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Sandia National Laboratories

Experiments to Improve Engineering Models of Molding Polyurethane Foams

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U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

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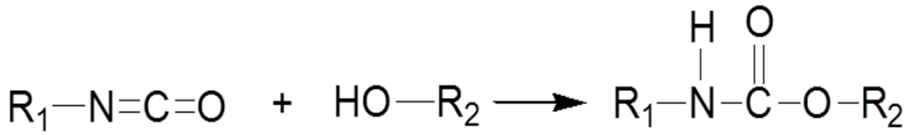
Overview

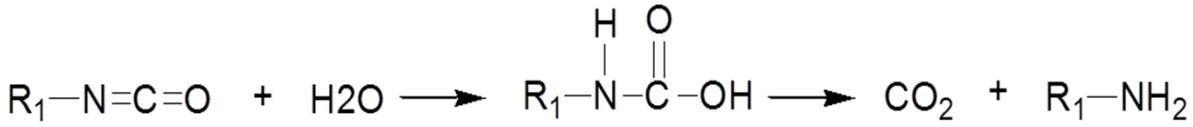
- Introduction
- Objectives
- Experiments
- Data/Analysis
- Conclusions and Discussion

Introduction

- Polyurethane Foams
  - Two part reactive mixture
  - Two main reactions: polymerization and gas generation



Urethane formation, crosslinking



Foaming reaction yields CO_2 and amine

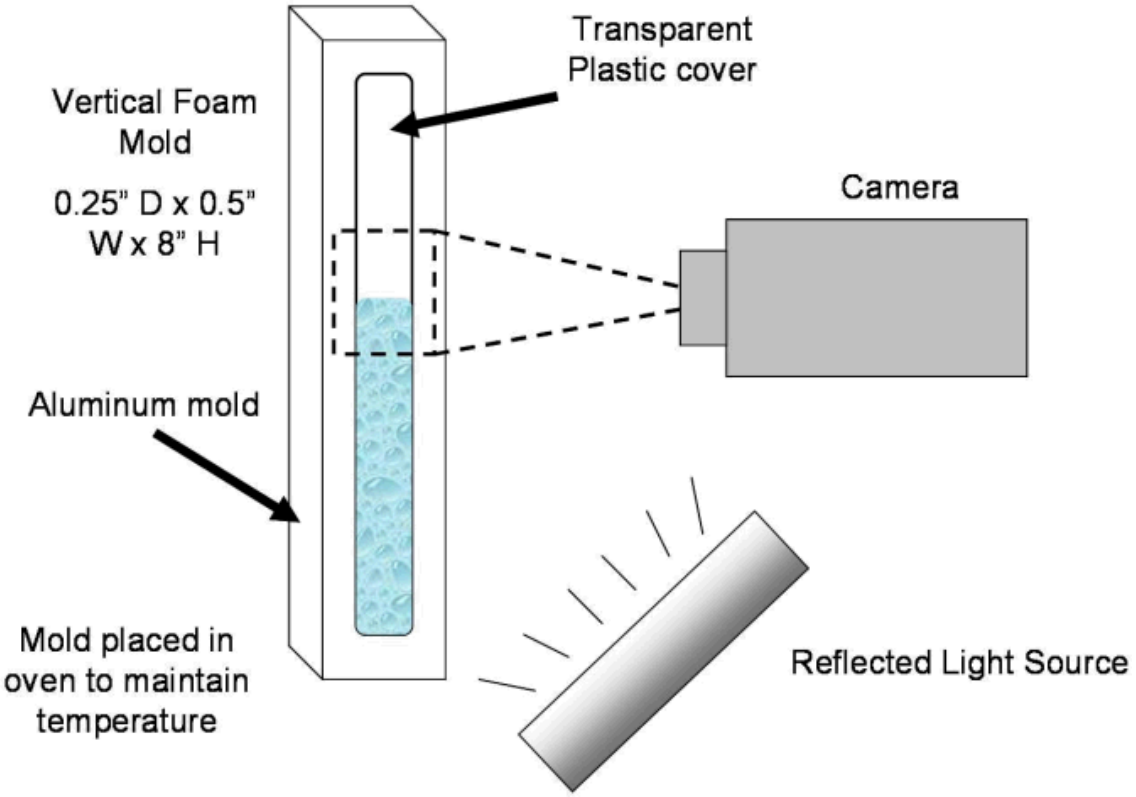
  - Uses: Structural support and encapsulation of important electronics

Objectives

- Overall Project: Provide a engineering model to fully predict the mold filling process
  - Kinetics: Experimentally determine the rate laws and rate law coefficients of major reactions
  - Compressibility: Provide a model that predicts compressibility of the reacting foam
  - Bubble Microstructure: Provide a model that describes bubble growth in the reacting foam

