COMPUTATIONAL FLUID DYNAMICS in CHEMICAL REACTION ENGINEERING V

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Computational Fluid Dynamics Model of Viscous Droplet Breakup

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Challenge

- Many high-viscosity mixing / blending processes result in the formation of droplets of one material inside a matrix of a second material
- The final application often requires that the droplet size be reduced to an acceptable range -
  - Properties or characteristics may depend on DSD
  - Reactions may be induced in one of the two phases
- There may be further process requirements
  - energy efficiency (low ΔP)
  - low capital cost
  - high throughput

Historic Droplet Breakup Literature:

- Breakup is impossible at high droplet to matrix viscosity ratios in simple shear flows
- However, breakup is possible in elongational flows

Capillary Number:

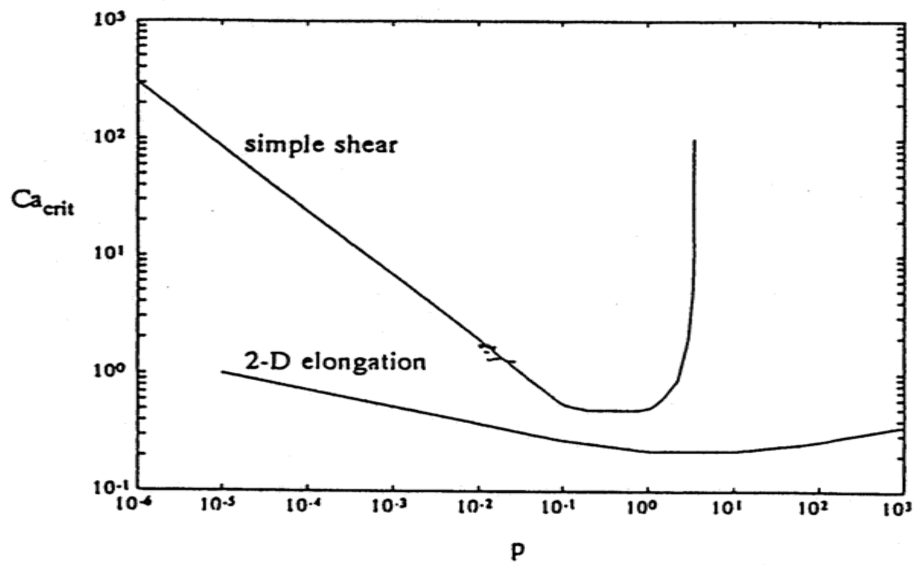
$Ca = \mu_m Ga/\sigma$

μ_m: matrix viscosity

G: deformation rate (shear or extensional)

a: droplet radius

σ: interfacial tension



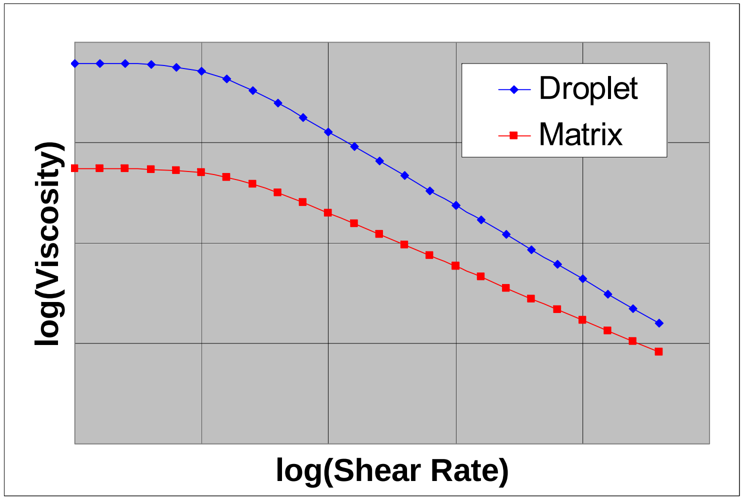
Critical Capillary number versus viscosity ratio p $(= \eta_d/\eta_c)$, in simple shear and in elongational flow (after Grace 1971).

Goals

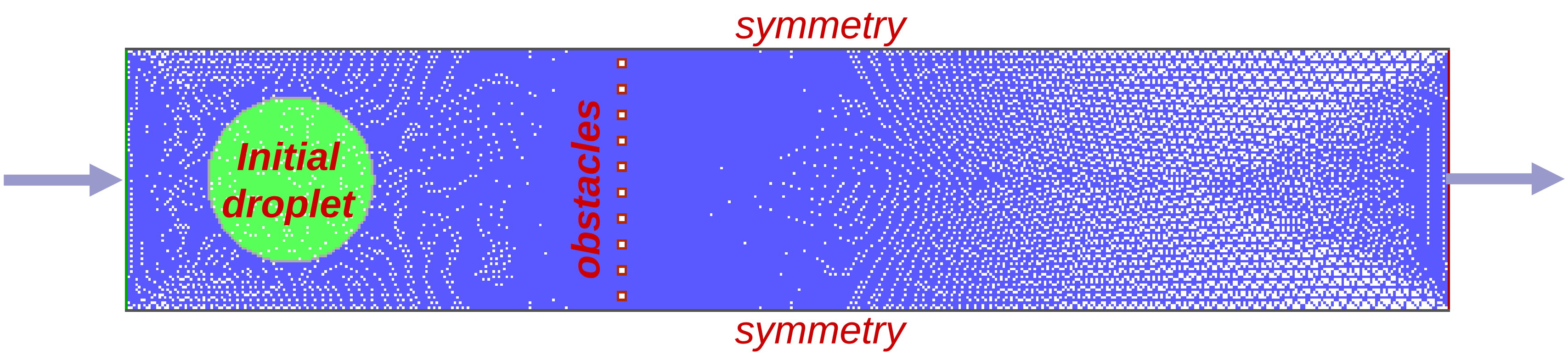
- Develop a validated model that can predict viscous droplet breakup in complex flow geometries
- Provide insights into the fundamental breakup mechanisms
- Design optimal flow geometries for effective droplet breakup with efficient energy input

