# Bench-scale experiments and CFD simulations for Low Aqueous Solvent with different packings


Zhijie (Jay) Xu, Pacific Northwest National Lab (PNNL)

Richard Zheng, Pacific Northwest National Lab (PNNL)

Christine Anderson-Cook, Los Alamos National Lab (LANL)

# Challenges & Objectives

## Challenges:

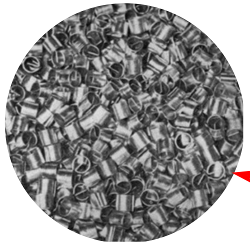
Packing characterization at device scale:

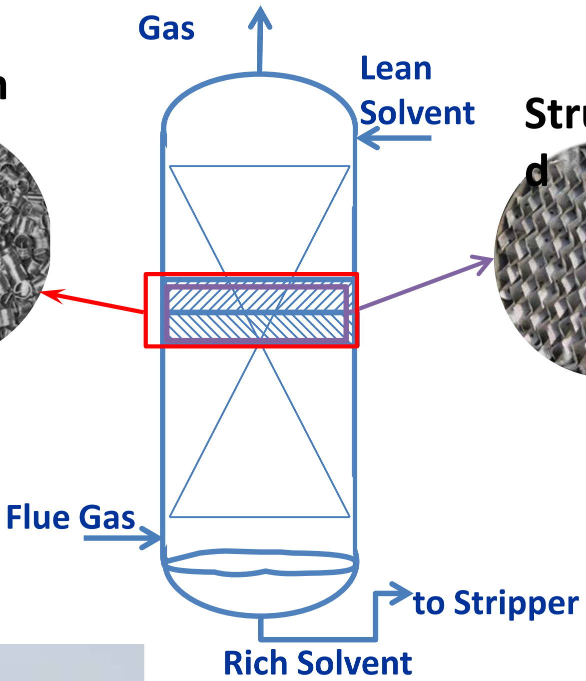
- Effective mass transfer area $a_e$
- Gas-film mass transfer coefficient $k_g$
- Liquid-film mass transfer coefficient $k_l$

## Objectives:

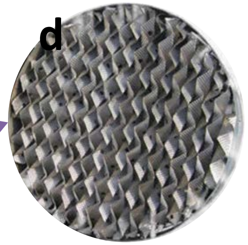
- Using CFD to
  - directly model mass transfer area at bench-scale
  - understand the local hydrodynamics /mass transfer with complex geometry
- Using bench-scale column exp. to
  - study the performance of solvent/packing
  - validate the CFD area model

**Random**

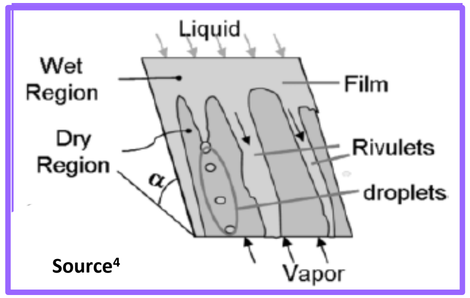





**Structured**



**Counter-current flow**




**Column:**
Φ ~10m
H ~30m

**Layer height:**
~20cm

**Corrugation height:**
O(10 mm)

**film thickness**
~ O(0.1mm)

# Outline

- Bench-scaled Packed Column (Overview)
- Experiments (EEMPA & MEA)
- CFD Simulations
  - 1:1 full size column CFD modeling
  - Representative column CFD modeling
- Experiment / CFD Comparison
- Plan for Sequential Design of Experiment (SDoE)
- Conclusion

# Outline

- Bench-scaled Packed Column Overview
- Experiments (EEMPA & MEA)
- CFD Simulations
  - 1:1 full size column CFD modeling
  - Small size  column CFD modeling
- Experiment/CFD Comparison
- Plan for Sequential Design of Experiment (SDoE)
- Conclusion

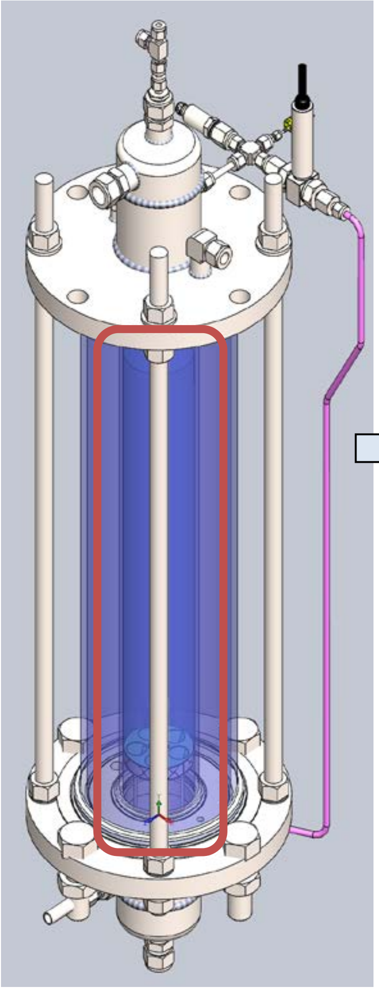
# Bench-scaled Packed Column Overview

**Bench-scale Column Design:**
- Glass Jacket Column
- Diameter 3'', Height 21''

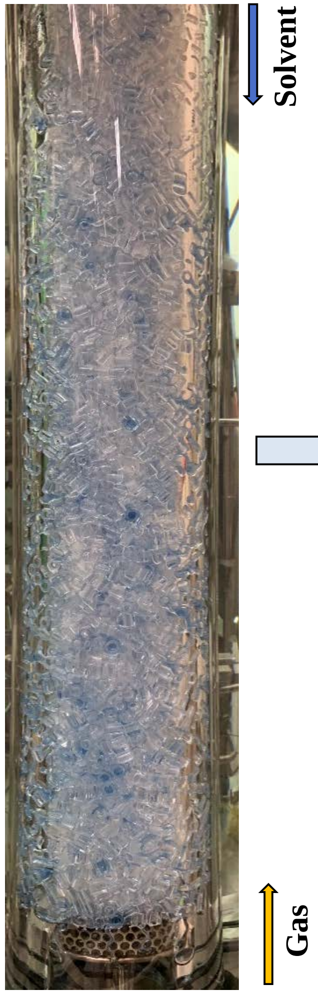
**Packing Type:**
- Raschig rings
  - Diameter: 6 mm
  - Height: 6 mm
- 8000-9000 rings
- Material: 316SS, Nylon 6
- Porosity: 68%
- Specific area: 835 $m^2/m^3$

**Solvents:**
- MEA
- EEMPA

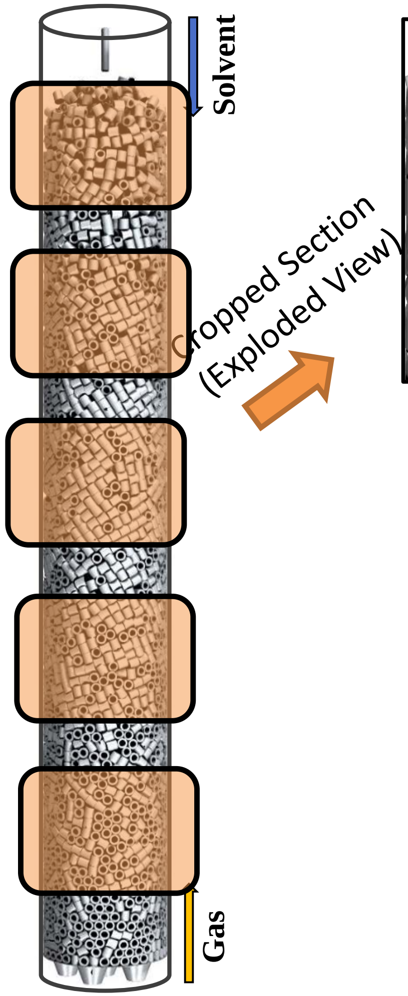
| | MEA | EEMPA |
|---|---|---|
| Viscosity $\mu$ [cP] | 1.4 | 7.1 |
| Surface Tension $\sigma$ [N/m] | 0.067 | 0.034 |



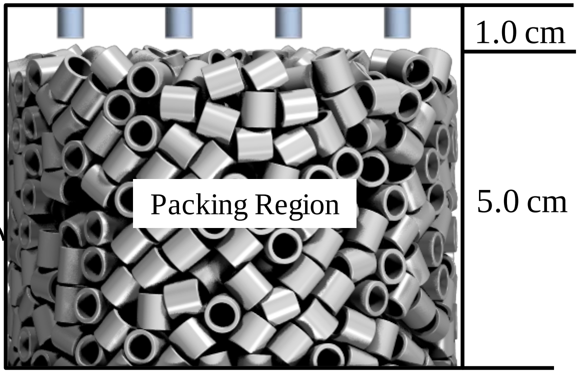
**Column Design**




**Experiment Column**




**1:1 Full Scale CFD Model**




**Representative Column Model**

**Sensitivity study and SDoE (Sequential Design of "Experiment")**

# Outline

- Bench-scaled Packed Column Overview
- Experiments (EEMPA & MEA)
- CFD Simulations
  - 1:1 full size column CFD modeling
  - Representative column CFD modeling
- Experiment/CFD Comparison
- Conclusion