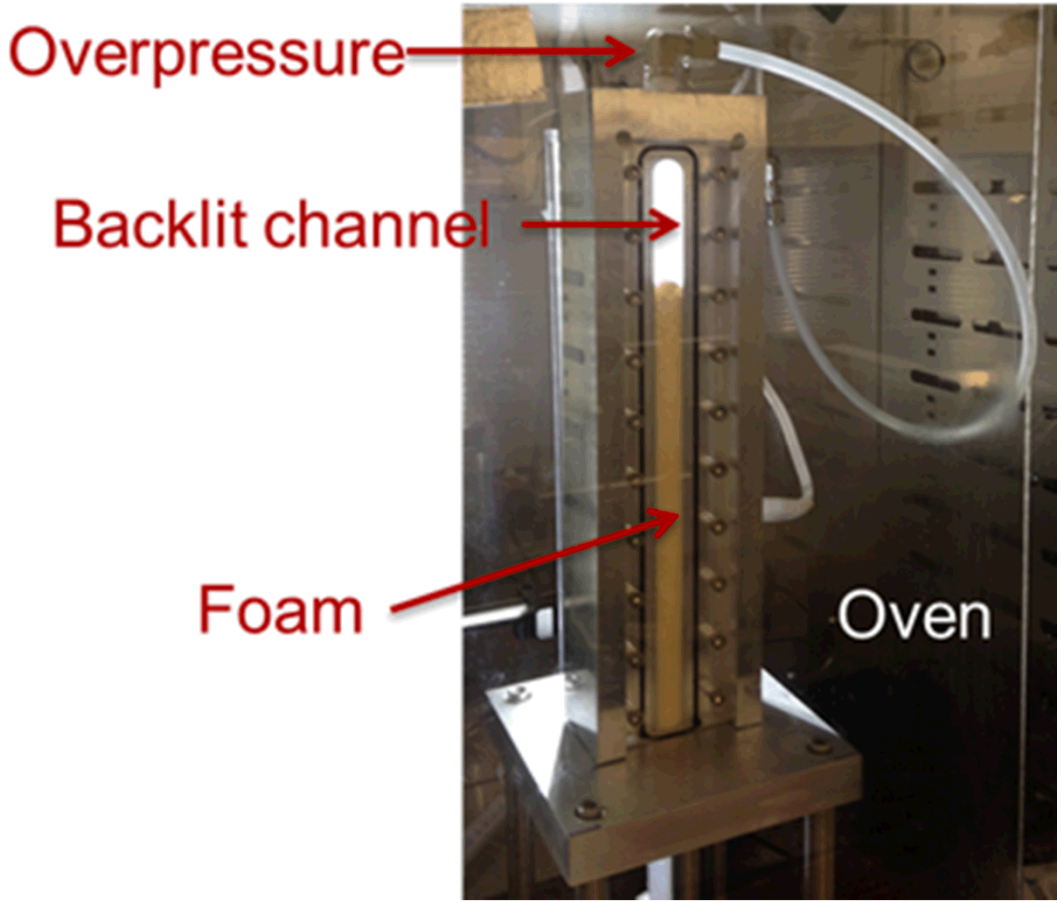
Experiments (Free Rise Column)

- Data being taken:
  - Temperature
  - Pressure
  - Camera (10 fps images)
- Used to track the gas generation reaction
- Image processing software used to quantify volume



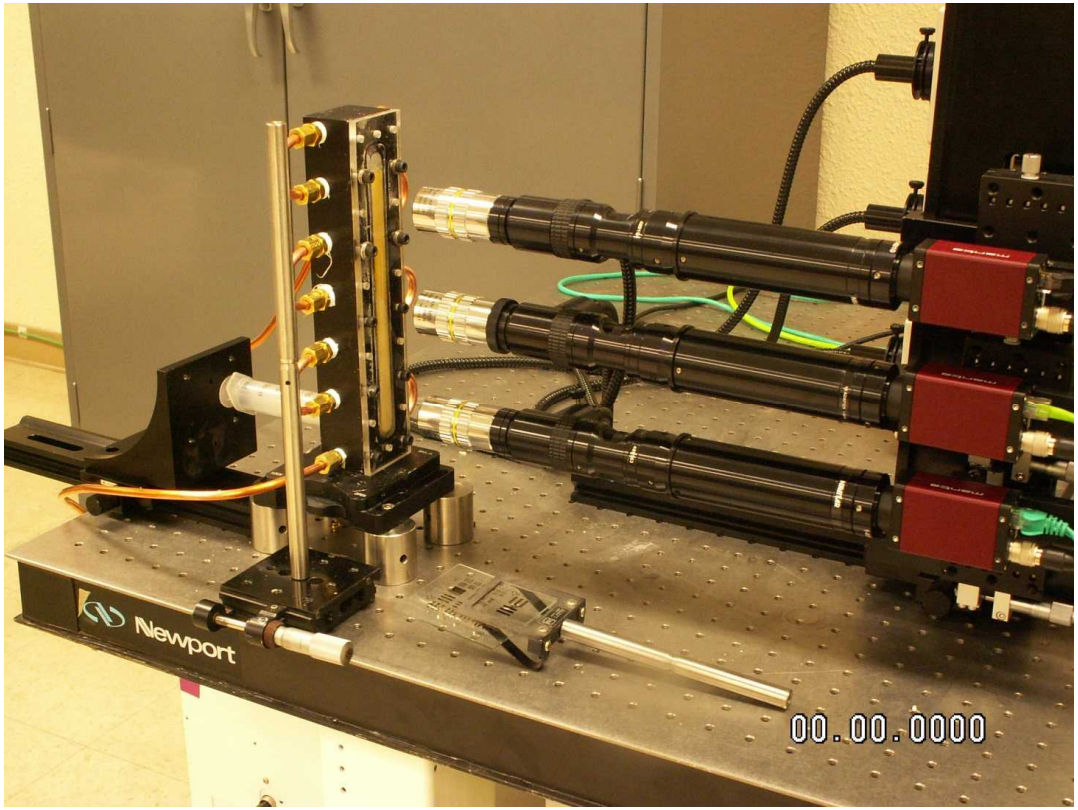
Experiments (Compressibility)