Modeling Methodology

- ***COMPUTATIONAL FLUID DYNAMICS SET-UP***
  - Code: FLUENT
  - Interface Tracking: "Volume of Fluids" Method (VOF)
  - Laminar / Transient
  - Geometry: SINGLE droplet flowing past obstacles
    - symmetry planes – captures effect of droplet number density
    - tight mesh to capture interface
- ***PROPERTIES***
  - Rheology: Carreau model
    - Shear Thinning
    - Droplet has higher viscosity than the matrix over the shear rates of interest
  - Density (droplet and matrix)
  - Interfacial tension *(No observed effect)*

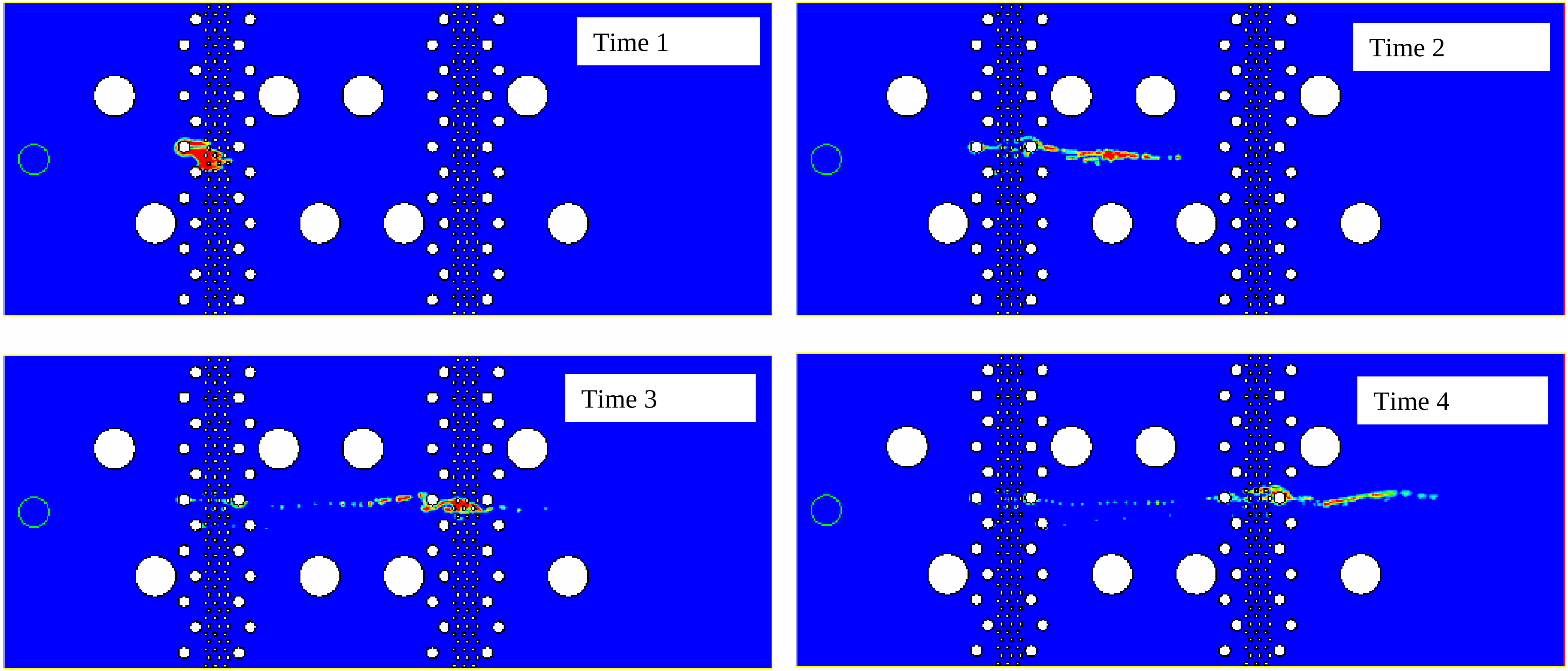


2D Modeling



- ***Vary***
  - □Obstacle Layout
  - □Initial droplet radius (circular / cylindrical)
  - □DROPLET Number density
  - □Mass flux (V_{in})
  - □Rheology
  - □Droplet – Obstacle Alignment

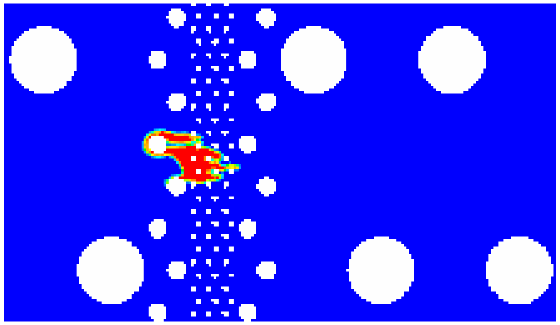
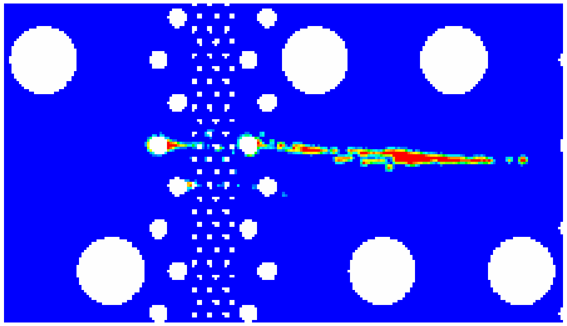
- *Follow droplet interface with time as it flows past obstacles*



Colors represent volume fraction of droplet phase

Multiple Mechanisms

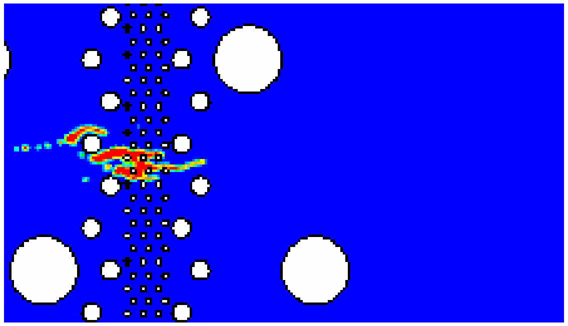
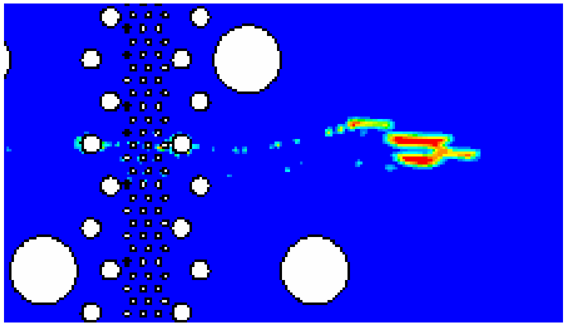
1) ***"Stick-and-Pull":***
Higher droplet-to-matrix viscosity ratios cause the droplet to "stick" to the obstacles more tightly so there is more stretching as it is pulled off.