# Experiments of Bench-scale Packed Column

## Solvent/packing pairs:

- MEA and 316SS
- EEMPA and 316SS
- MEA and Nylon 6
- EEMPA and Nylon 6

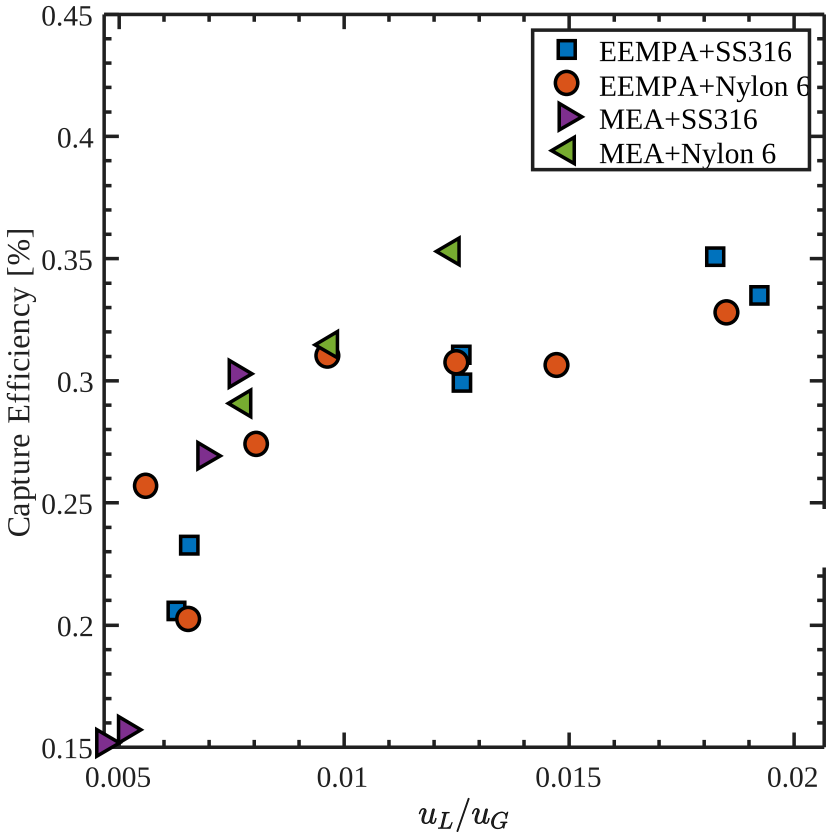
## Packing Material

- 316 Stainless Steel
- Nylon 6

H = 6mm
OD= 6mm
Wall=0.82 mm

## Measured Carbon Capture Efficiency (CE)

- CE increase with $u_L/u_G$
- Effective area back out from CE

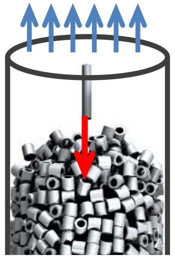


# Outline

- Bench-scaled Packed Column Overview
- Experiments (EEMPA & MEA)
- CFD Simulations
  - 1:1 full size column CFD modeling
  - Representative column CFD modeling
- Experiment/CFD Comparison
- Conclusion

# 1:1 Full Size CFD Model

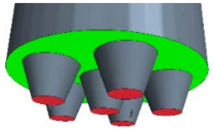
## Full Size CFD Model Setup



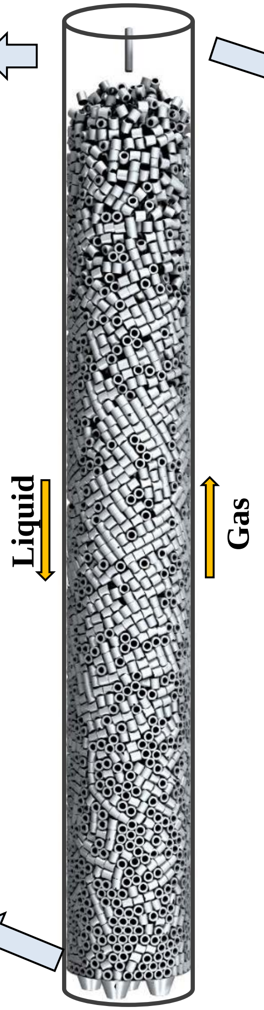

Top Boundary

Packed Column Dimension:
ID: 3''
Height=21''