- Column attached to pressurized tank
- Solenoid valve opened every 5 seconds for 1 second
- Small pressure applied (0.5 or 1.0 psig)
- Volume monitored by camera

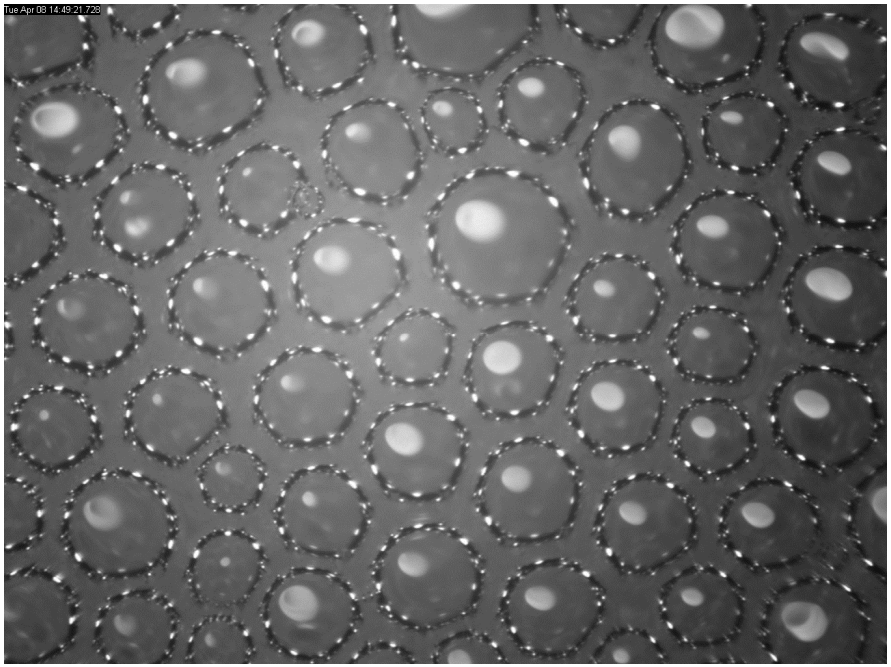


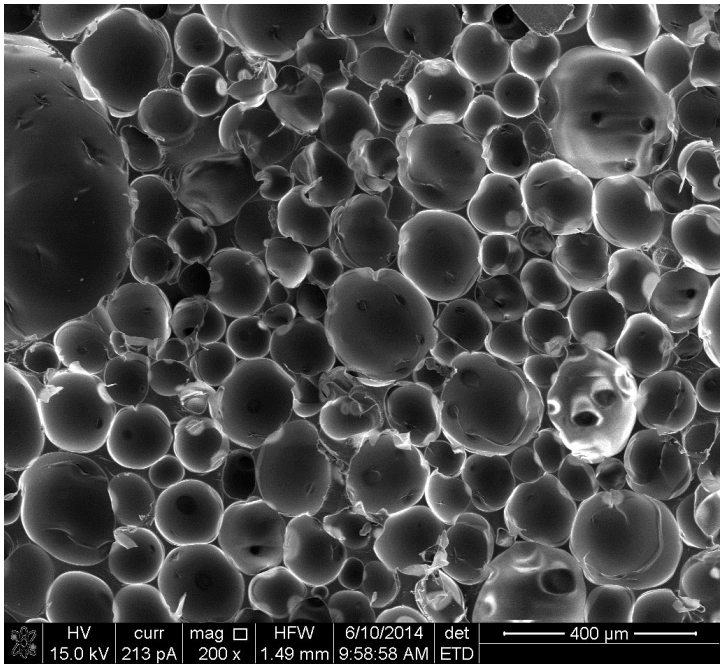
Experiments (Bubbles)