Time 1

Time 2

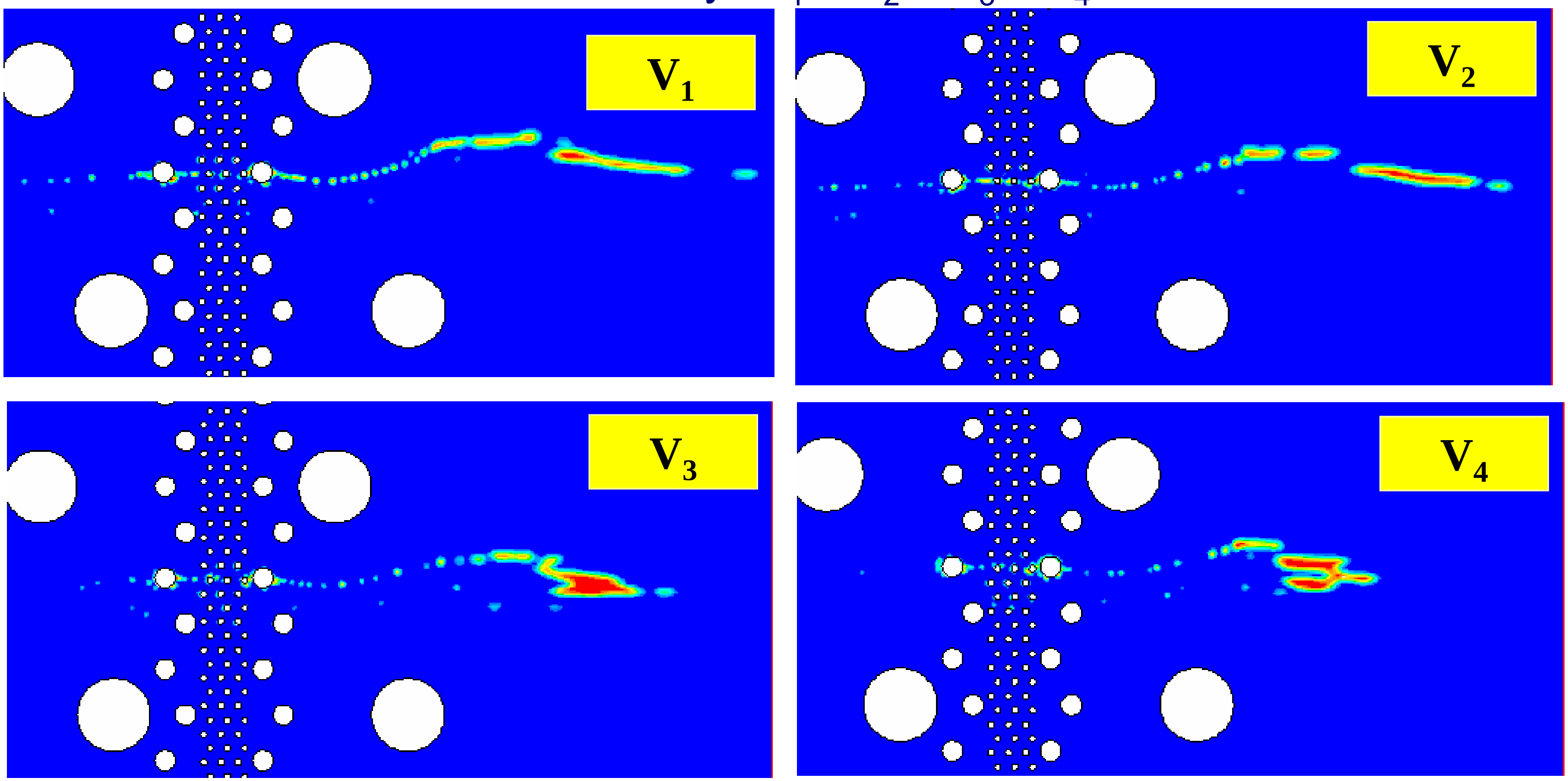
2) ***"Wire-Spreading":***
Lower droplet to matrix viscosity ratios are more easily spread apart by the obstacles and less likely to flow back together.

"Stick-and-Stay"

Compare Breakup at Different Flow Rates
(different shear rates → different viscosity ratios)