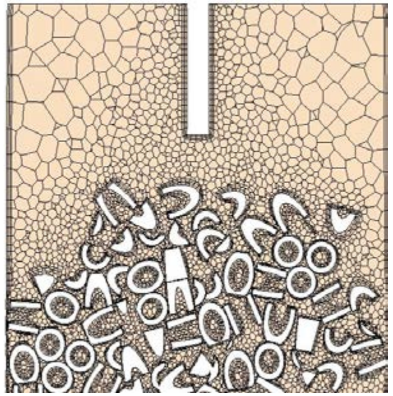
Bottom Boundary



Green: Gas Inlet
Red: Solvent Outlet




Arrangement of Raschig Rings

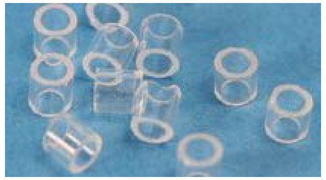


Sectional plane view

## Numerical Packing Process

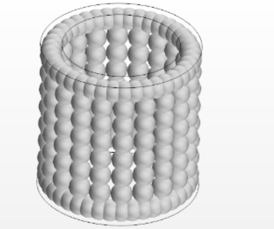
Stainless Steel

Glass Ring



H = 6mm, OD= 6mm, Wall=0.82 mm

Composite Particle Model

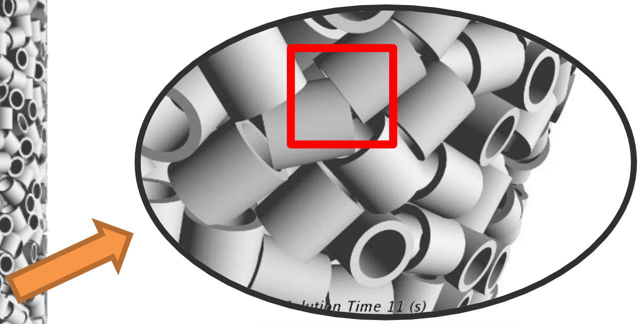


200 Small Ball (D=0.82 mm)

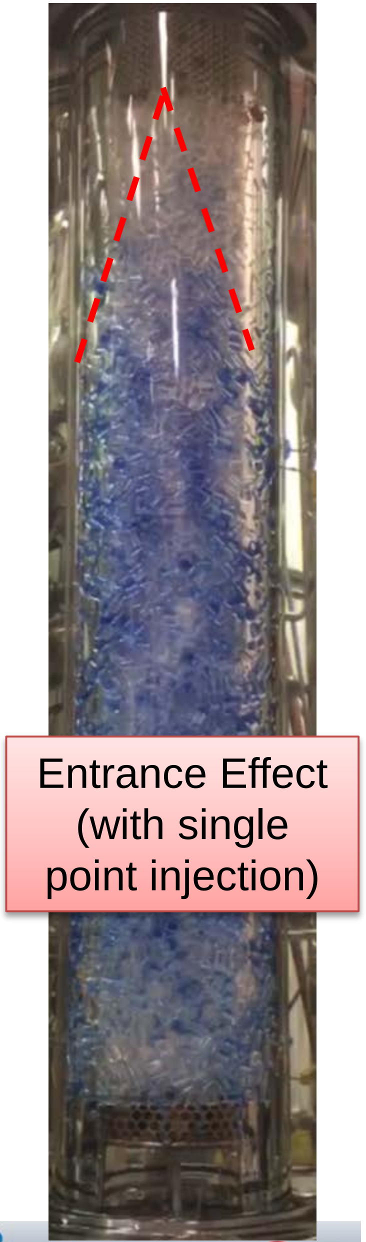
Experiment Packing

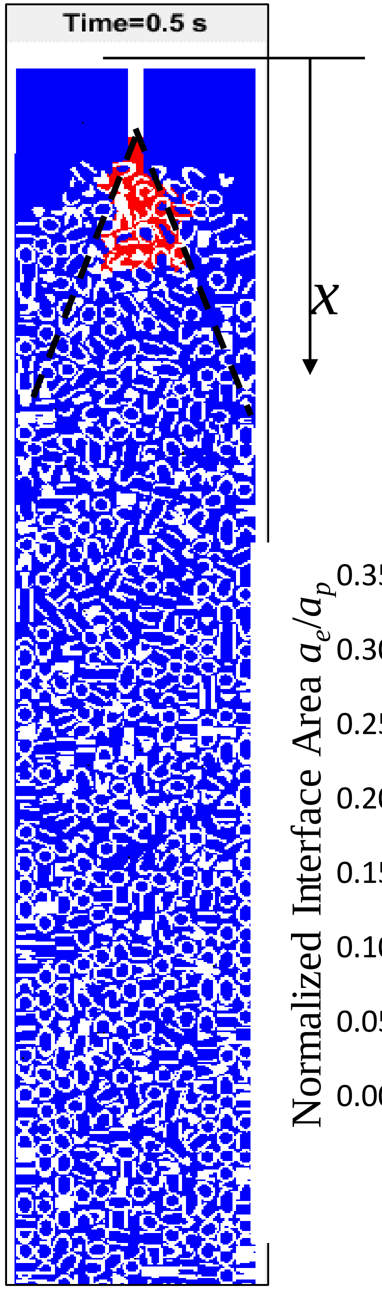
CFD Simulated Packing

**Improved ring contact modeling**



# 1:1 Full-size CFD Model



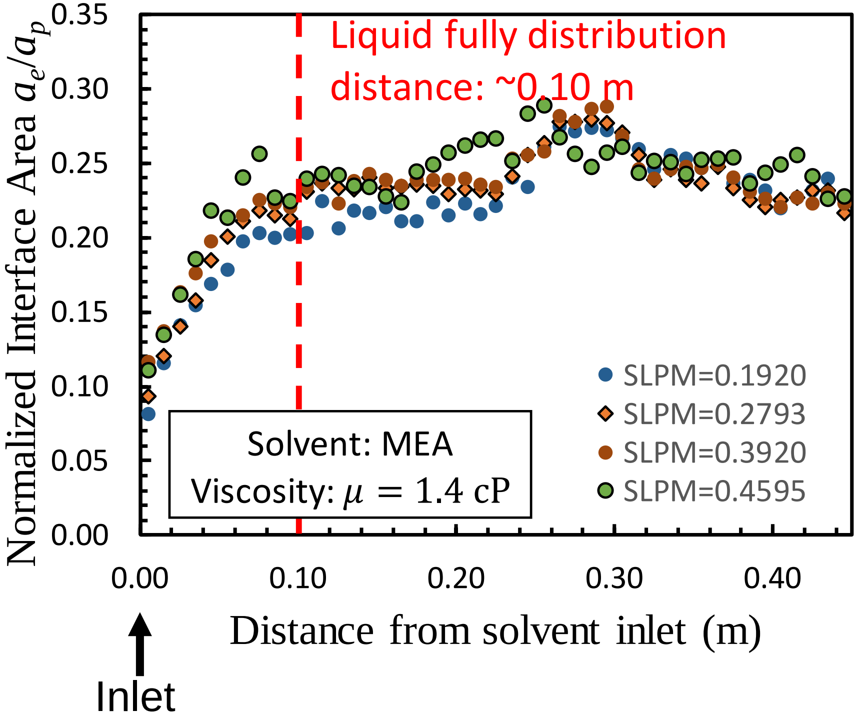



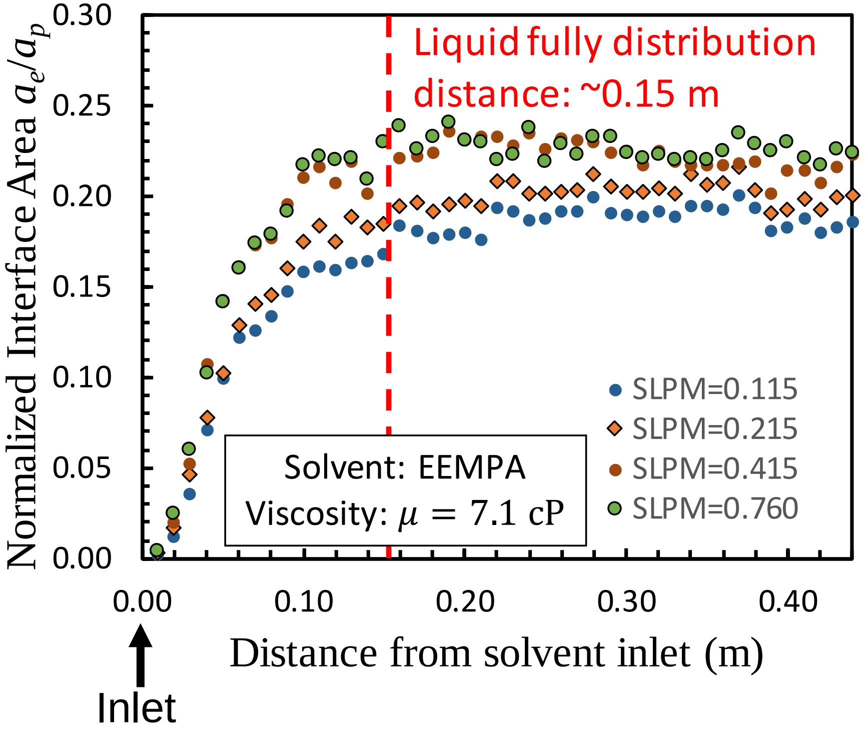

## Simulation Conditions:

- Total 9434 Rings
- Total ring surface area: 1.99 m2
- Liquid flow rate: 0.1-0.8 SLPM
- Gas flow rate: 25 SLPM
- Solvent viscosity: [1.4, 7.1] cP

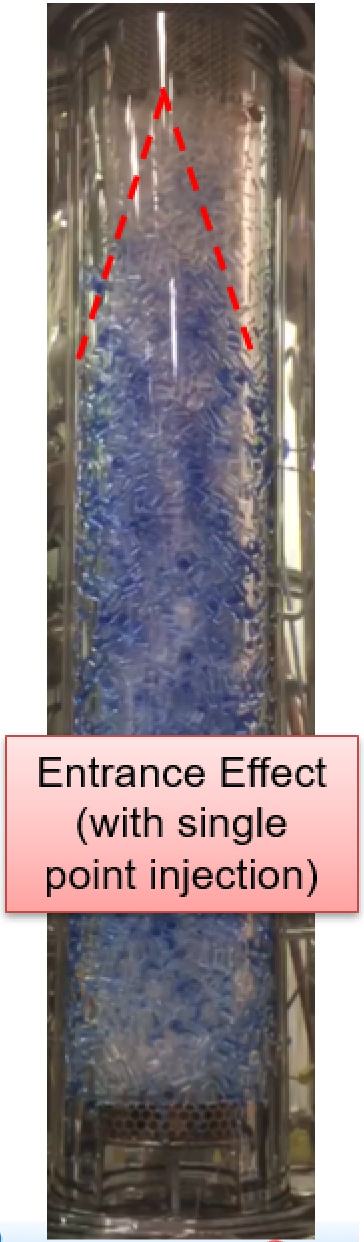
## Findings:

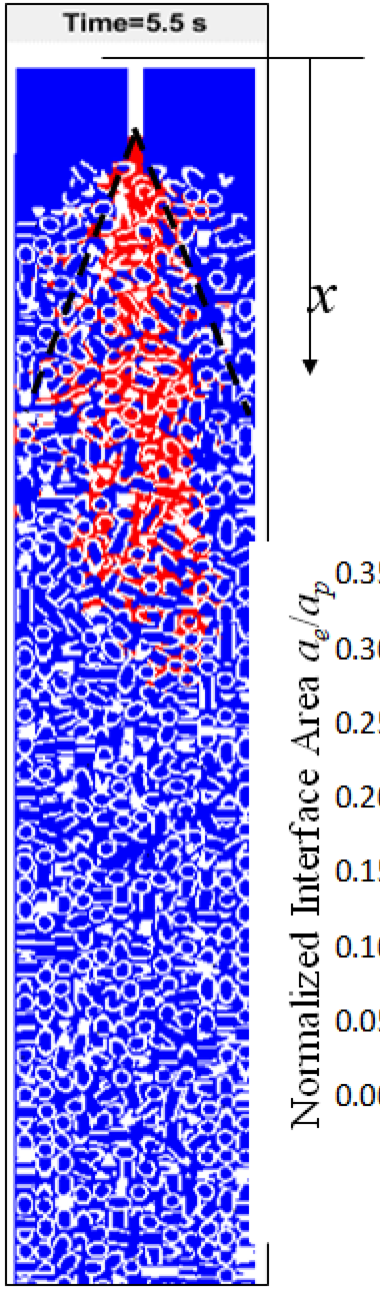
- Significant entrance effect for single point injection, distributor required.
- 20% to 30% of column height before reach fully distribution
- Stronger entrance effect for more viscous solvent



