Using CFD to Optimize Cavitation Yield for Degradation of Lignocellulistic Biomass

Cody Jacobucci

Outline

- Motivation
- Previous Optimization Studies
- This study
  - Methods used
  - Results
  - Next steps

Motivation

Motivation

AD and Lignin

Cavitation

This study

- Reviewed experiments and simulations of cavitating devices
- Created Multiphase Cavitation model in Fluent
- Validated model against experimental results.

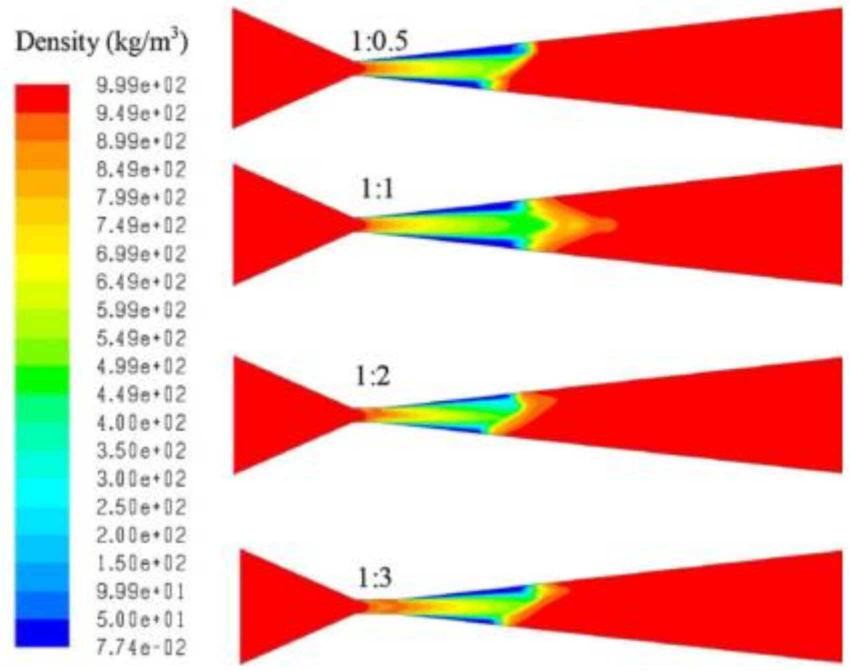
How can CFD help design cavitating devices?

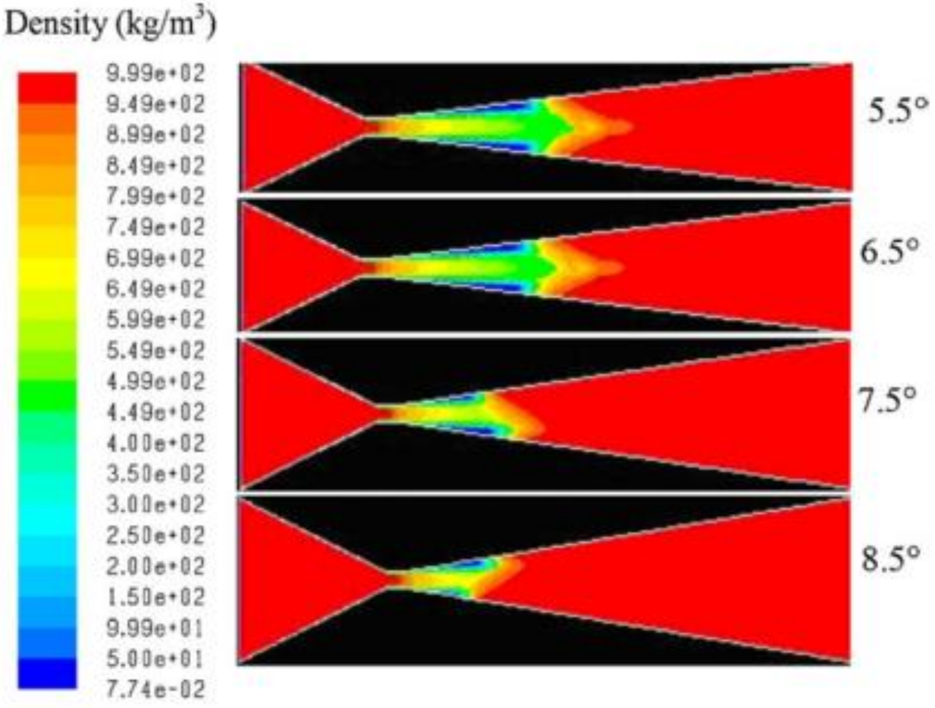
- Much research has gone into how to prevent cavitation
  - Any pressurized/warm/moving system has the chance to encounter it
  - Take what they say and do the opposite!
- Intense optimization study to optimize geometry of venturi and orfice plate cavitation devices based on “cavitation yield” (Bashir at al. 2011)
- Experiments run by Saharan et al. using optimized geometry for degradation of Orange-G (2012)