Inlet velocity: $V_1 < V_2 < V_3 < V_4$

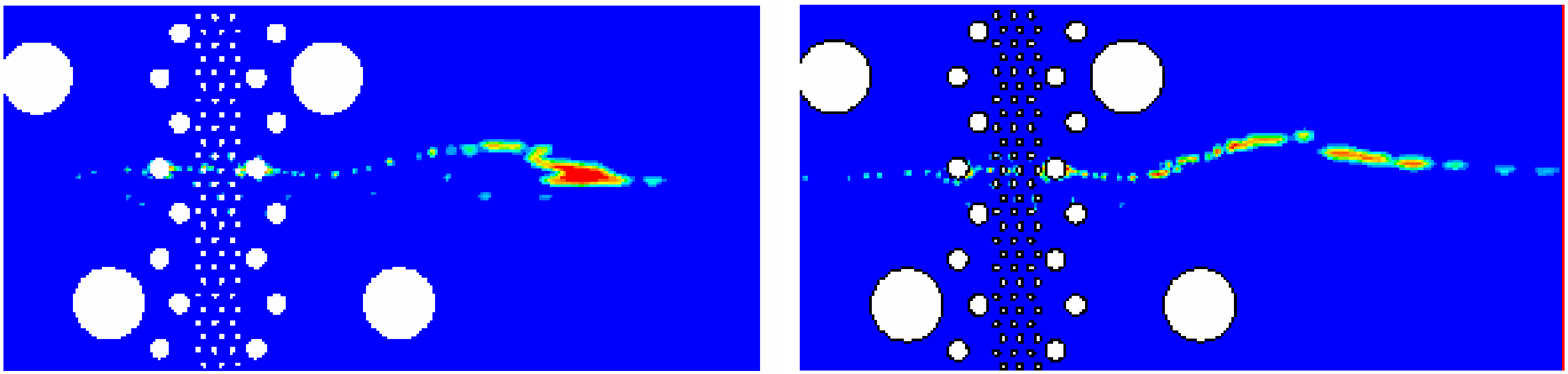


Experimental Observation: break-up is more efficient at lower and higher rates

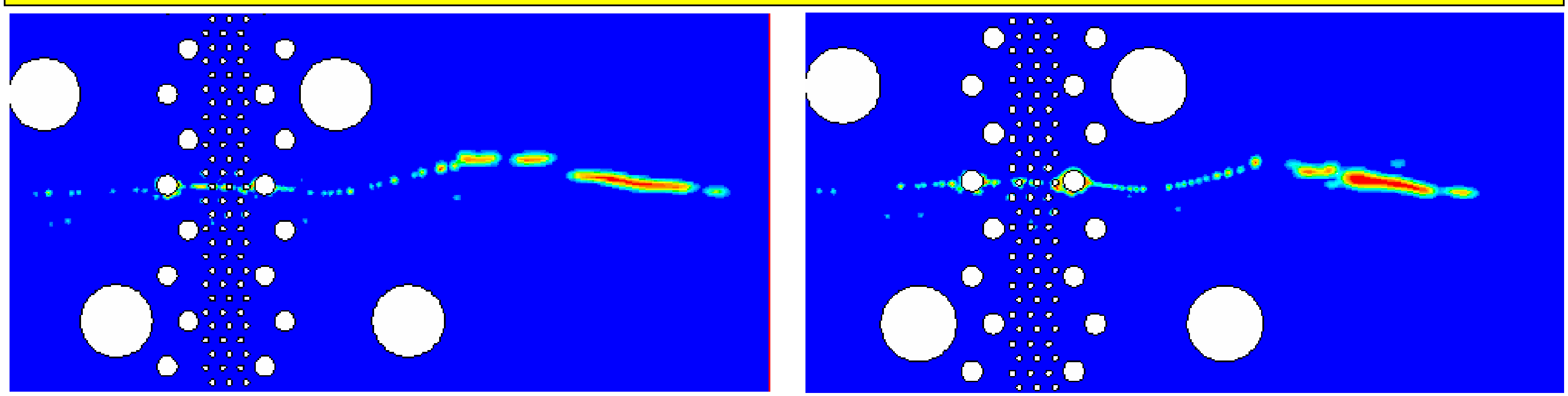
Compare Two Different Droplet/Matrix Systems

System A	SystemB

Same Flow Rate



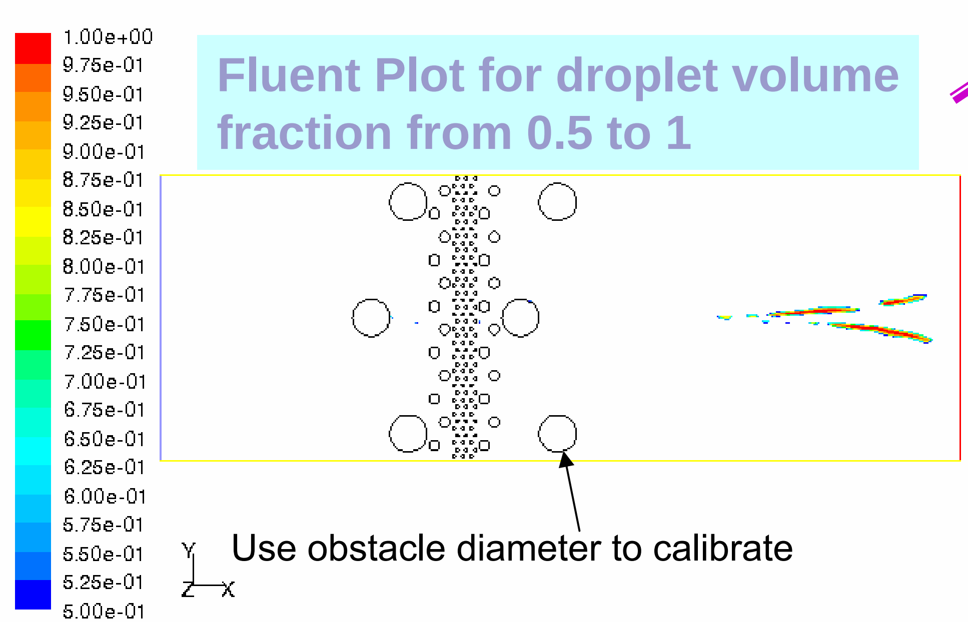
Similar Droplet-to-Matrix Viscosity Ratios



2D Model Validation

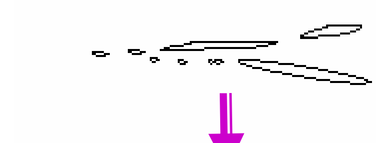
- Compare the droplet breakup predicted by the model with experimental data:
  - Experimental Data is in the form of droplet size distributions (DSD) for both the upstream and downstream mixtures
  - Model needs to account for initial DSD and determine final DSD
    - use ImageJ software

