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

\[
\frac{J}{N} = \frac{2\pi}{3\eta} \left( \frac{M'}{T^2} \right) \exp \left( \frac{-1}{4\pi N \eta T} \right)
\]

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Nucleation Rate

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

<table>
<thead>
<tr>
<th>Case</th>
<th>P (bar)</th>
<th>T (K)</th>
<th>N</th>
<th>J (Pa)</th>
</tr>
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<tbody>
<tr>
<td>4a</td>
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Analysis: The Sandia sCO₂ compressor modeled with the non-equilibrium phase change model

Super-critical inlet conditions (305.4 K, 78.43 bar)

sCO₂ Power Cycle

- **Objective:** To develop an integrally geared compressor-expander in a sCO₂ recompression cycle for a 10 MW e 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

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 (γ ~ φ) thermodynamic model developed to predict the compositions of the saturated liquid and vapor phases within the window of operation:

\[
y_i \frac{T}{P} \phi_i(\gamma P, \gamma T, \gamma) = x_i H_{2}(T, P)
\]

\[
y_2 \frac{T}{P} \phi_2(\gamma P, \gamma T, \gamma) = x_2 f_{2}(T, P)
\]

\[
\phi_i(T, P, \gamma) = \text{Boltzmann Constant}
\]

\[
\phi_2(T, P, \gamma) = \text{VLE of carbon dioxide}
\]

\[
\rho(T, P, x_2) = 1/n(T, P, x_2)
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