Bashir et al. 2012

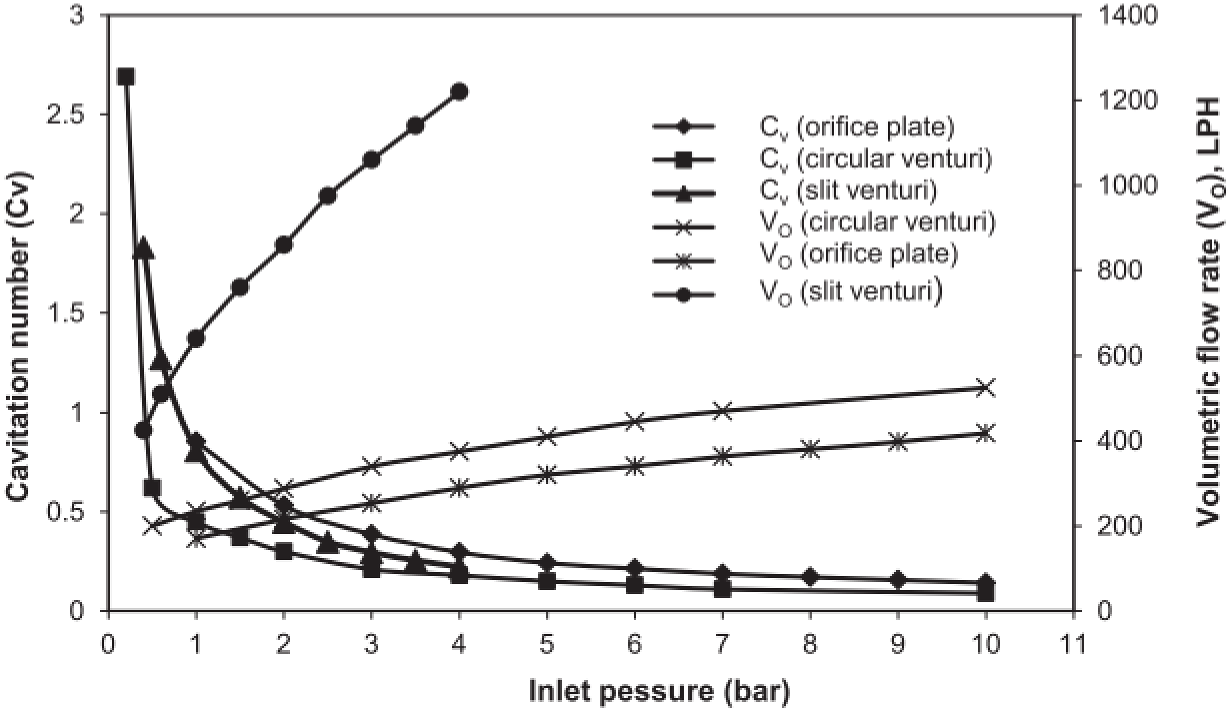
3 step process

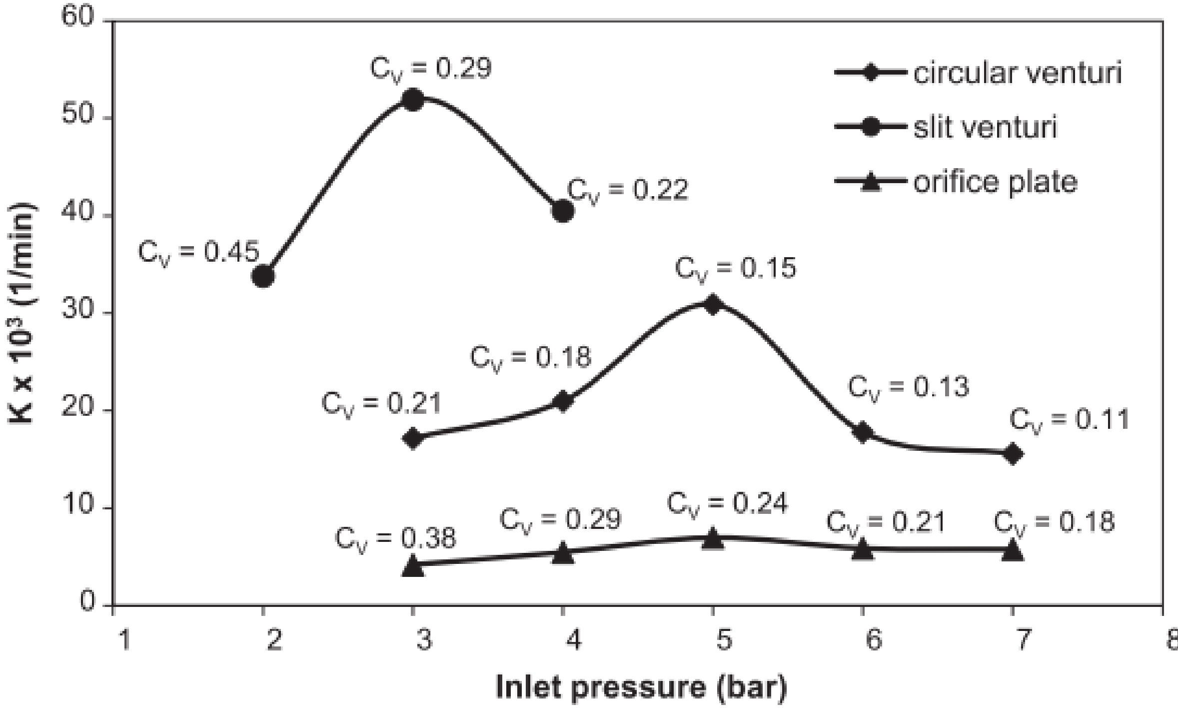
- Predict bulk pressure and veloicty based on Singhal et al. (2002)
- Predict movement of individual cavities using discrete phase model
- FLUENT eliminates acceleration term from the R-P equation (reduces min time step from 10^-9 s to 10^-4 s), use in house code for complete R-P to predict collapse intensity.