- Three zoomed cameras monitor evolving foam microstructure
- Image processing software used to analyze bubble microstructure
- SEM images used to compare outer bubbles to inner bubbles



Experiments (Bubbles)





- Dotted lines are bubble boundaries
- SEM images

Kinetic Fitting

- Two major reaction → Two rate laws

Polymerization Kinetics

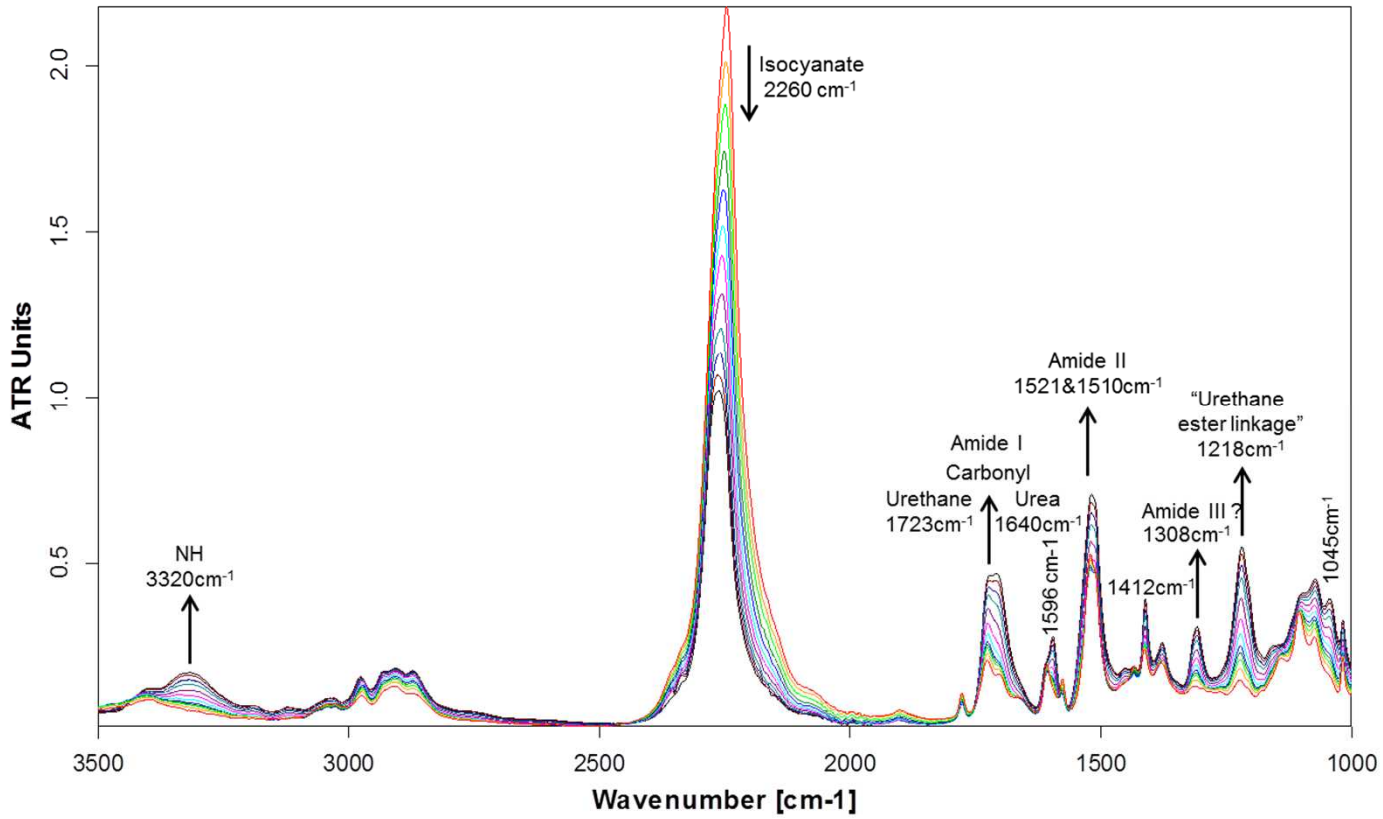
$$\frac{d\xi}{dt} = k_0 e^{-\frac{E_a}{RT}}(1-\xi)^n(A+\xi^m)$$