Fluent Plot for droplet volume fraction from 0.5 to 1



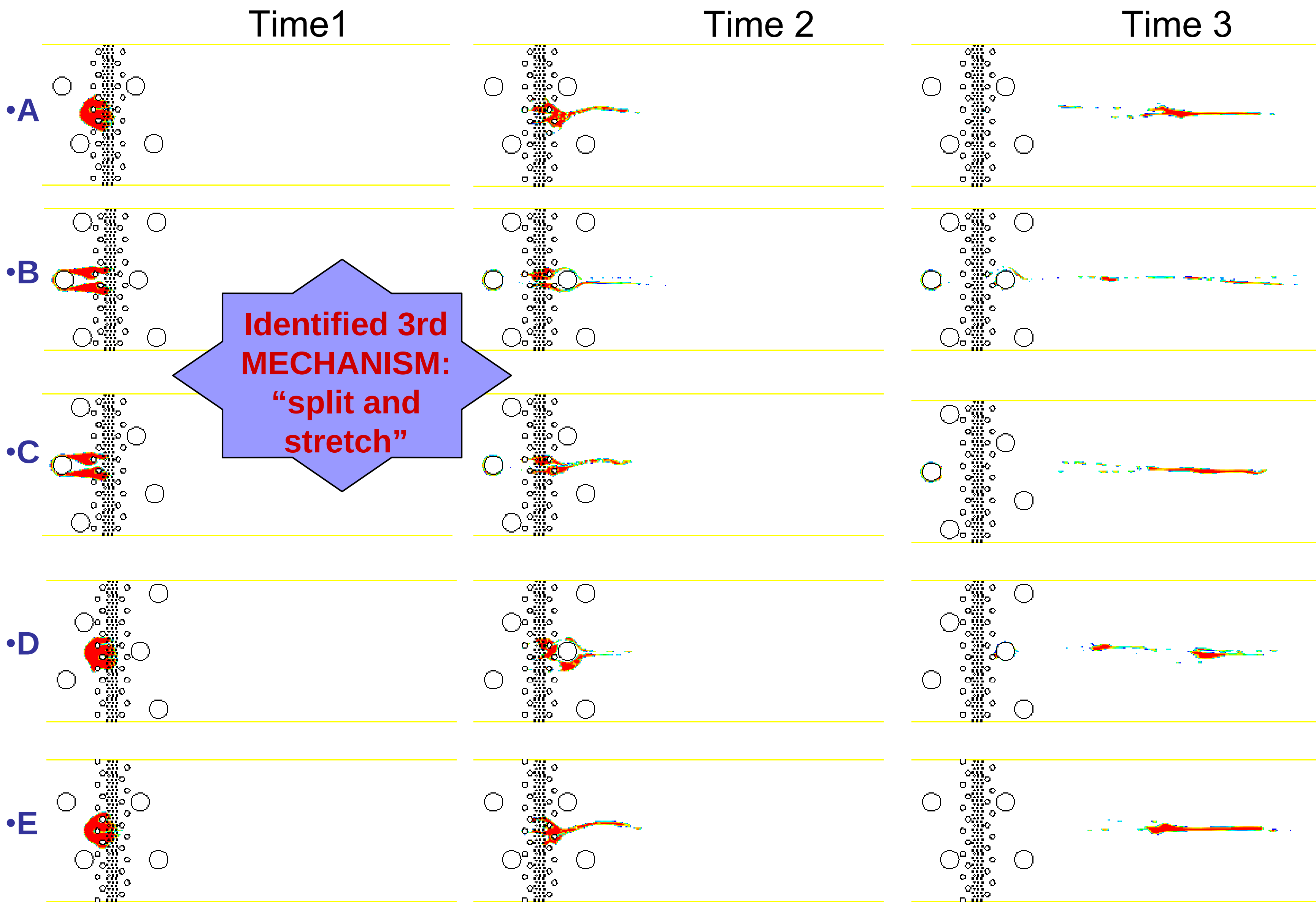
rendering of droplets to be analyzed

Equivalent ellipses



Obtain Predicted DSD and Aspect Ratios

Effect of Obstacle Position



Overall DSD Methodology

- *Run the CFD droplet breakup simulation for*
  - *5 different obstacle alignment cases (A-E)*
  - *8 different starting droplet diameters (80-1200 μm)*
- *Use the Image analysis tool to get the DSD for each case*
- *Account for possible elongational breakage*
  - *Droplet Aspect Ratio > "Break-up Aspect Ratio" (BAR)*

    → droplet will break up into the minimal number of equal parts so that the aspect ratio of each part is less than the BAR value
- *Determine the overall DSD for each initial droplet size using probabilities of droplet-obstacle contact for each alignment*
- *Determine the combined DSD for all of the droplet sizes using the experimental values for the number of starting droplets in each size bin*
- *Compare to the experimental DSD values*

Droplet-Wire Contact Probabilities

Determine probabilities for droplet "hitting" large wires in the two rows

- Define "hitting" to mean the droplet edge crosses the wire center
- Event R = droplet "hits" first wire

  Event S = droplet "hits" last wire

  Assume R and S are independent
- P(R) = P(S) = G/L

  where G = droplet diameter

  L = distance between wire centers
- B: $P(R \cap S) = P(R) * P(S)$

  C: $P(R \cap S^C) = P(R) * (1-P(S))$

  D: $P(R^C \cap S) = (1-P(R)) * P(S)$

  A: $P(R^C \cap S^C) = (1-P(R)) * (1-P(S))$

Droplet Size	P(R) = P(S)	B	C and D	A (split w/ E)
microns	%	%	%	%
1200	100	60	20	0
700	55.12	30.38	24.74	20.14/2
550	43.31	18.76	24.55	32.14/2
450	35.43	12.56	22.88	41.69/2
350	27.56	7.60	19.96	52.48/2
250	19.69	3.88	15.81	64.50/2
150	11.81	1.40	10.42	77.77/2
78	6.14	0.38	5.76	88.09/2