Saharan et al. 2012





Model Theory

Fluent has 3 models

- Singhal et al. (2002)
  - Mixture based, reduced R-P equation, considers first order effects like phase change, bubble dynamics, non-condensable gases, turbulent pressure fluctuations
  - “Complete Cavitation Model”
- Zwart et al(2004)
  - Reduced R-P, assumes large bubbles of equal size, interphase mass transfer rate determined by bubble size and density
- Schnerr and Sauer (2001)
  - Mass transfer driven by pressure differential, can model rentrant jet and sheet to cloud.

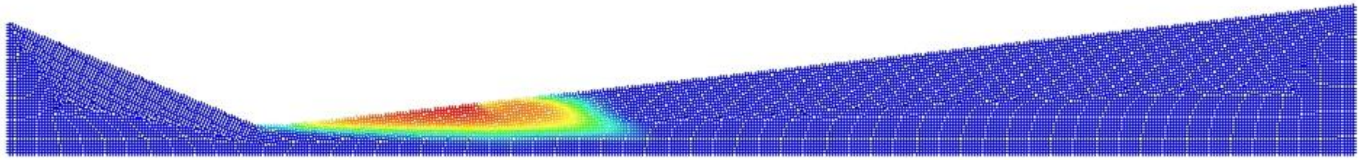
$$R\frac{d^2R}{dt^2}+\frac{3}{2}\left(\frac{dR}{dt}\right)^2+\frac{4\nu_L}{R}\frac{dR}{dt}+\frac{2\gamma}{\rho_L R}+\frac{\Delta P(t)}{\rho_L}=0$$

Current Model

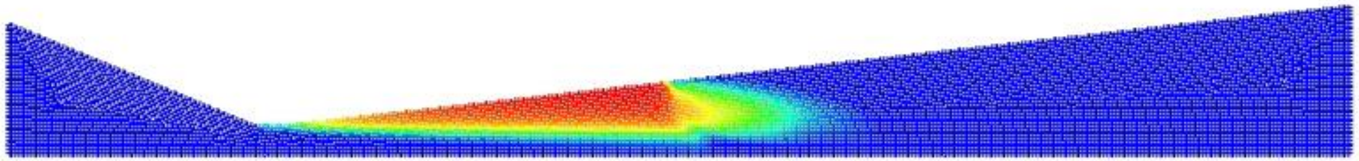
Parameter	Value
BCs	Pressure (P_in, P_out = 1 atm)
Elements	100,000 and 500,000
Model	Schnerr
Iterations	Steady: 500, unsteady: 200, 200 time steps at 1e-5 s
Turbulence	2nd Order k-epsilon