Gas Generation Kinetics

$$\frac{d\alpha}{dt} = \frac{Nk(1-\alpha)^n}{(1-\alpha)^m + M}$$

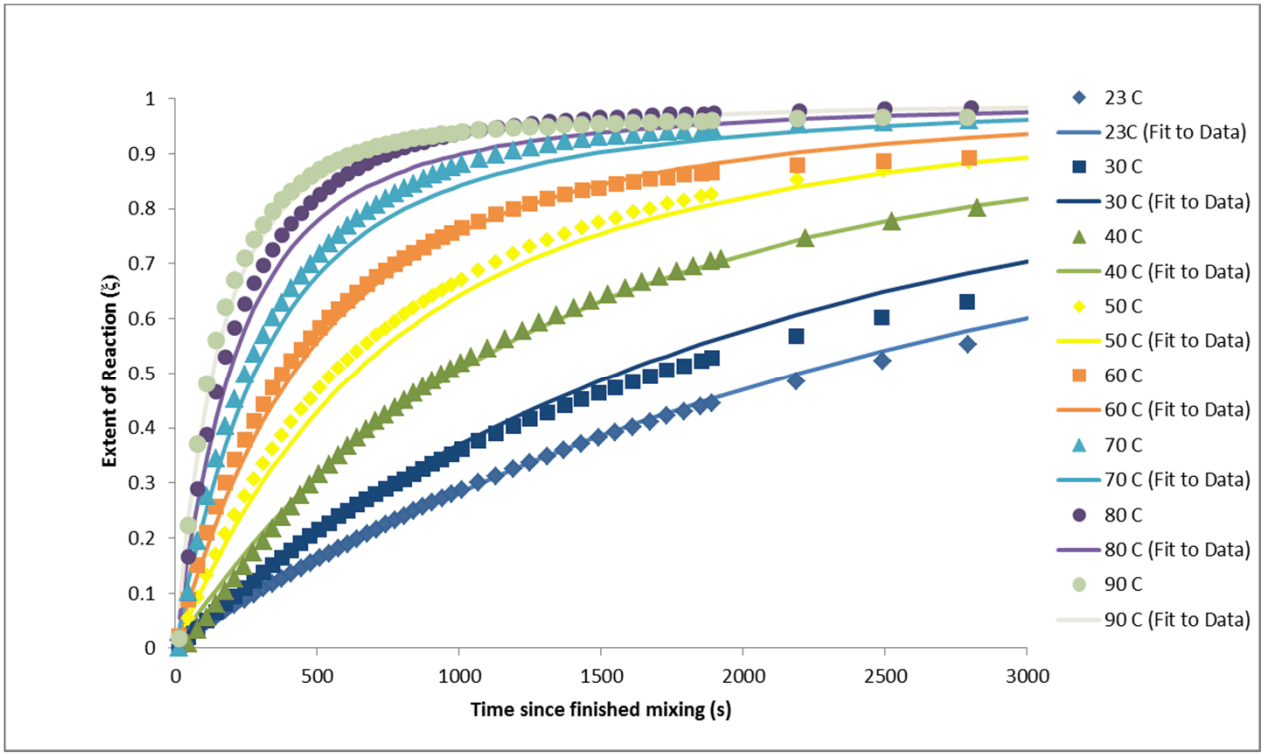
- Polymerization → Fitting to empirical IR data
- Gas Generation → Fitting to calculated α from column rise experiments

Polymerization Kinetics- IR Data



- 1218 cm^{-1} Urethane linkage peak used
- Values are normalized across all temperatures

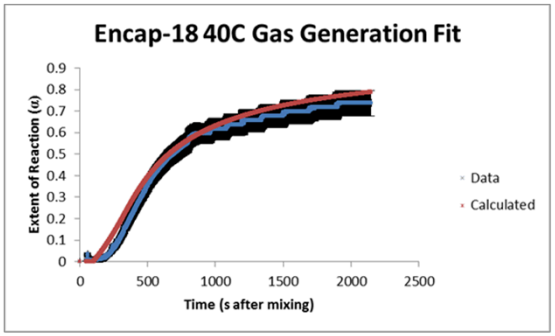
Polymerization Kinetics

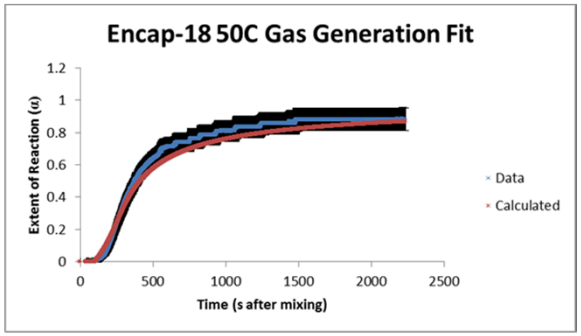


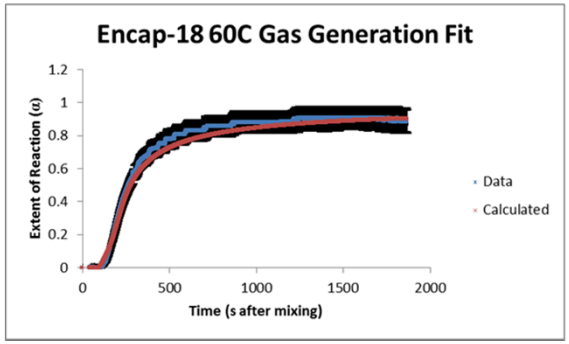
$$\frac{d\xi}{dt} = k_0 e^{-\frac{E_a}{RT}}(1-\xi)^n(A+\xi^m)$$