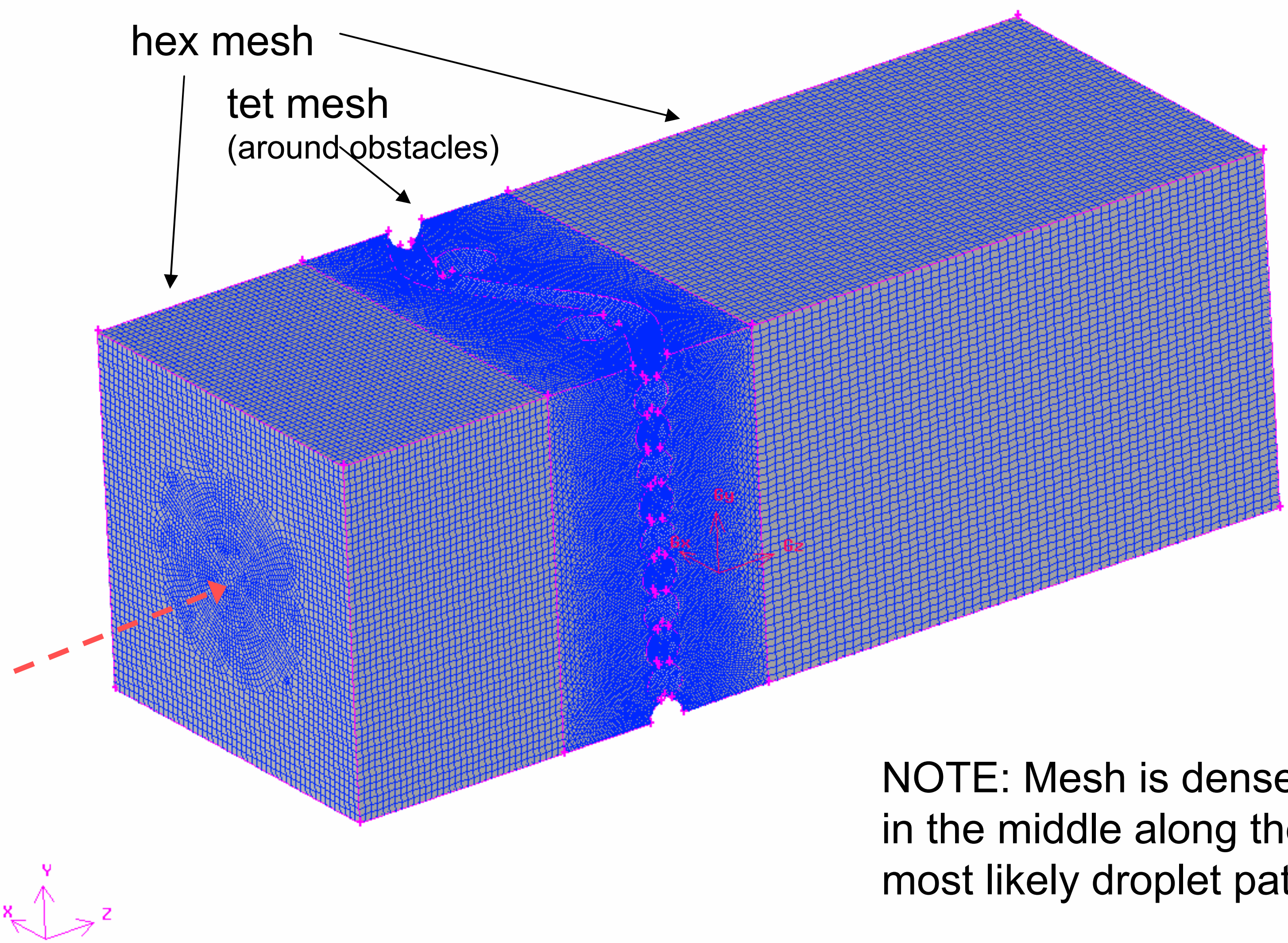
- Allow cases A and E to be weighted evenly