Cavitation zone increases with decreasing Cv

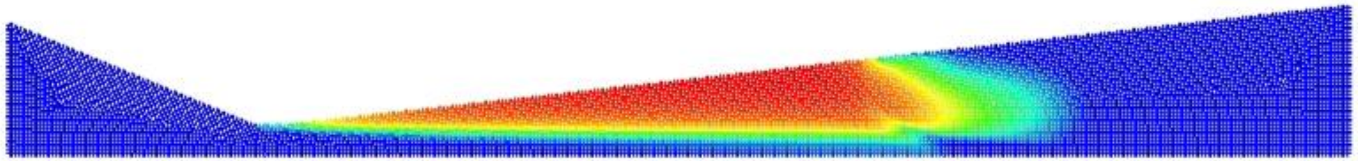
2 atm



3 atm

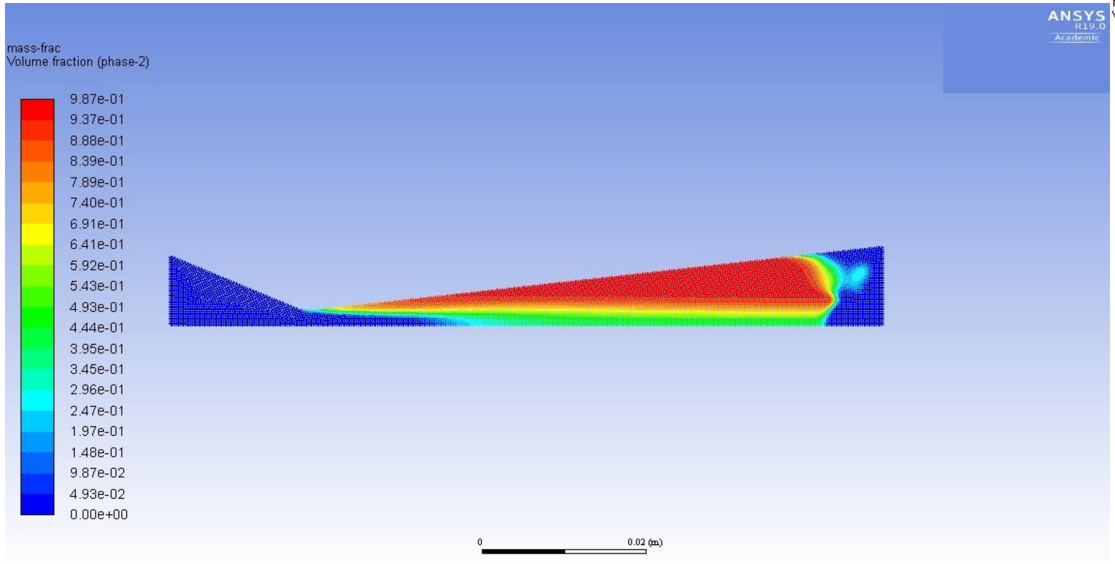


4 atm

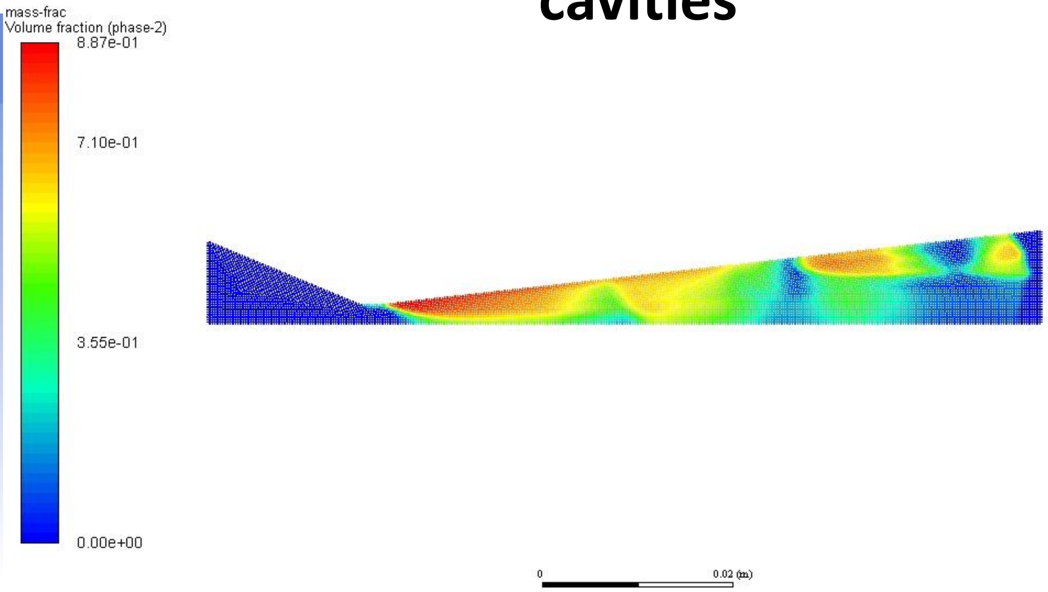


Model Captures Complex Behaviour

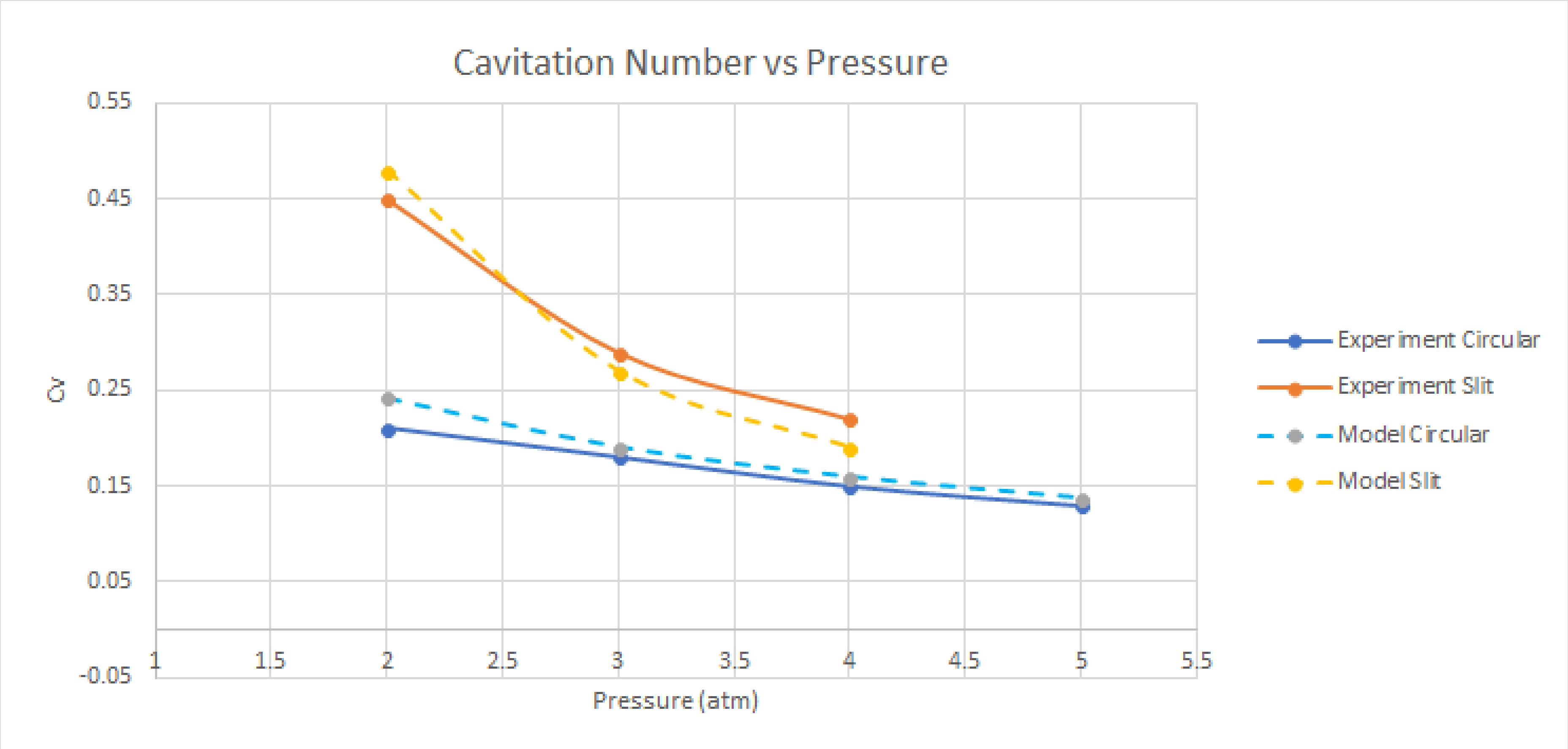
Sheet to Cloud