# 1:1 Full-size CFD Model



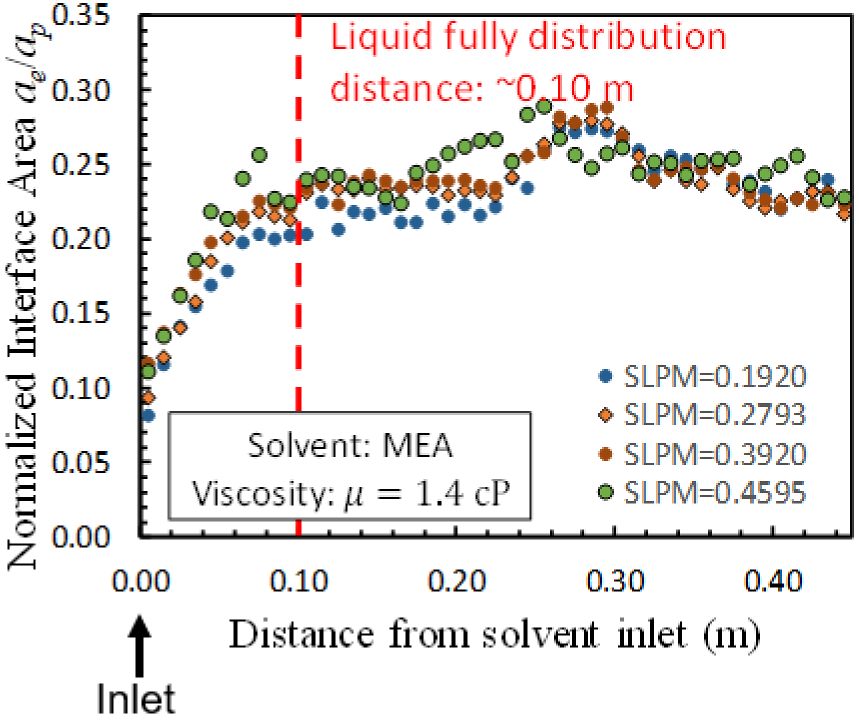



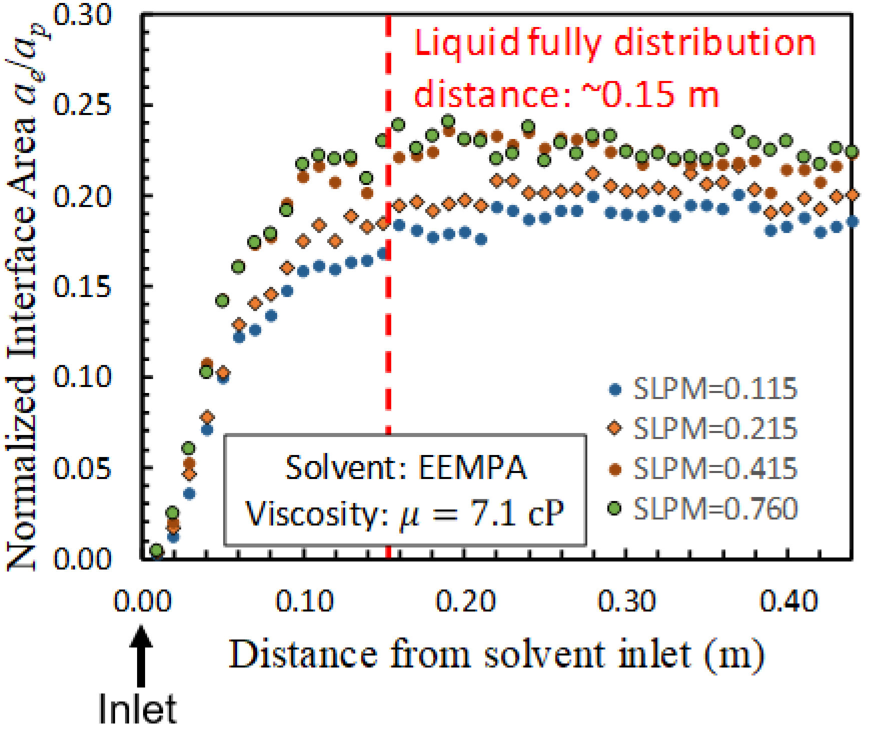

## Simulation Conditions:

- Total 9434 Rings
- Total ring surface area: 1.99 m2
- Liquid flow rate: 0.1-0.8 SLPM
- Gas flow rate: 25 SLPM
- Solvent viscosity: [1.4, 7.1] cP

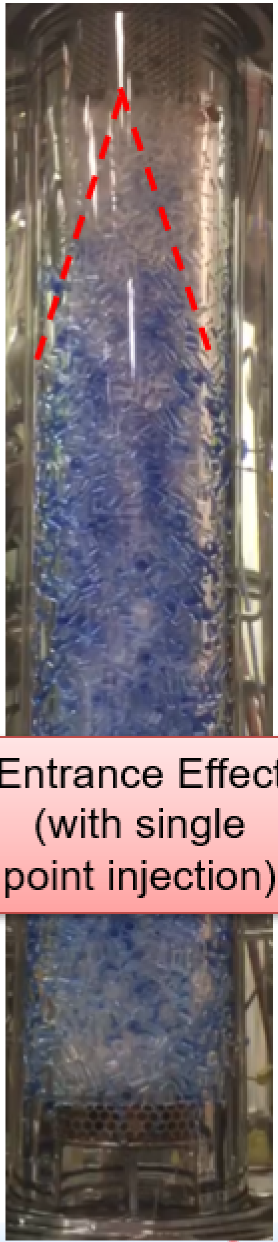
## Findings:

- Significant entrance effect for single point injection, distributor required.
- 20% to 30% of column height before reach fully distribution
- Stronger entrance effect for more viscous solvent

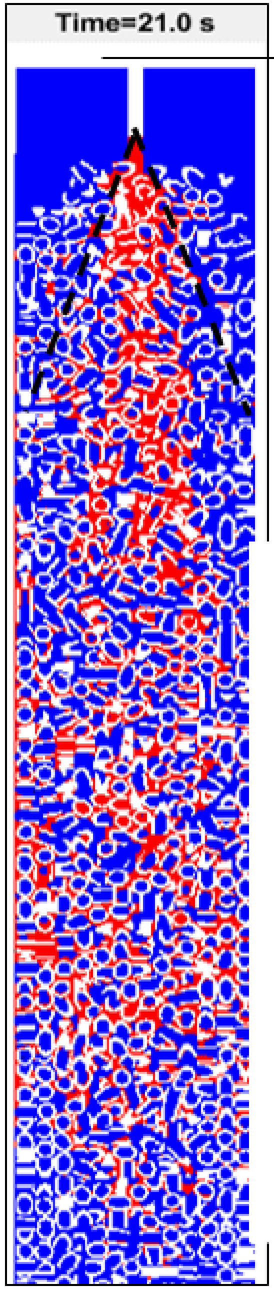


# 1:1 Full-size CFD Model



Entrance Effect (with single point injection)

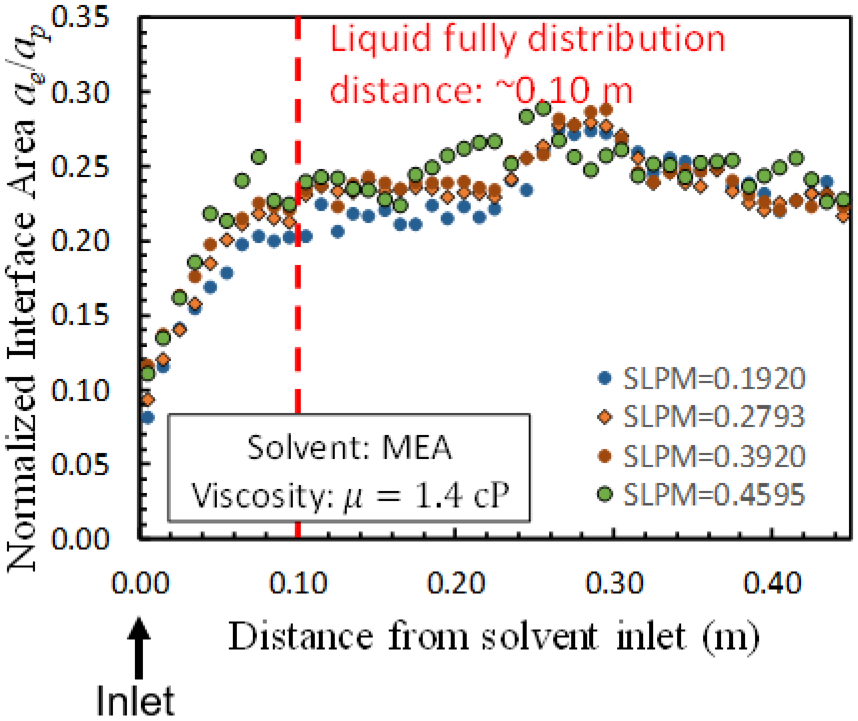


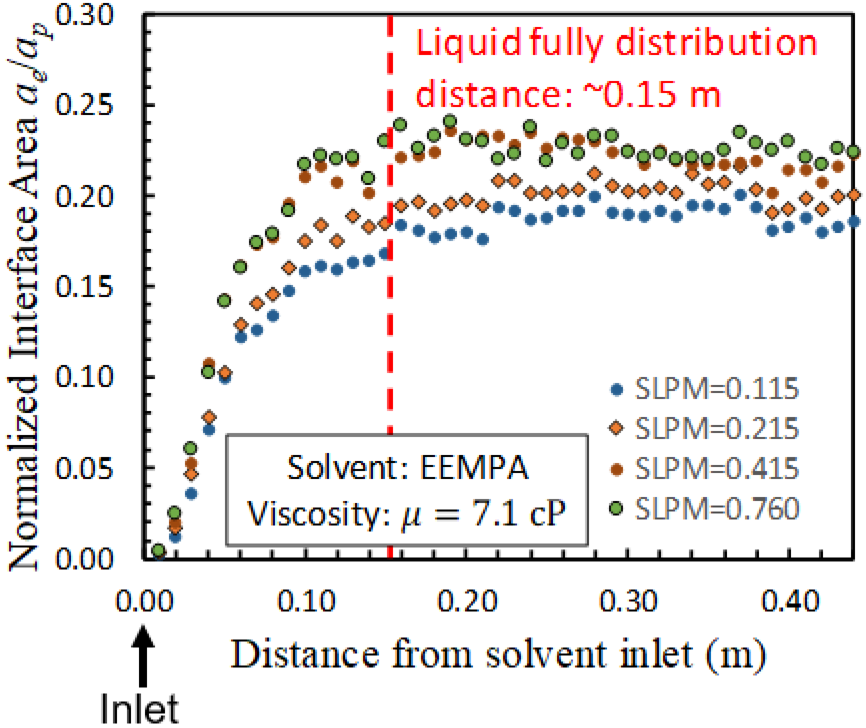

## Simulation Conditions:

- Total 9434 Rings
- Total ring surface area: 1.99 m2
- Liquid flow rate: 0.1-0.8 SLPM
- Gas flow rate: 25 SLPM
- Solvent viscosity: [1.4, 7.1] cP