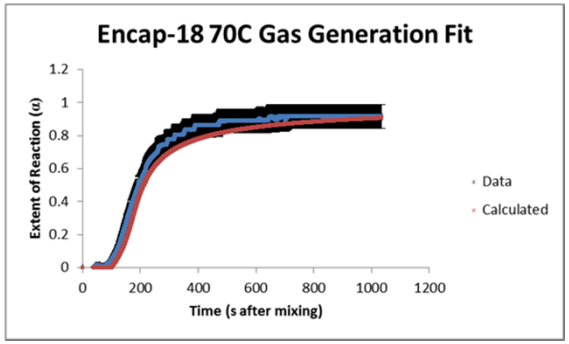
- Fits reasonably well for ~2000 seconds
- At t>2000 seconds, some divergence is observed

Gas Generation Kinetics









$$\frac{d\alpha}{dt} = \frac{Nk(1-\alpha)^n}{(1-\alpha)^m + M}$$

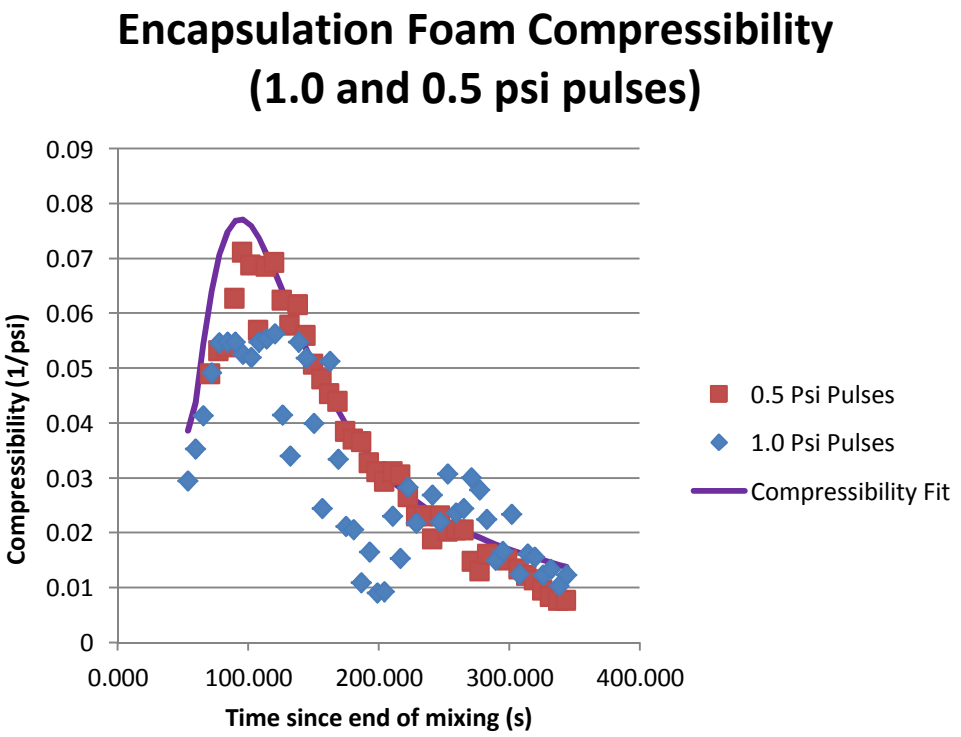
$$K = A_1 e^{E_1/RT}$$

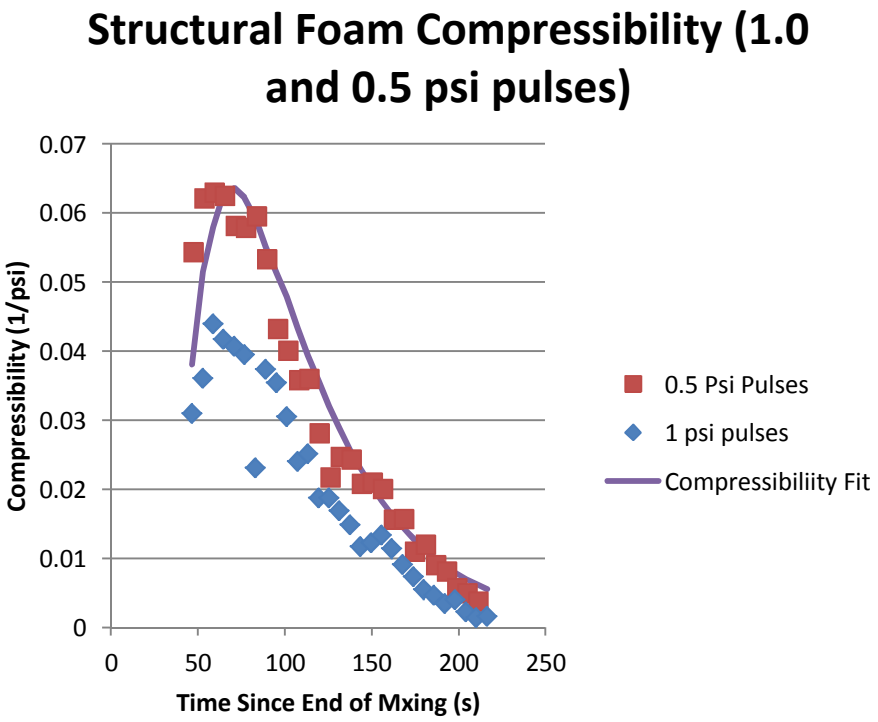
$$M = A_2 e^{E_2/RT}$$

$$N = 0.5(1 + \tanh(t - t_{nucleation}))$$