Collapse to form more cavities

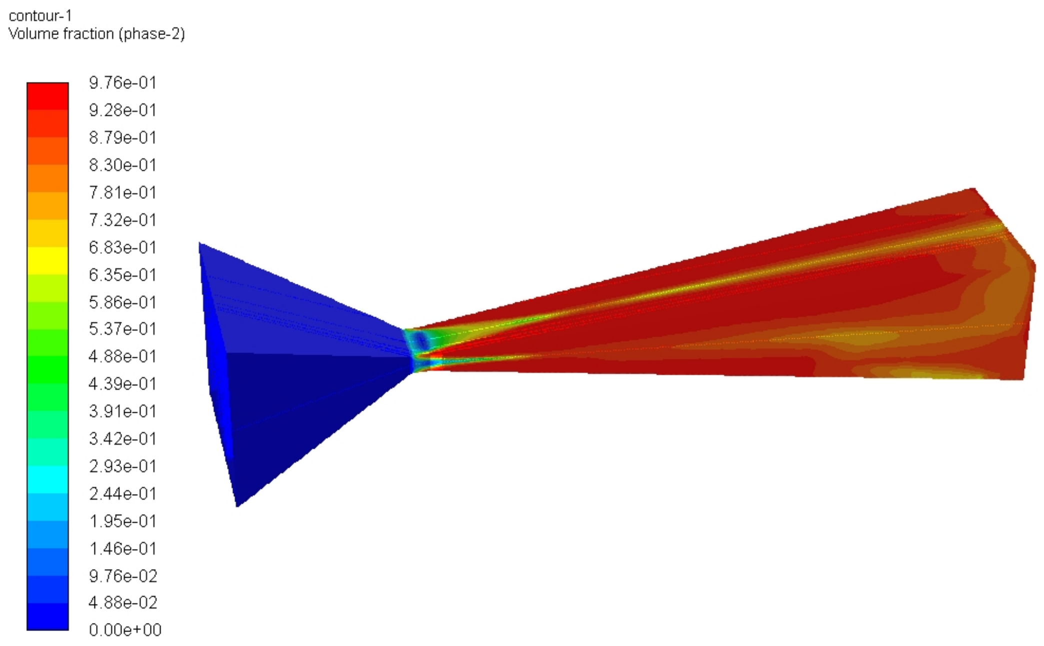


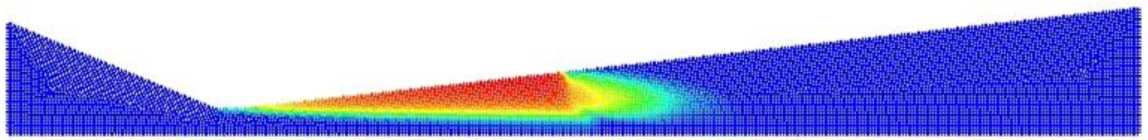
Results



Cavitation Number vs Pressure
0.55
0.45
0.35
0.25
0.15
0.05
-0.05
Cv
1
1.5
2
2.5
3
3.5
4
4.5
5
5.5
Pressure (atm)
Experiment Circular
Experiment Slit
Model Circular
Model Slit