## Findings:

- Significant entrance effect for single point injection, distributor required.
- 20% to 30% of column height before reach fully distribution
- Stronger entrance effect for more viscous solvent



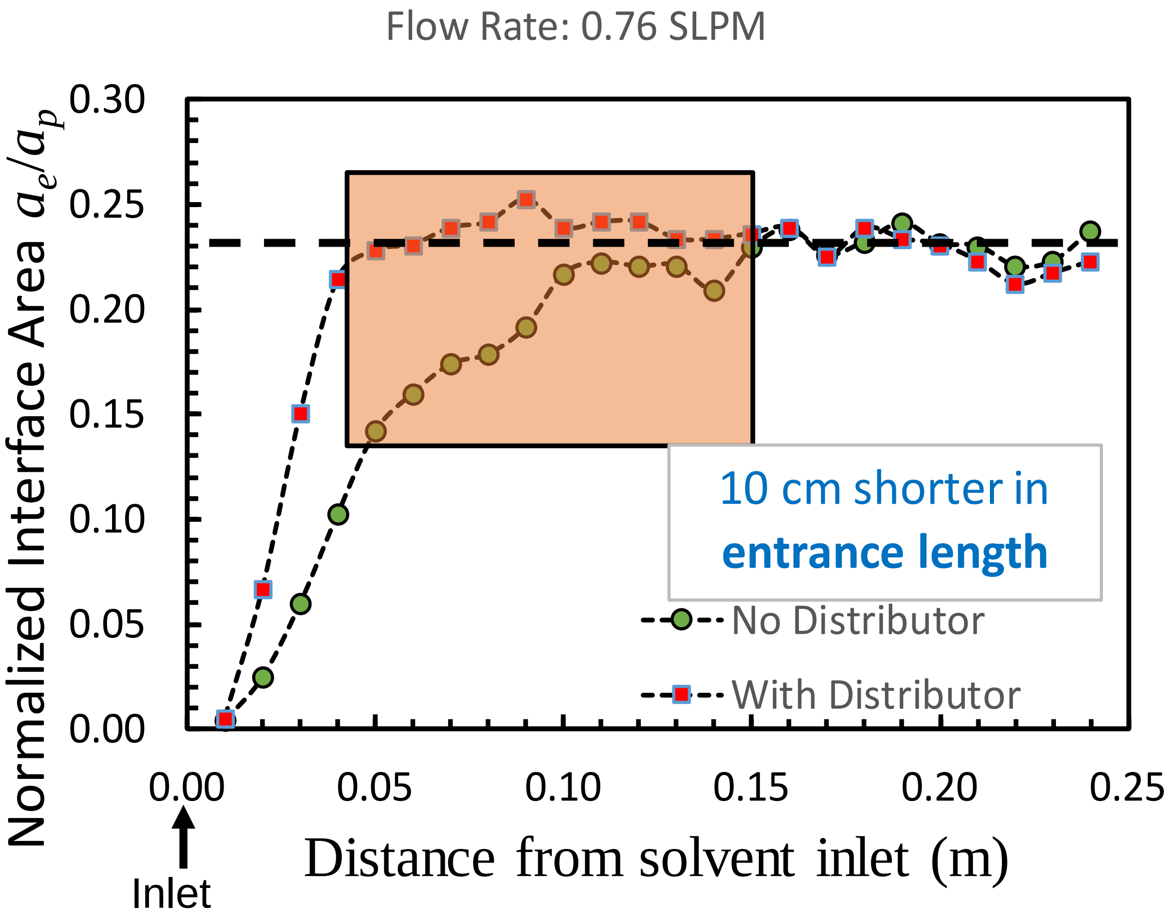




CCSI2 Carbon Capture Simulation for Industry Impact

NATIONAL ENERGY TECHNOLOGY LABORATORY | Berkeley Lab | Lawrence Livermore National Laboratory | Los Alamos National Laboratory | Pacific Northwest National Laboratory | West Virginia University | The University of Texas at Austin | U.S. Department of Energy

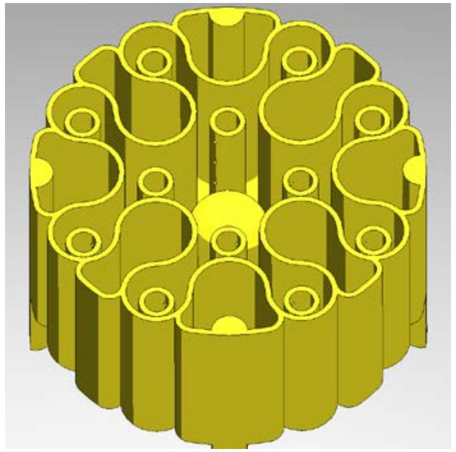
# 1:1 Full-size CFD Model

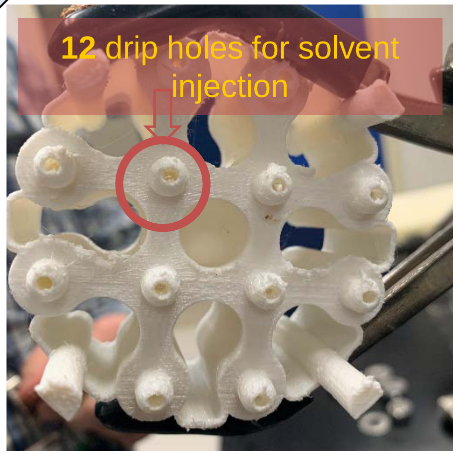
## CFD Comparison w and w/o Distributor




**Distributor will be used for all experiments**

## Distributor design in experiment






3D Printed Distributor

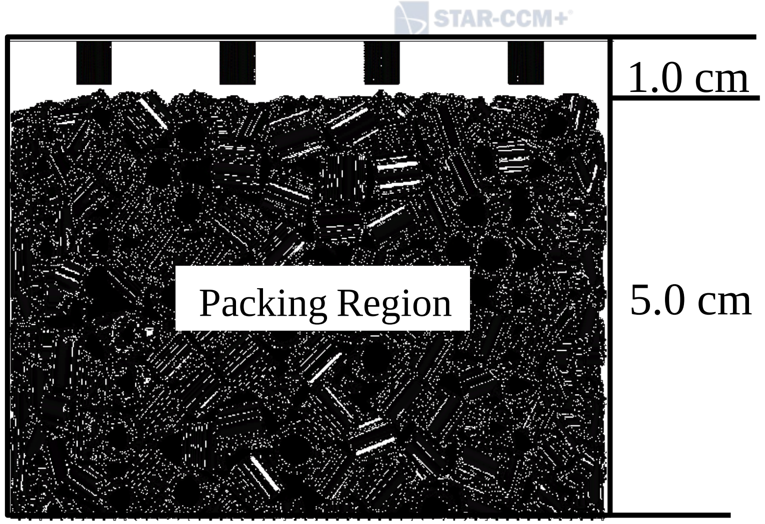
# Outline

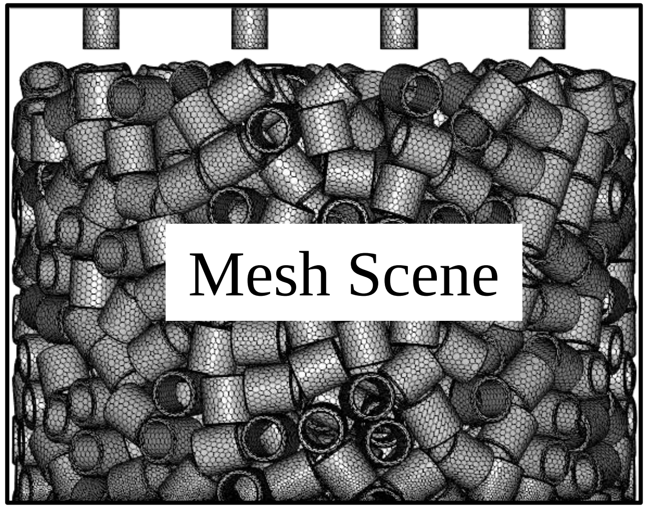
- Bench-scaled Packed Column Overview
- Experiments (EEMPA & MEA)
- CFD Simulations
  - 1:1 full size column CFD modeling
  - Representative column modeling
- Experiment/CFD Comparison
- Conclusion