- α calculated assuming ideal gas law with collected T,P, and V values

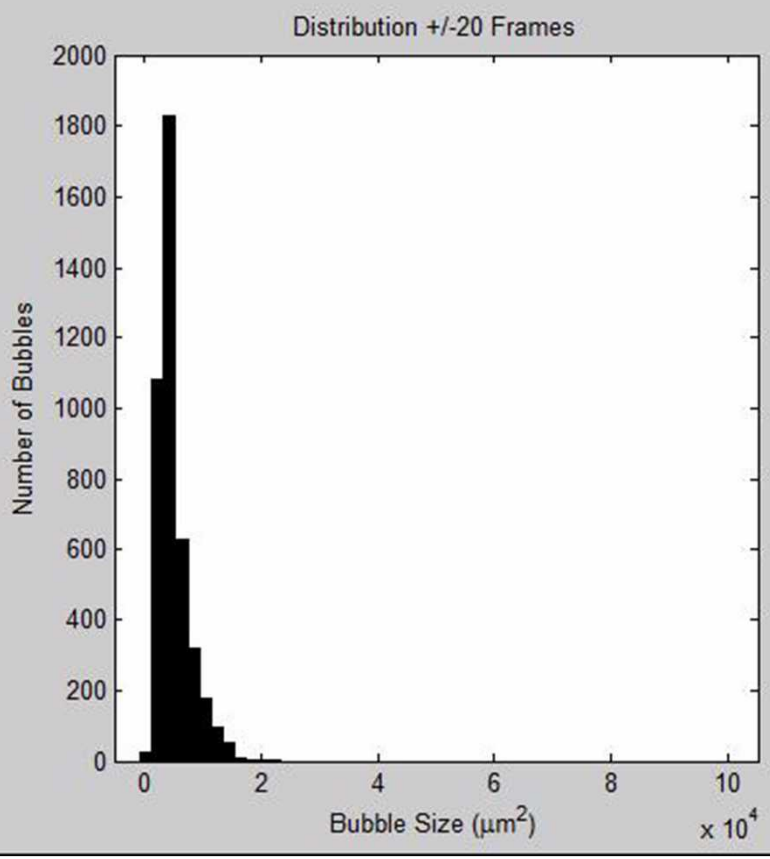
Compressibility





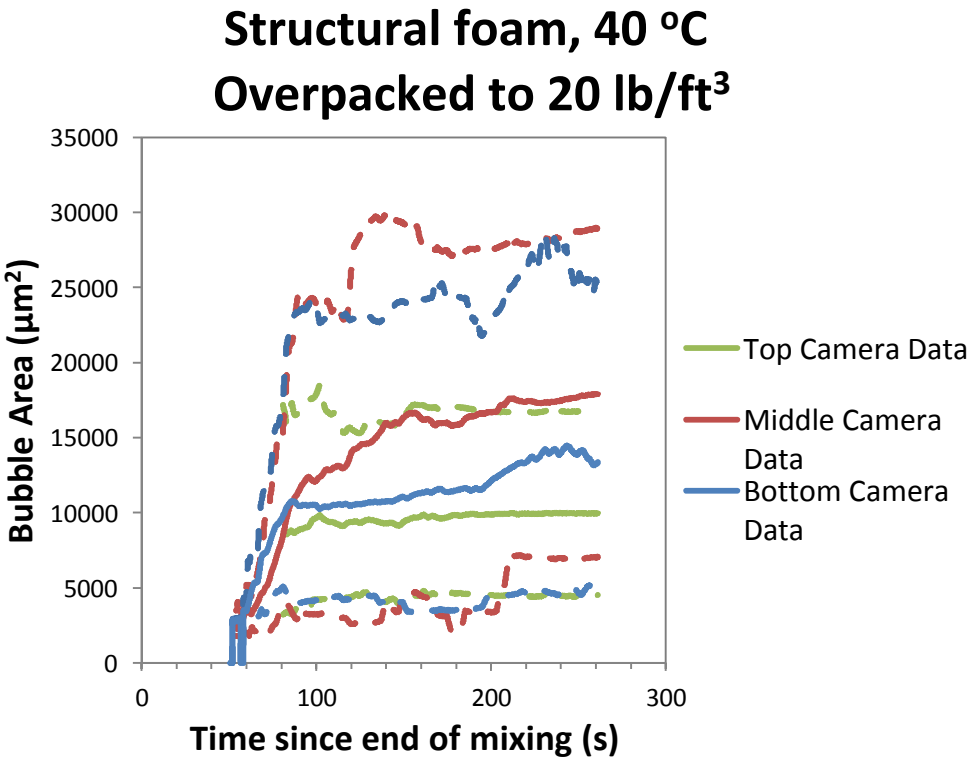
$$\beta_{Foam} = \beta_{Ideal\ Gas}\varphi[K_1(\xi_{Max} - \xi)^n + K_2(\xi_{Max} - \xi)^m]$$

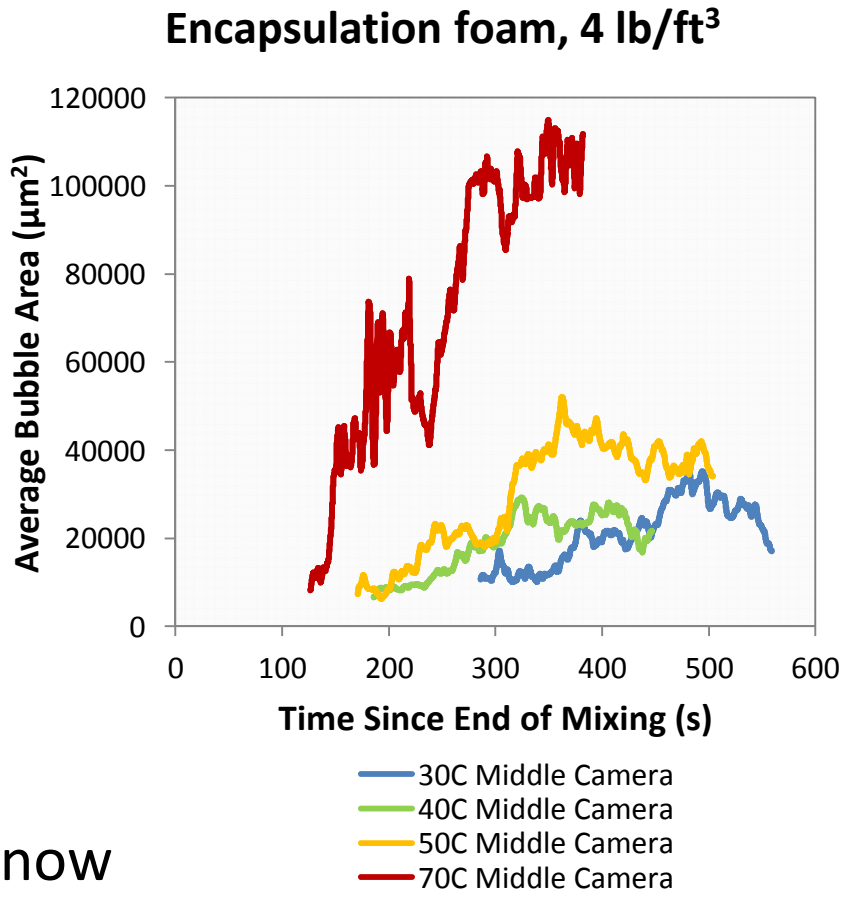
Bubble Microstructure Analysis



- Code works well for certain sections
- Manual analysis to fill gaps

Bubble Microstructure Analysis





- Qualitative conclusions only right now
- Integrating code analyzed and manually analyzed

Conclusions & Discussion

- Kinetic Models
  - Kinetic coefficients determined for both reactions
  - Polymerization fit limitations
- Compressibility
  - General form determined
  - Issues with higher pressures
- Bubble Sizing
  - Large difference between inner and outer bubbles
  - Qualitative conclusions about bubble growth