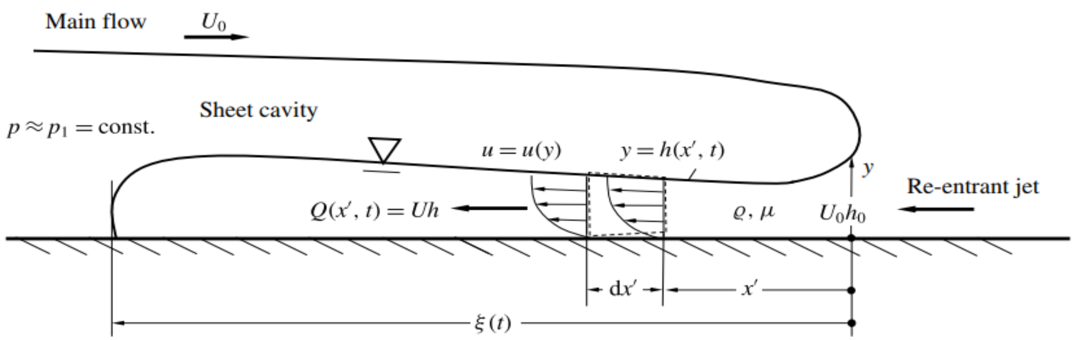
Cavitation Zones by Geometry





Re-entrant Jet

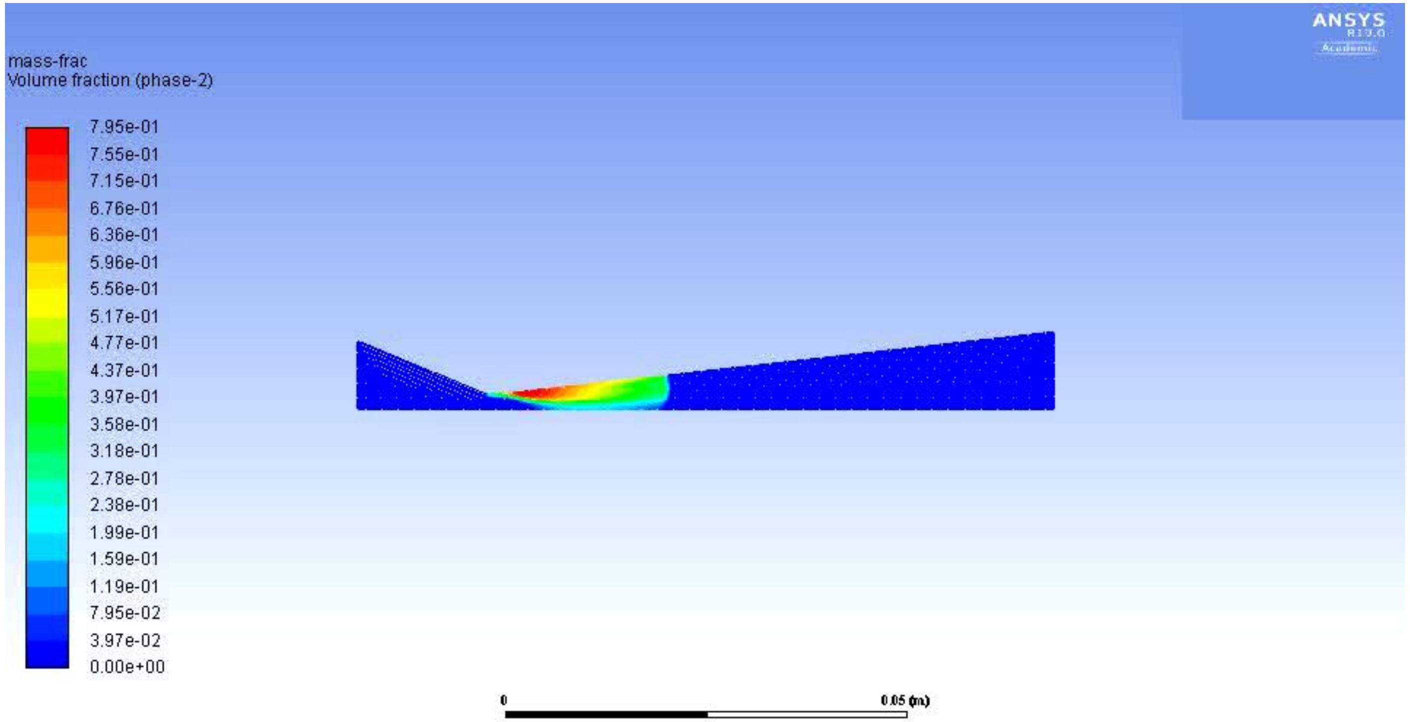
- Model captures Re-etrance jet
  - This thin spreading viscous film is typically 15-35% of cavity thickness (Callenaere et al. 2001)
  - Most people want to stop this, I want it!
    - Can explore the effect of geometry for breaking this up earlier to create cloud cavitation
    - Keep surface smoother so there are no obstacles to block jet