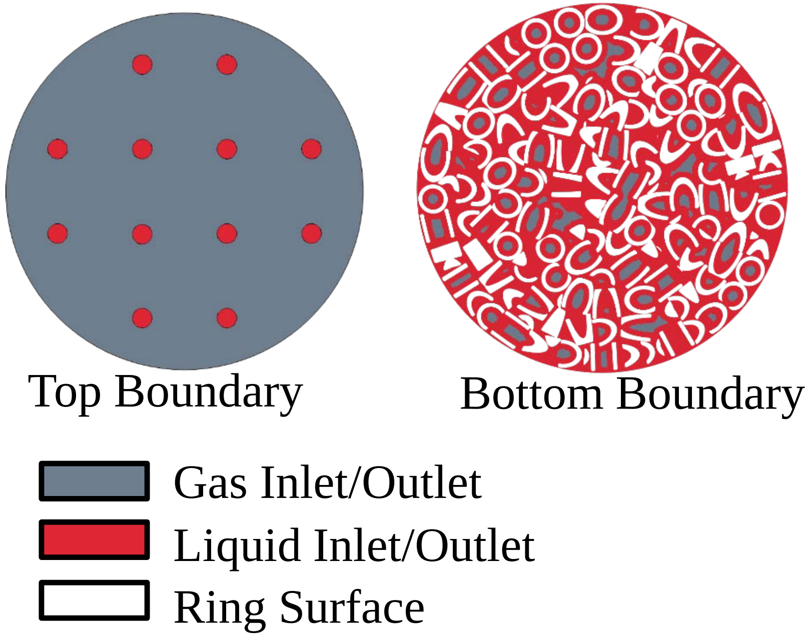
# Representative Column Model

## Representative Column Setup

- Column Size: H = 6 cm, OD= 7.62 cm
- Packing Height Z =[0 5] cm
- Raschig Ring Size 6 mm
- Specific Area $a_p$ = *857* $\mathrm{m}^2/\mathrm{m}^3$




- 2.9 million mesh with mesh size
- Run to 8s (3 hours Simulation) for converged solution
- Good size for sensitivity study

# Representative Column Model

## Sensitivity Study For Solvent Parameters

- Fixed Parameter:

$\rho_L = 1077\ \mathrm{kg/m^3}, u_L = 1.46 \times 10^{-3} \mathrm{m/s}$

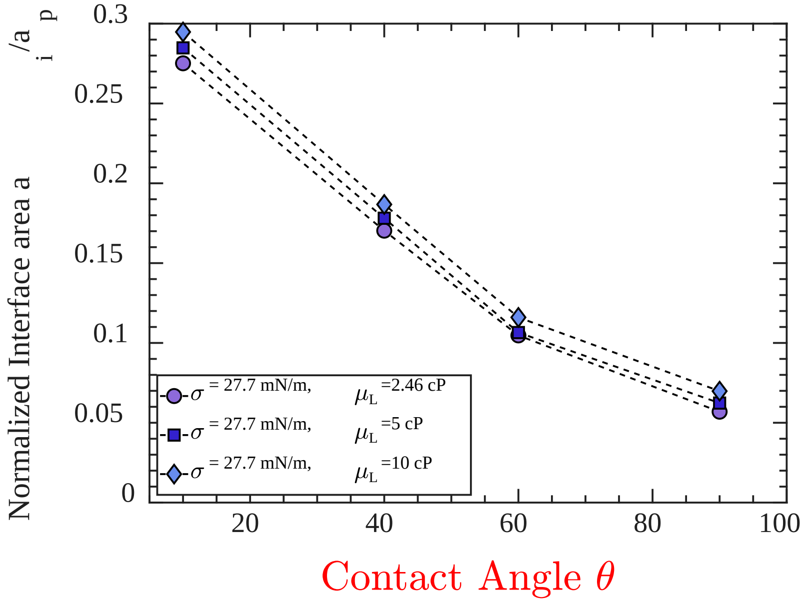
- Varying one parameter at a time (~30 runs);

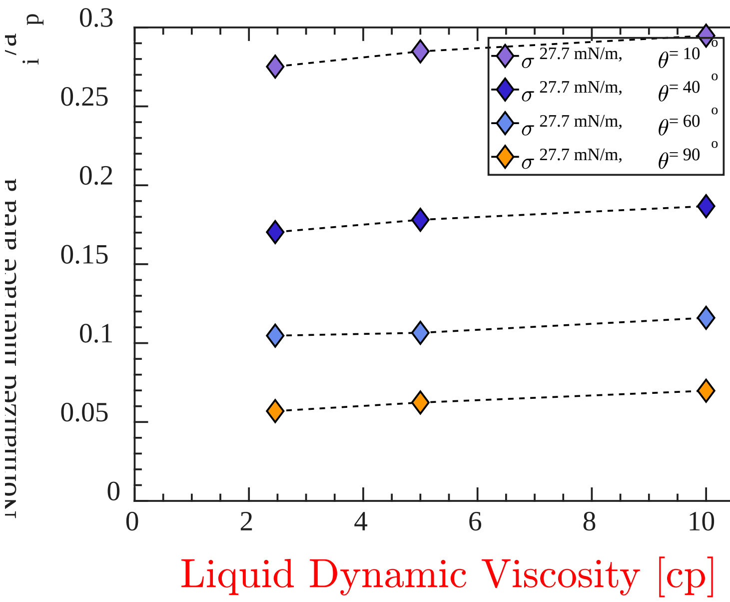
## Range covers MEA and EEMPA:

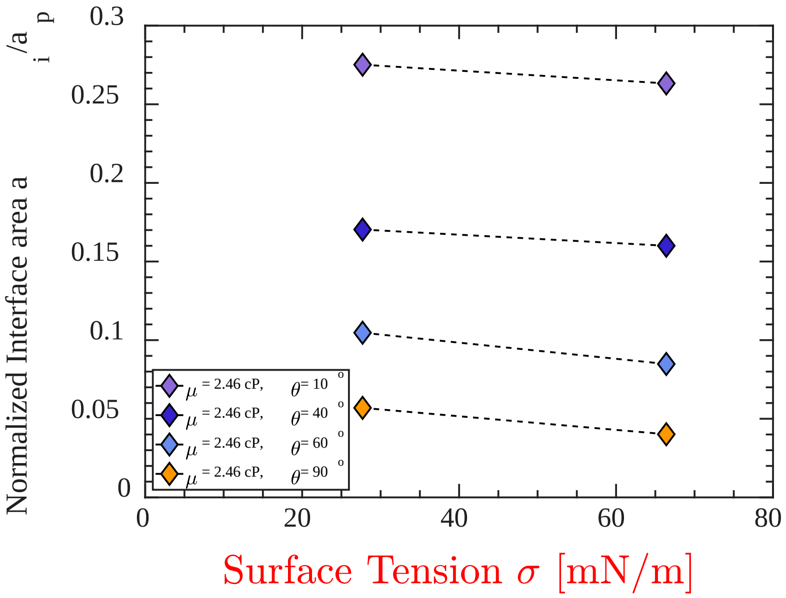
Contact angle $\theta$ [10º 90º]

Surface tension $\sigma$ [25 70] N/m

Solvent viscosity $\mu_L$ [2 10] cP



# Representative Column Model

## Sensitivity Study For Solvent Parameters

- Fixed Parameter:

$\rho_L = 1077\ \mathrm{kg/m^3}, u_L = 1.46 \times 10^{-3}\mathrm{m/s}$

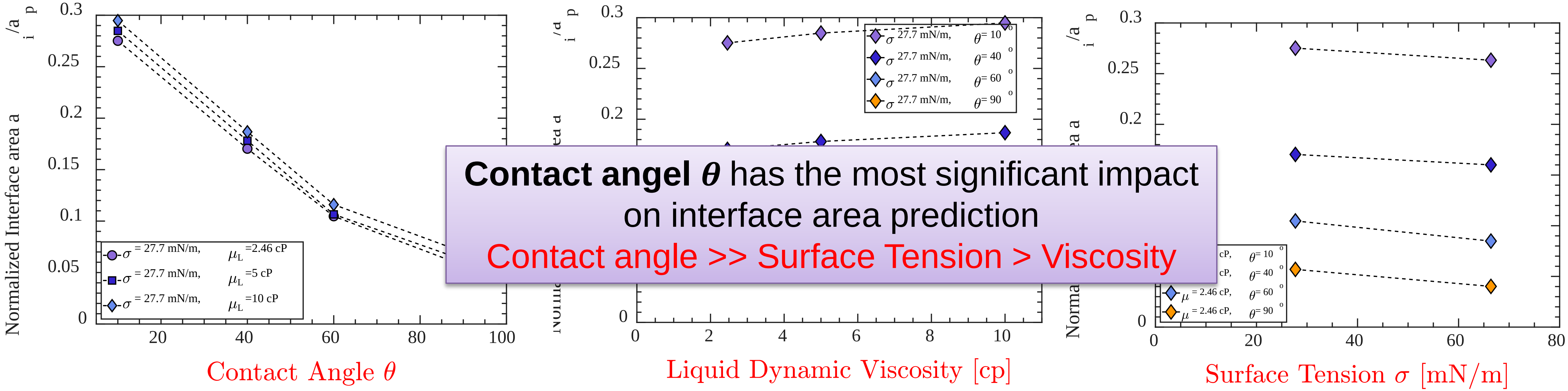
- Varying one parameter at a time (~30 runs);

## Range covers MEA and EEMPA:

Contact angle $\theta$ [10º 90º]