•Note: Probability of droplet hitting smaller wires is always 100%

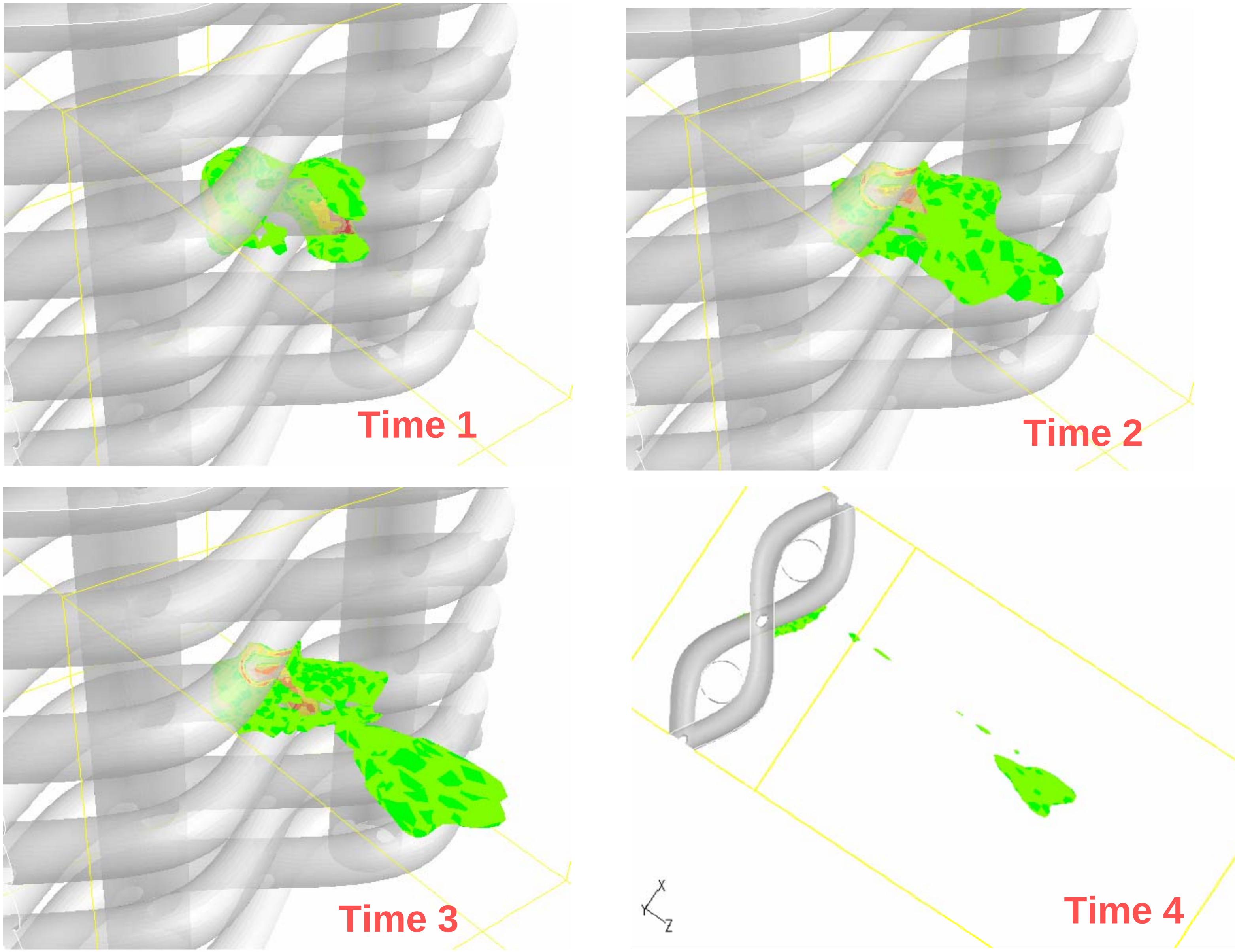
Prediction vs. Experiment

Droplet Size Bins (um)		Droplet Breakup Simulation DSD Predictions							Exp DSD
		Breakup Aspect Ratio (BAR)							
Range	Ave.	1	2	3	4	5	6	inf	
7 to 54	30	21157.66	**18739.04**	**18573.55**	**18526.43**	**18526.43**	**18526.43**	**18634.32**	**13651**
55 to 100	78	13493.22	5578.46	**4832.53**	**4719.96**	**4719.96**	**4719.96**	**4826.91**	**3960**
101 to 200	150	**1525.10**	11814.66	12155.64	10384.53	10024.79	10024.79	10091.32	**1543**
201 to 300	250	33.84	**43.83**	**555.31**	2501.26	2818.70	2338.51	1847.68	**141**
301 to 400	350	0.00	**33.84**	**75.79**	**44.76**	**56.65**	506.44	839.57	**49**
401 to 500	450	0.94	0.00	0.94	**0.00**	**30.40**	60.81	247.78	**9**
501 to 600	550	0.03	0.00	**0.00**	**32.90**	32.90	32.90	108.10	**2**
601 to 800	700	0.03	0.94	0.03	0.00	0.00	**0.00**	**26.79**	**4**
801 to 1600	1200	0.00	0.05	0.96	0.99	0.99	**0.99**	**18.00**	**9**