Source: Pelz et al. 2017

Problems

- Not enough nodes on student version
- Backflow



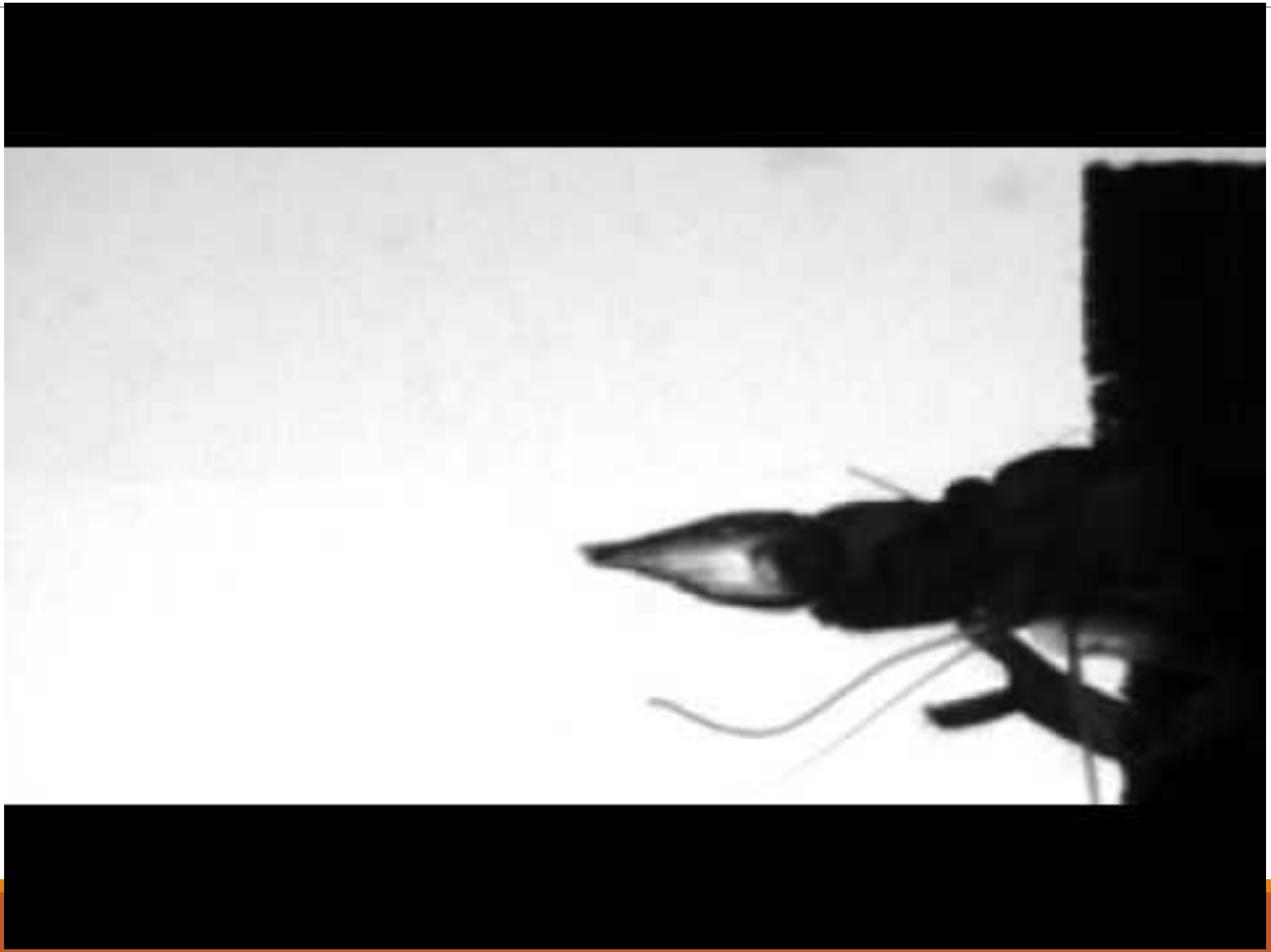
Lessons Learned and Next Steps

- Learned how to download OpenFOAM
- Learned FLUENT replaces all of it’s pictures and animations for each run
- Effect of cavitation number on sheet length
- Slit Venturi induces greater cavitation

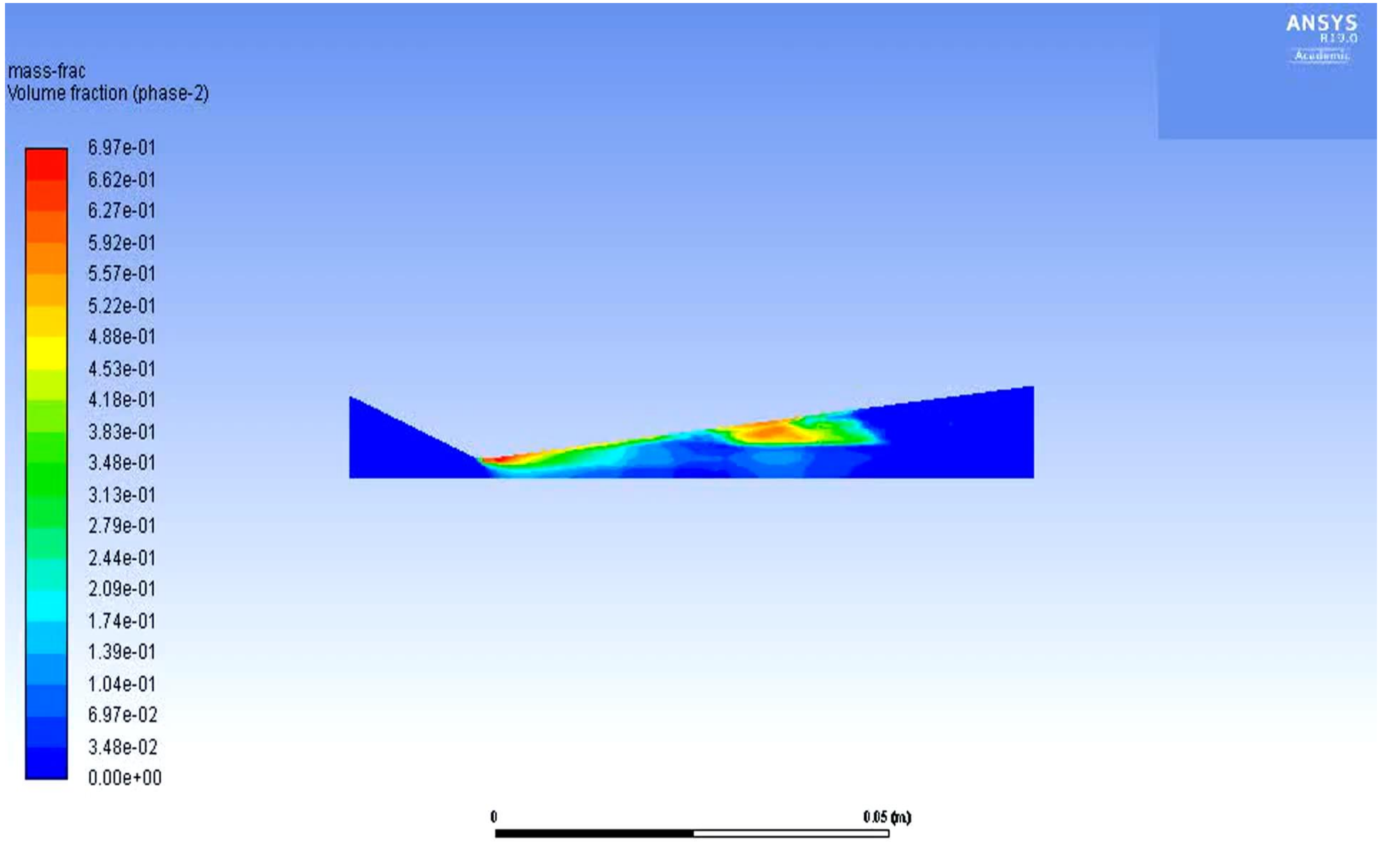
Next

- Build DPM to track cavity paths
- Build larger model to eliminate backflow
- Begin coding in-house code to determine collapse intensity
- Study geometries with higher alpha
  - Tradeoff of cavity density and size

Thanks! Questions?