Surface tension $\sigma$ [25 70] N/m

Solvent viscosity $\mu_L$ [2 10] cP




**Contact angel $\theta$** has the most significant impact on interface area prediction

Contact angle >> Surface Tension > Viscosity

# Representative Column Model

## SDoE for CFD

- Initial 50 runs to explore 5-dim parameter $(u_L, u_G, \mu_L, \sigma, \theta)$ space
- Selected to cover bench experiment conditions

| CFD Parameters | Range |
|---|---|
| Viscosity $\mu_L$ [cP] | [5 15] |
| Surface Tension $\sigma$ [N/m] | [0.01 0.04] |
| Contact Angle $\theta$ [°] | [5 80] |
| Solvent Flow Rate $u_L$ [L/min] | [0.1 0.9] |
| Gas Flow Rate $u_G$ [SLPM] | [10 100] |

## Statistical Analysis of 50 CFD Runs

| Effect Summary | Sensitivity Score | Sensitivity Rank |
|---|---|---|
| Contact Angle | 27.341 | 1 |
| **Solvent Flow Rate** | 13.375 | 2 |
| **Surface Tension** | 9.434 | 3 |
| Solvent Flow Rate* Solvent Flow Rate | 6.484 | |
| Others | … | |

CCSI[2] Carbon Capture Simulation for Industry Impact
NATIONAL ENERGY TECHNOLOGY LABORATORY
BERKELEY LAB
Lawrence Livermore National Laboratory
Los Alamos NATIONAL LABORATORY EST.1943
Pacific Northwest NATIONAL LABORATORY
West Virginia University
THE UNIVERSITY OF TEXAS AT AUSTIN
U.S. DEPARTMENT OF ENERGY

# Outline

- Bench-scaled Packed Column Overview
- Experiments (EEMPA & MEA)
- CFD Simulations
  - 1:1 full size column CFD modeling
  - Small size column CFD modeling
- Experiment/CFD Comparison
- Conclusion

# Experiment / CFD Comparison

<u>Physical Properties of Solvent</u>

- Solvent type: MEA, EEMPA
- Three key parameters:
  - ❑ Viscosity $\mu_L$
  - ❑ Surface tension $\sigma$
  - ❑ Contact angle $\theta$ (much larger uncertainty)
- Three data sources:
  - ❑ Measured at PNNL
  - ❑ Aspen predicted
  - ❑ Existing correlation
- Identify the range of these parameters in packed column
- Quantify the uncertainty in CFD interface area prediction

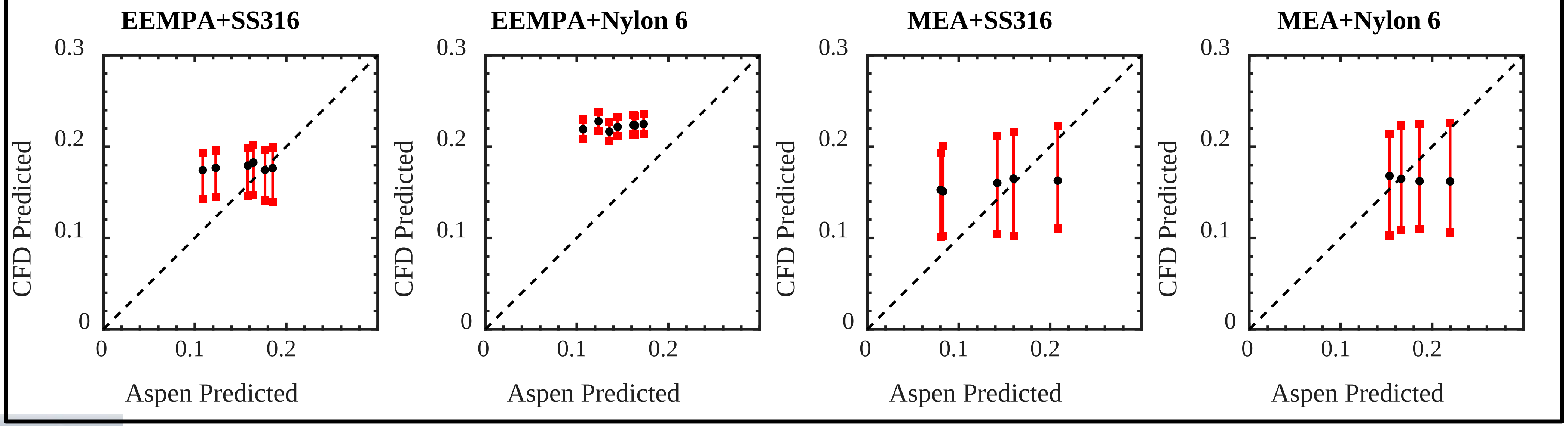
# Experiment/CFD Results Comparison

Contact angle in column:
(difficult to precisely determine)

- Roughness
- Geometry
- Loading
- Temperature, etc.

| Experiment Pair | Contact Angle [º] (Best Guess) | Surface Tension [N/m] (From Aspen & Paper) | Liquid Viscosity [cP] (From Aspen & Paper) |
|---|---|---|---|
| EEMPA+SS316 | [30, 46] | [0.026, 0.038] | [6.2, 7.6] |
| EEMPA+Nylon6 | [15, 23] | [0.026, 0.038] | [6.2, 7.6] |
| MEA+SS316 | [19.8, 52.6] | [0.054, 0.07] | [1.38, 2.54] |
| MEA+Nylon6 | [19.8, 52.6] | [0.054, 0.07] | [1.38, 2.54] |

**Normalized Interface Area $a_i/a_p$ Comparison**

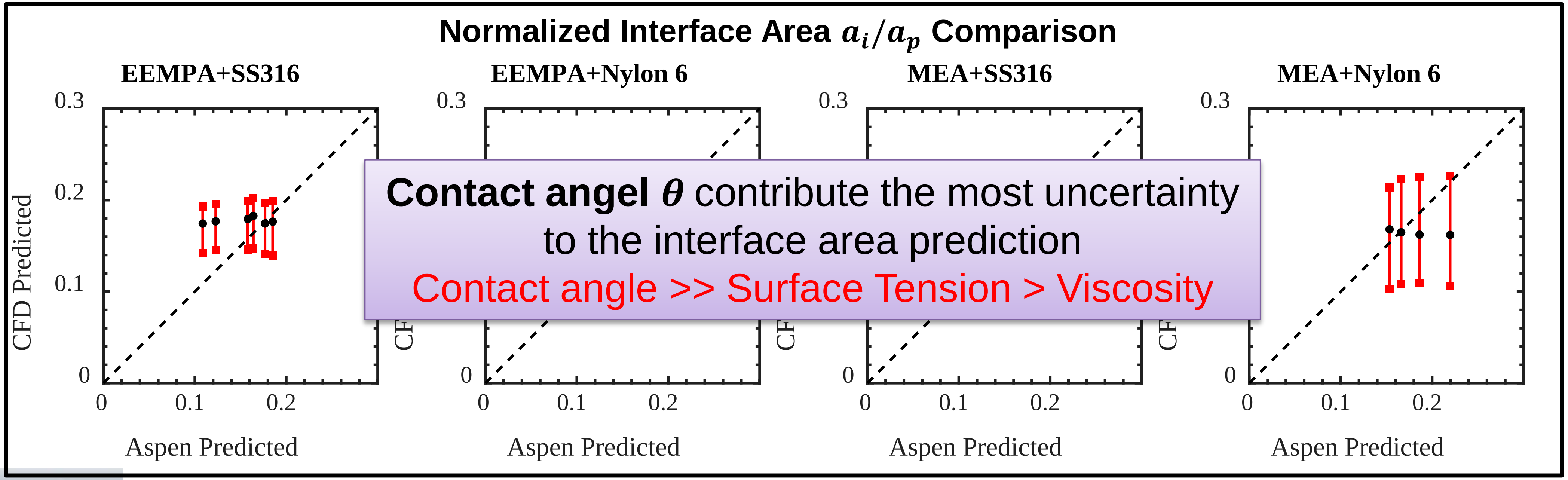


# Experiment/CFD Results Comparison

Contact angle in column:
(difficult to precisely determine)

- Roughness
- Geometry
- Loading
- Temperature, etc.

| Experiment Pair | Contact Angle [º] (Best Guess) | Surface Tension [N/m] (From Aspen & Paper) | Liquid Viscosity [cP] (From Aspen & Paper) |
|---|---|---|---|
| EEMPA+SS316 | [30, 46] | [0.026, 0.038] | [6.2, 7.6] |
| EEMPA+Nylon6 | [15, 23] | [0.026, 0.038] | [6.2, 7.6] |
| MEA+SS316 | [19.8, 52.6] | [0.054, 0.07] | [1.38, 2.54] |
| MEA+Nylon6 | [19.8, 52.6] | [0.054, 0.07] | [1.38, 2.54] |