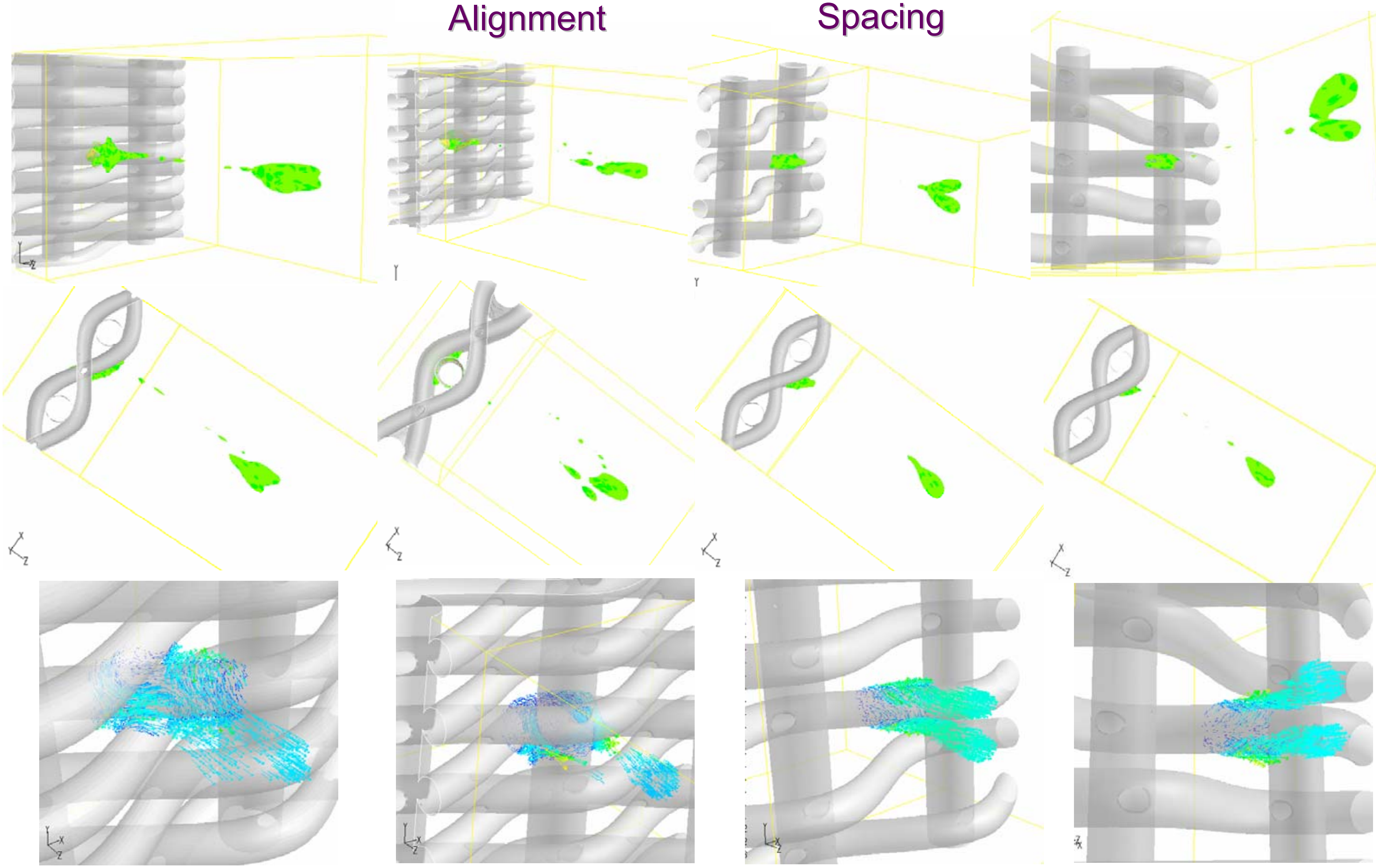
3D Modeling



NOTE: Mesh is denser in the middle along the most likely droplet path


Time 1
Time 2
Time 3
Time 4

Base Case	Change Droplet Alignment	Change Wire Spacing	Change Wire Size



Double layer

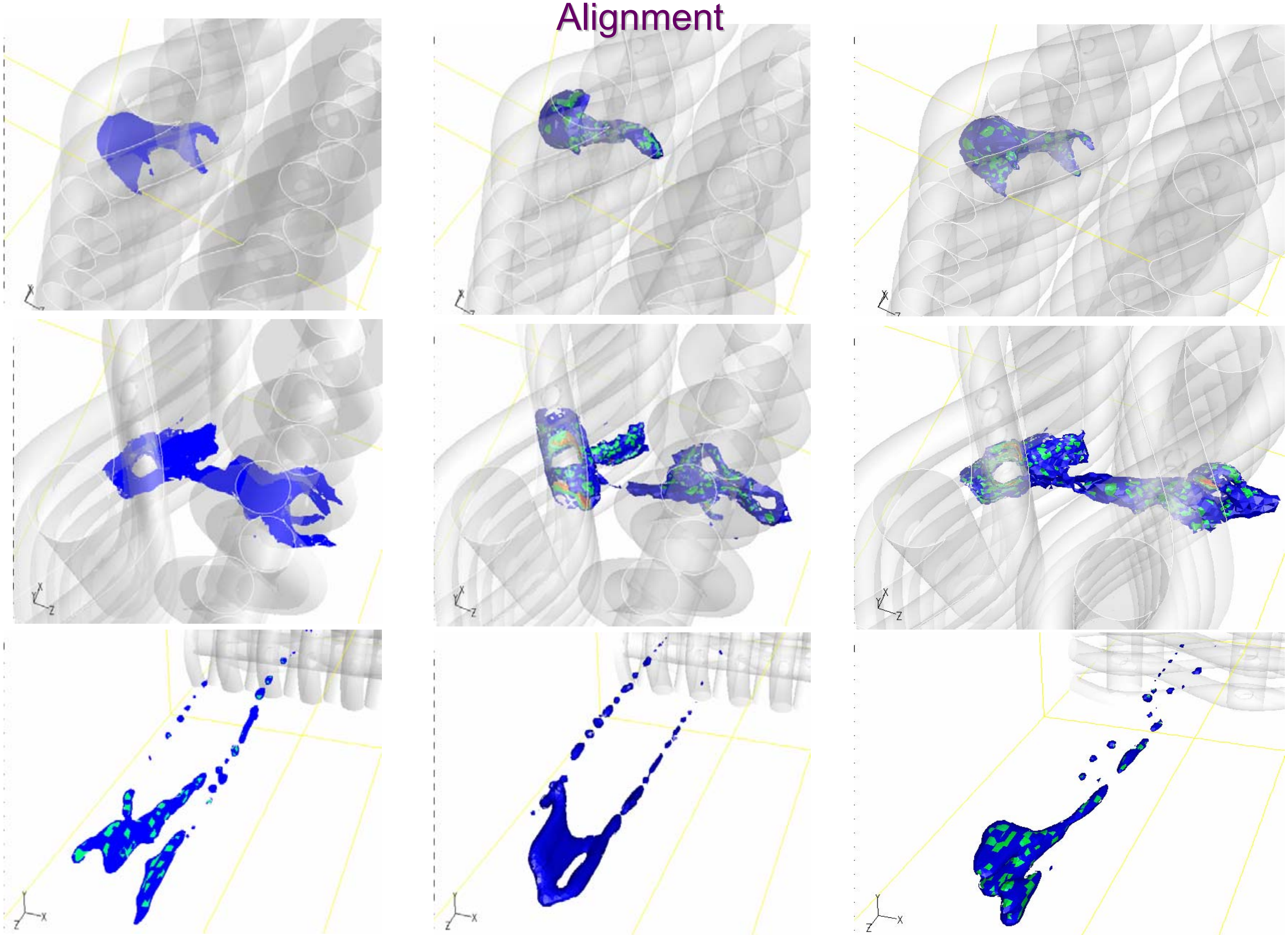
Change Droplet Alignment

Change Wire Alignment

Time 1

Time 2

Time 3



Potential Model Enhancements / Challenges

- Multiple starting droplets in single model
  - *degree of interaction depends on droplet number density*
  - *requires large mesh and computational resources*
- Miscibility / Diffusion effects
  - *VOF method treats the phases as immiscible*
- **Elongational and/or viscoelastic viscosity models**
  - ***Variations in Literature Observations concerning the Effect of Viscoelasticity on Droplet Breakup***
  - ***We do not currently have a code that has both viscoelastic modeling capability and a VOF method***

Viscoelasticity Effect - Literature Observations

- *Trends:*
  - Droplet elasticity → stabilizing
  - Matrix elasticity → destabilizing
- *Break-up Mechanisms:*
  - stretching along flow axis
  - erosion
  - tip streaming
  - elongation in vorticity direction

e.g., PS droplet in PE matrix in simple shear (Couette) flow*:

- at low shear rates, viscous shearing forces dominate → drop elongates a small amount in the flow direction
- as shear rates increase, normal stresses induce secondary flow perpendicular to flow direction → droplet takes on a diamond shape
- at high shear rates, get competition between normal stresses and shear stresses → drops align perpendicular to flow direction
- at high enough shear rates → droplet elongates and breaks along vorticity axis

*Frej Mighri, Michel Huneault; *In Situ Visualization of Drop Deformation, Erosion,and Breakup in High Viscosity Ratio Polymeric Systems under High Shearing Stress Conditions*; J. Applied Polymer Science, 100, 2006, pp 2582-91

Summary

- The model has provided insights into some of the mechanisms that can cause droplet breakup
  - *Helps to explain some puzzling observed phenomena*
- We have generated ideas for new obstacle geometries
  - *Some have been implemented*
- Although the 2D model results do not perfectly match the experimental data, they do seem to capture the trends
- The 3D model results provide further understanding of the complex interactions between the droplet and obstacles
- Next Step: Develop ability to evaluate the effect of viscoelasticity on the droplet breakup in complex geometries
  - *Requires new modeling capabilities*