Appendix


mass-frac
Volume fraction (phase-2)
6.97e-01
6.62e-01
6.27e-01
5.92e-01
5.57e-01
5.22e-01
4.88e-01
4.53e-01
4.18e-01
3.83e-01
3.48e-01
3.13e-01
2.79e-01
2.44e-01
2.09e-01
1.74e-01
1.39e-01
1.04e-01
6.97e-02
3.48e-02
0.00e+00
ANSYS
0
0.05 (m)

Model formulation (Chian and Chen 2016)

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \mathbf{u}_m) = 0 \qquad (1)$$

$$\frac{\partial}{\partial t}(\rho_m \mathbf{u}_m) + \nabla \cdot (\rho_m \mathbf{u}_m \mathbf{u}_m) = -\nabla p + \nabla \cdot \left[\mu_m \left(\nabla \mathbf{u}_m + \nabla \mathbf{u}_m^T\right)\right] + \nabla \cdot \left[\sum_{\kappa=1}^{2} \alpha_\kappa \rho_\kappa \mathbf{u}_{dr,\kappa} \mathbf{u}_{dr,\kappa}\right] \qquad (2)$$

$$\rho_m = \sum_{\kappa=1}^{2} \alpha_\kappa \rho_\kappa , \qquad (3)$$

$$\mathbf{u}_m = \frac{\sum_{\kappa=1}^{2} \alpha_\kappa \rho_\kappa \mathbf{u}_\kappa}{\rho_m} , \qquad (4)$$

$$\mu_m = \sum_{\kappa=1}^{2} \alpha_\kappa \mu_\kappa . \qquad (5)$$

Full Cavitation

$$\frac{\partial}{\partial t}(\rho_2\alpha_2) + \nabla \cdot (\rho_2\alpha_2\mathbf{u}_2) = R_e - R_c \qquad (6)$$

For the full cavitation model, if $p < p_v$,

$$R_e = C_e \frac{\sqrt{k}}{\sigma} \rho_2 \rho_1 \sqrt{\frac{2}{3}\left(\frac{p_v - p}{\rho_1}\right)}(1 - f_2 - f_g), \qquad (6)$$

and, if $p > p_v$,

$$R_c = C_c \frac{\sqrt{k}}{\sigma} \rho_2 \rho_1 \sqrt{\frac{2}{3}\left(\frac{p - p_v}{\rho_1}\right)} f_2. \qquad (7)$$

Zwart-Gerber-Belamri

For the Zwart-Gerber-Belamri cavitation model, if $p < p_v$,

$$R_e = C_e \frac{3\alpha_{nuc}(1-\alpha_2)}{R_B}\rho_2\sqrt{\frac{2}{3}\left(\frac{p_v - p}{\rho_1}\right)}, \tag{8}$$

and, if $p > p_v$,

$$R_c = C_c \frac{3\alpha_{nuc}\alpha_2}{R_B}\rho_2\sqrt{\frac{2}{3}\left(\frac{p - p_v}{\rho_1}\right)}. \tag{9}$$

In the above two expressions, C_e and C_c take the values of 50 and 0.01, respectively; R_B is the radius of bubble and is assumed to be 10^{-6} m; α_{nuc} represents the nucleation site volume fraction and its default value is assumed to be 5×10^{-4}.

Schnerr-Sauer

$$R_e = \frac{\rho_2 \rho_1}{\rho_m} \alpha(1-\alpha) \frac{3}{R_B} \sqrt{\frac{2}{3}\left(\frac{p_v - p}{\rho_1}\right)}, \tag{10}$$

and, if $p > p_v$,

$$R_e = \frac{\rho_2 \rho_1}{\rho_m} \alpha(1-\alpha) \frac{3}{R_B} \sqrt{\frac{2}{3}\left(\frac{p - p_v}{\rho_1}\right)}, \tag{11}$$

where the volume fraction is defined as

$$\alpha = \frac{n_b \frac{4}{3} \pi R_B^3}{1 + n_b \frac{4}{3} \pi R_B^3}. \tag{12}$$

with n_b being the number of bubbles per volume of liquid which is assumed to be 10^{13}.

It is noted that for the Zwart-Gerber-Belamri model and the Schnerr-Sauer model, the non-condensable permanent gas is not accounted for.

Models to look into

- Saito et al. 2007: Uses theory of evaporation/condensation on plane surface
- Okita and Kajishima 2002: mass transfer in the form of volume fraction
- Kunz et al. 2000: mass transfer depends on proportion of pressure below the vapor pressure for liquid to gas. Gas to solid modeled by third order polynomial function of volume fraction

For fine detail analysis: can resolve flow down to level of bubble radius

- BEM
- Front-tracking Method
- Interface Tracking Methods

Multiscale Models

- Ma et al. 2016: multi-scale, macroscale based on continuum based phase averaged two-phase model. Small bubble and liquid interaction considered with E-L coupling scheme.
  - Level-Set method for larger bubbles due to large free surface deformations, DSM for all unresolved bubbles (Lagrangian singularities)