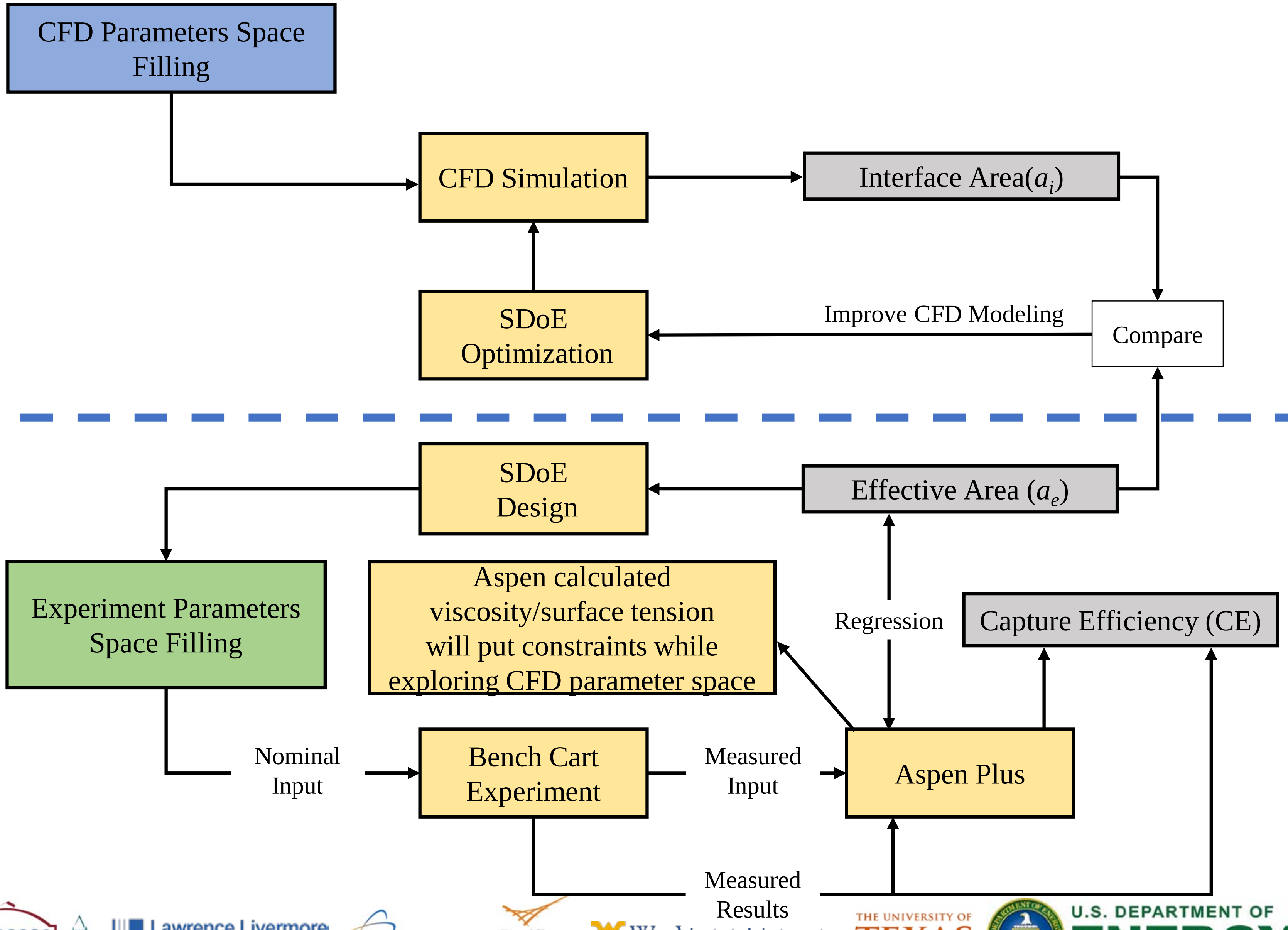



**Contact angel $\theta$** contribute the most uncertainty to the interface area prediction

Contact angle >> Surface Tension > Viscosity

# Next Step: Plan for SDoE

| CFD Parameters | Range |
|---|---|
| Viscosity $\mu_L$ [cP] | [5 15] |
| Surface Tension $\sigma$ [N/m] | [0.01 0.04] |
| Contact Angle $\theta$ [°] | [5 80] |
| Solvent Flow Rate [L/min] | Same as Exp |
| Gas Flow Rate [SLPM] | Same as Exp |




| Experiment Parameters | Range |
|---|---|
| Solvent Flow Rate [L/min] | [0.1 0.9] |
| Gas Flow Rate [SLPM] | [10 100] |
| Loading/Reboiler Temperature | <135°C |
| Absorber Temperature [°C] | [30 60] |

# Conclusion

Validation Against Bench-cart Column Experiment

- Solvents: MEA, EEMPA
- Packing: SS316, Nylon 6
- Leverage Aspen prediction of properties

CFD Approach Optimized

- Direct calculation of interface area
- Full-size column for entrance effect:
  - Viscous solvent has stronger effect
  - Liquid distributor will reduce 2/3 of the effect
- Computationally efficient representative column model

Sensitivity Study

- Contact angle $\theta$ has the largest impact to the CFD interface area prediction.
- We need better understanding of its role and influential factors.

# Acknowledgements

**PNNL**: Dushyant Barpaga, Charlie Freeman, David Heldebrant, Jie Bao, Rajesh Singh, Chao Wang, Yucheng Fu

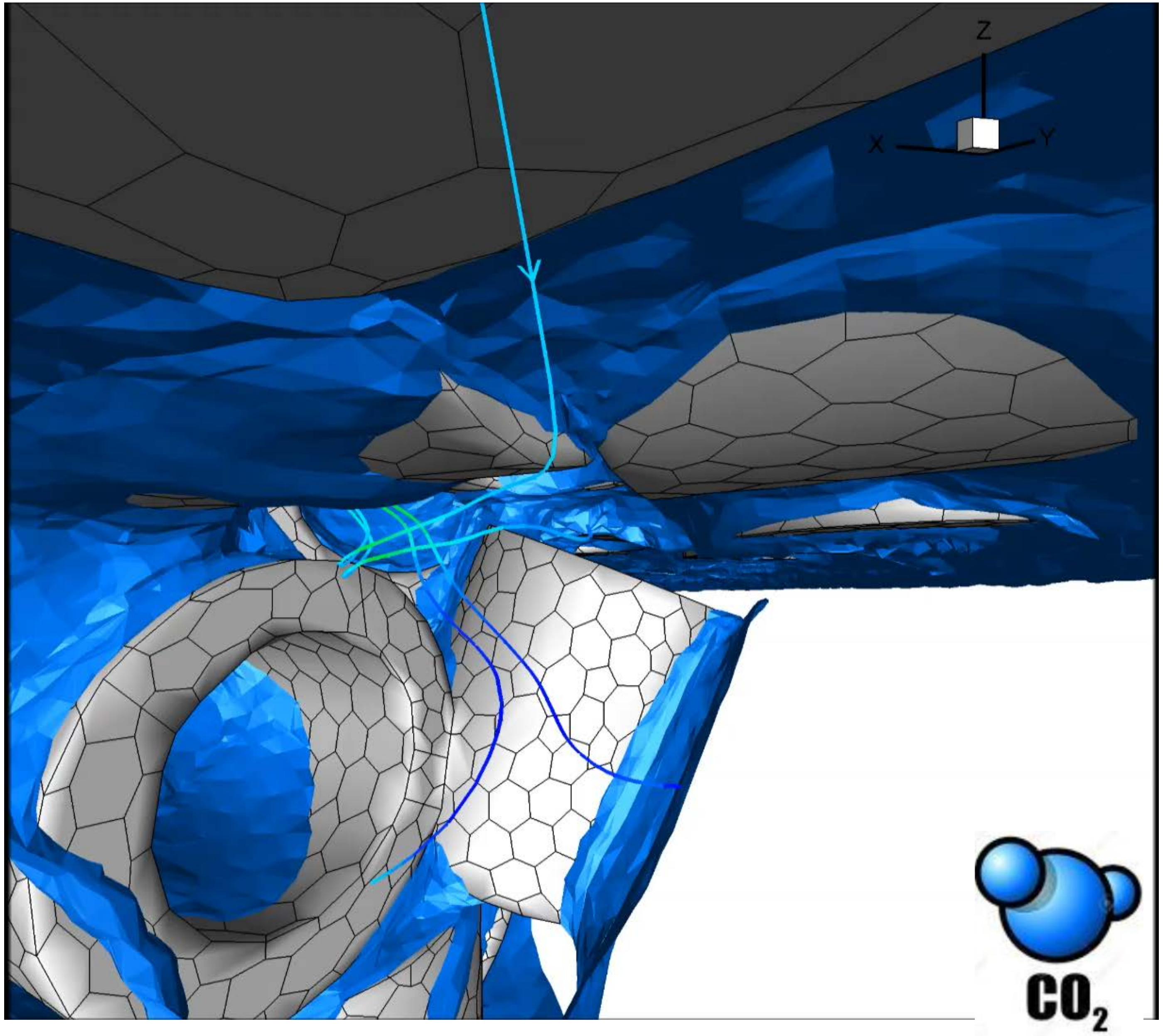
**LANL**: Christine Anderson-Cook, Sham Bhat, John Baca, Christopher Russell

**NETL**: Michael Matuszewski, Benjamin Omell, Joshua Morgan, Grigorios Panagakos

**UT Austin**: Gary Rochelle

**For more information**
**https://www.acceleratecarboncapture.org/**

Your Contact Info
Zhijie.Xu@pnnl.gov


**OUR RESEARCH FEATURED IN I&EC JOURNAL (POSTERS)**