T, P)$ is the fugacity of pure liquid water at T and P

$$\ln H_{1,2}(T, P) = \ln H_{1,2}^0(T) + \frac{\bar{V}_1^\infty(P - P^0)}{RT}$$

$$f_2^L(T, P) = P_2^{sat} \cdot \exp\left[\frac{v_2^{sat}}{RT}(P - P_2^{sat})\right]$$



Pressure-CO₂ composition VLE of carbon dioxide-water mixture at 323 K

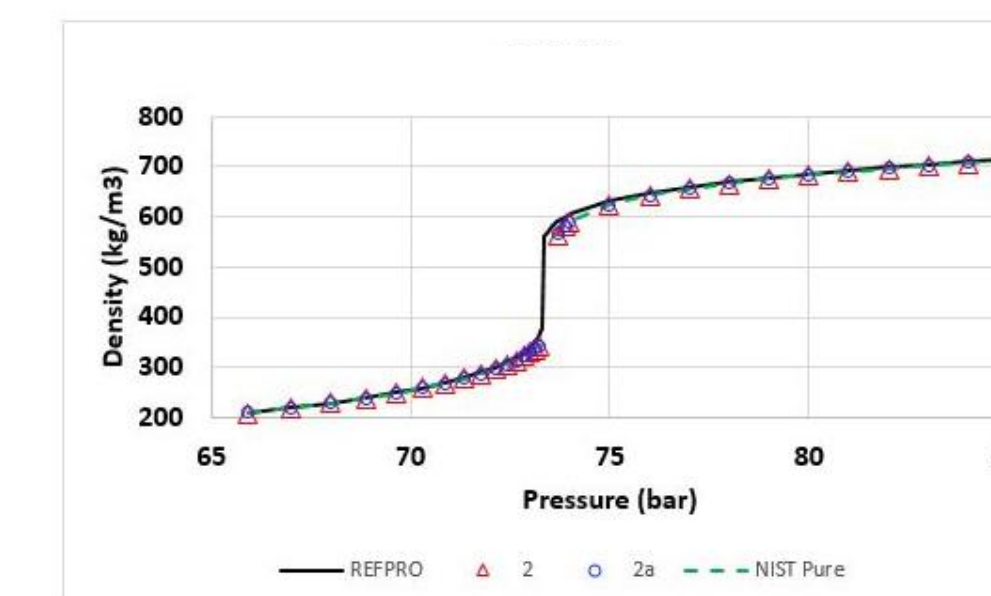
- Linear models are developed to predict the mixture density
- e.g. CO₂ rich vapor or liquid phase molar volume defined as:

$$v = v_2 + x_1(\bar{V}_1^\infty - v_2)$$

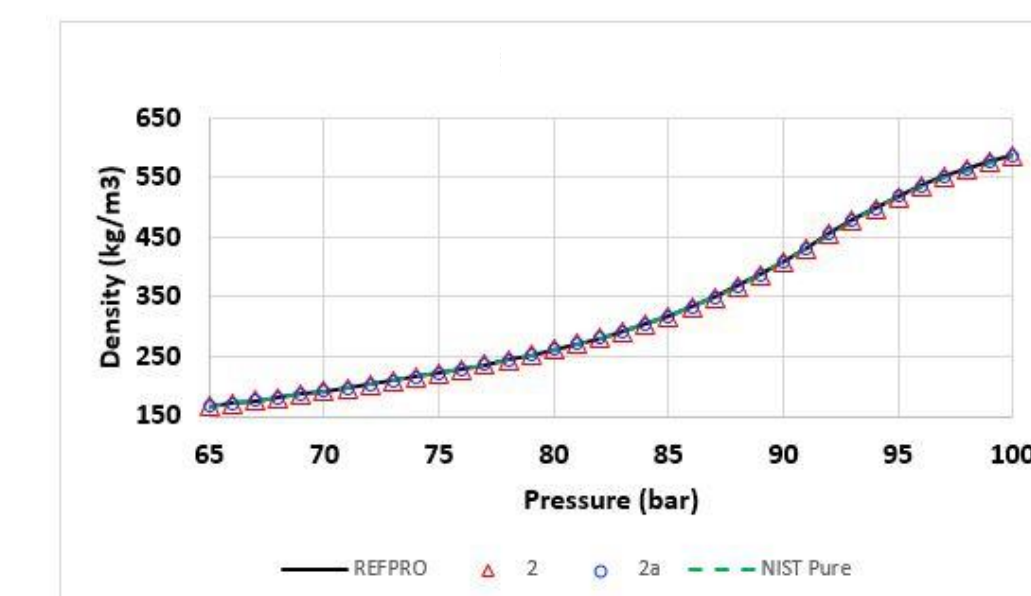
- $\bar{V}_1^\infty(T, P)$ represents the partial molar volume of carbon dioxide in water at infinite dilution

- $v_2(T, P)$ is the molar volume of pure solvent water

$$\rho(T, P, x_1) = 1/v(T, P, x_1)$$



Density of CO2-water mixture
 $y_1=0.9985$ and 304 K



Density of CO2-water mixture at
 $y_1=0.9995$ and 315 K