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Development of a Vapor Liquid Equilibrium (VLE) Model for Aria

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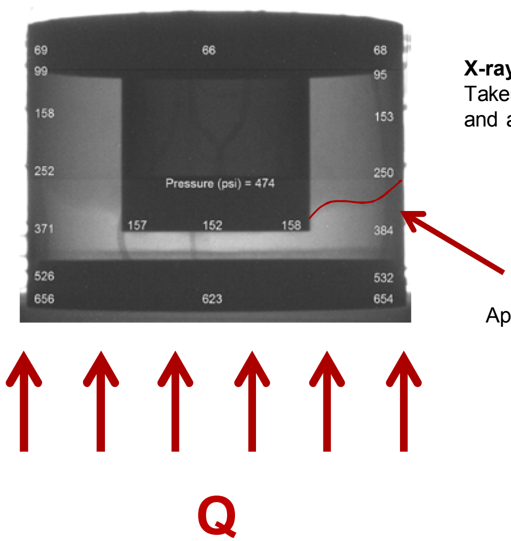
Motivation

- Foam In a Can (FIC) Experiment
  - Foam thermally degrades producing gaseous and liquid products
  - As gaseous products accumulate they pressurize the space

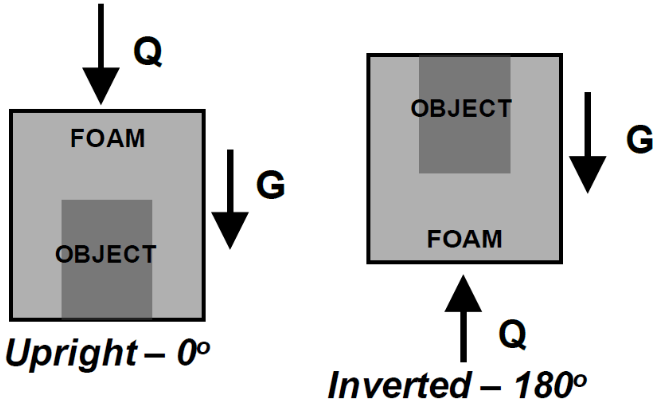


X-ray image of FIC experiments
Taken from [1] with permission and annotated in red.

Approximate Foam/Fluid interface

Motivation

- Upright vs. Inverted Tests
  - Different results for different orientations
  - Dripping?
- Goal for the summer:
  - Investigate applicability of VLE to FIC experiments
  - Create a numerical tool to investigate the effect of a vapor/liquid split in Foam In a Can experiments



Taken from [1] with permission

Vapor Liquid Equilibrium Theory

- Equilibrium occurs when Gibbs free energy is minimized
  - For VLE: Occurs when the chemical potentials of both phases of each material are equal

$$\mu_{v,i} = \mu_{l,i}$$

- Can be expressed using a simplified equation
  - Raoult's Law:

$$y_i P = P_i^{sat}(T) x_i$$

  - Henry's Law:

$$y_i P = H_i(T) x_i$$

Vapor Liquid Equilibrium Theory

- Flash equation:

$$F = L + V$$
$$Fz_i = Lx_i + Vy_i$$

- Continuity:

$$\sum_i y_i = \sum_i x_i = 0$$

- Calculate the vapor split, $\frac{V}{F}$, of the mixture:

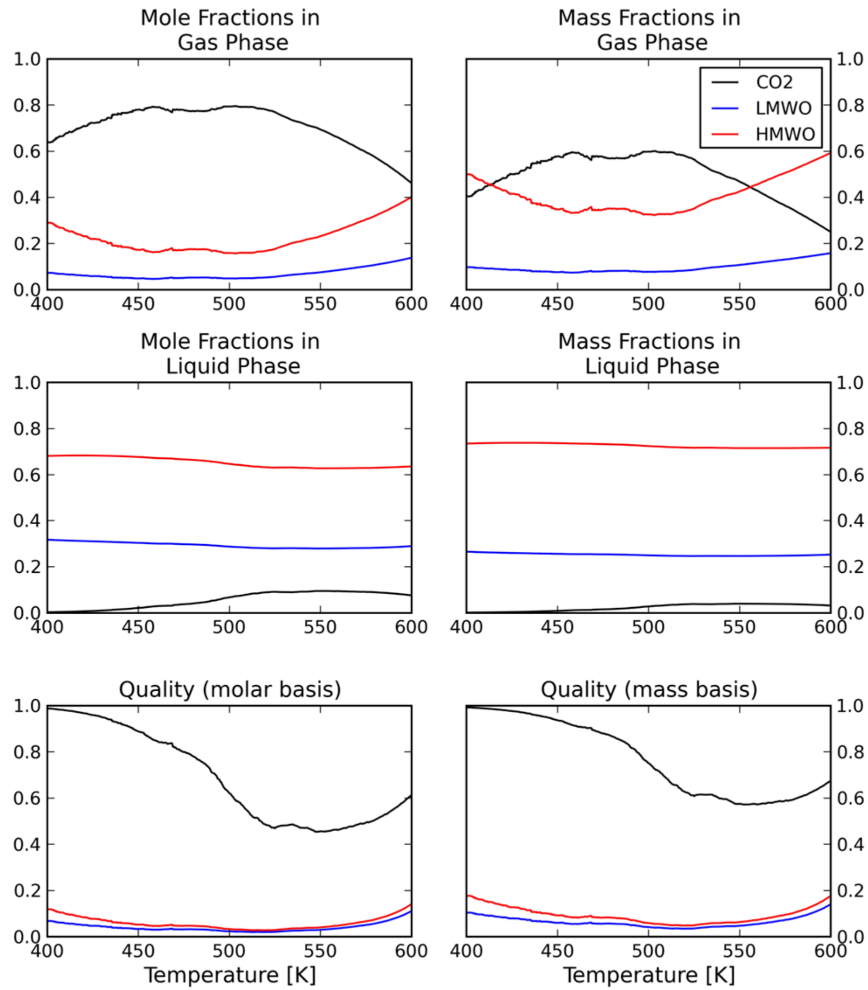
$$\sum_i \frac{z_i\left(\frac{H_i}{P} - 1\right)}{1 + \frac{V}{F}\left(\frac{H_i}{P} - 1\right)} = 0$$

VLE Solver Implementation

- Determine if the fluid mixture is in a state where VLE is possible
- Calculate the VLE concentrations
- Create fictitious ODE model:
  - $\dot{y}_j = \frac{y_{j,VLE} - y_j(t)}{\tau_{VLE}}$ $\dot{x}_j = \frac{x_{j,VLE} - x_j(t)}{\tau_{VLE}}$
  - We choose a small value of τ_{VLE} so it will arrive at VLE quickly
  - Treated as a chemical reaction

Python VLE Description & Results

- Made a simplified VLE model
  - Uses experimental temperature and pressure data as inputs
  - Calculates VLE of the mixture:
    - CO_2, LMWO, and HWMO
- Python VLE model Results:
  - Products of the foam are in both liquid and vapor phases
  - Heavier molecular weight species are more likely to be in the liquid phase



Overall Progress

- Investigate importance of VLE with a simplified python VLE model … Done
- Make VLE Solver into C++ … Done
- Make compatible with Sierra-Aria … In progress
- Evaluate performance of this VLE solver (accuracy, speed, etc.) … Soon

Thank You

- Questions?
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- References:

1. Scott, Sarah N and Dodd, Amanda B. "Uncertainty Quantification for Experimental and Model Results of Pyrolyzing and Pressurizing Polyurethane Foam at Varying Heating Rates." MCS 9, Rhodes, Greece, 2015