Computational Analysis of the Effect of Structured Packing Design on Absorption Column Hydrodynamics for Post-Combustion Carbon Capture Applications

NATIONAL ENERGY TECHNOLOGY LABORATORY

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Carbon Capture Simulation for Industry Impact

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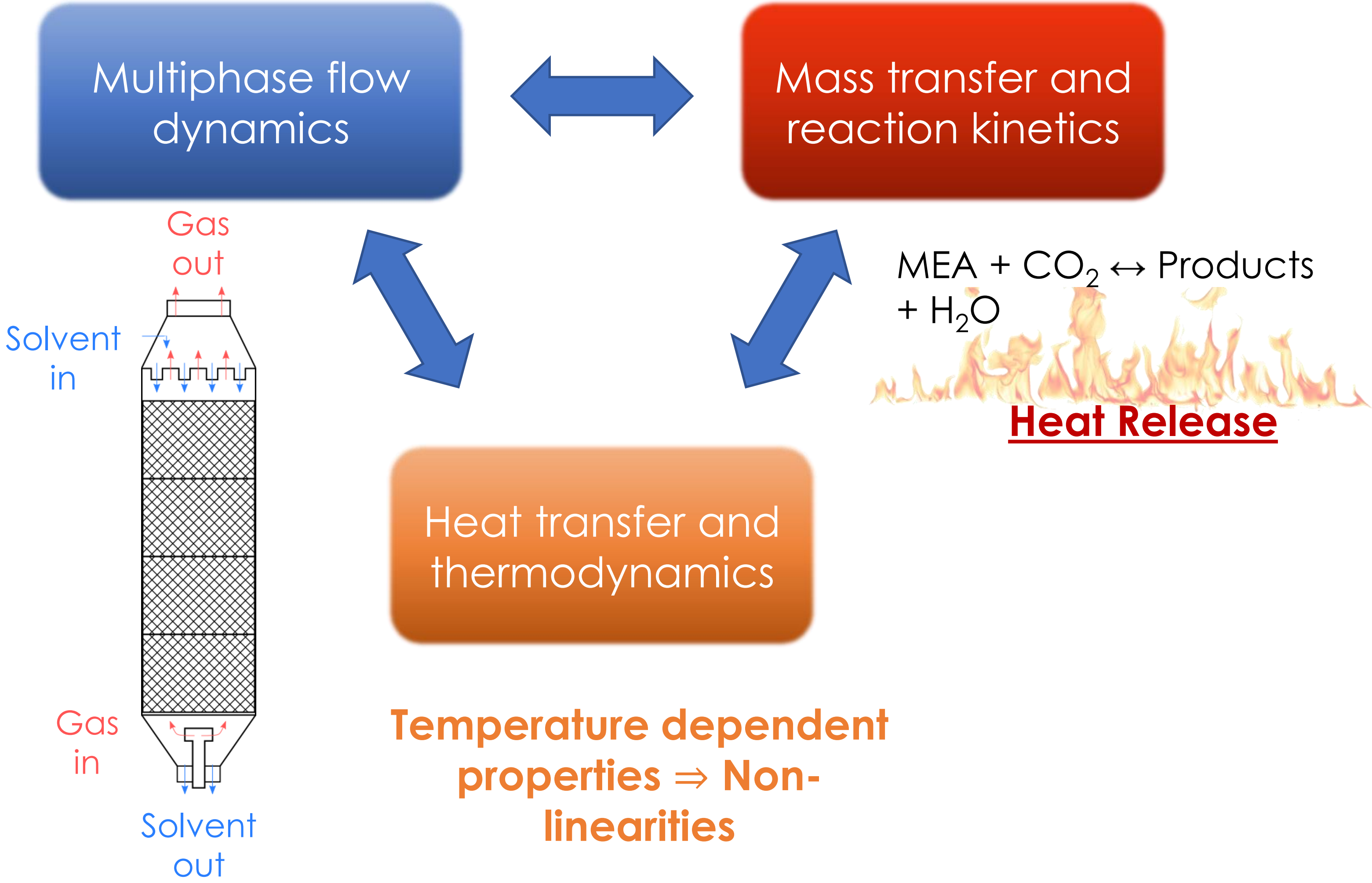
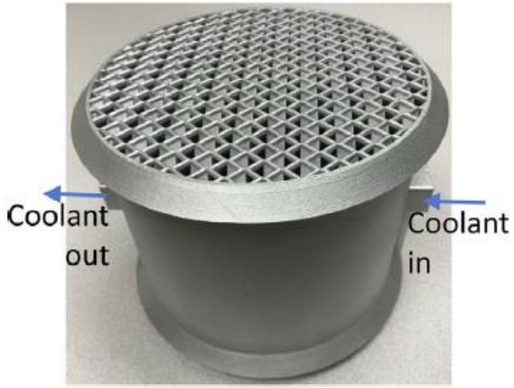
Dynamics Underlying Absorption Columns

- **Multiphase flow dynamics**
  ⇒ Solvent/gas flow interactions with geometry impact interfacial, wetted areas
- **Mass transfer and reaction kinetics** ⇒ Variations in interfacial area impact mass transfer
  ⇒ Exothermic reactions with Monoethanolamine (MEA) lead to heat release
- **Heat transfer and thermodynamics** ⇒ Temperature rise introduces variations to reaction rates and solvent physical properties (density, viscosity, surface tension, etc.)

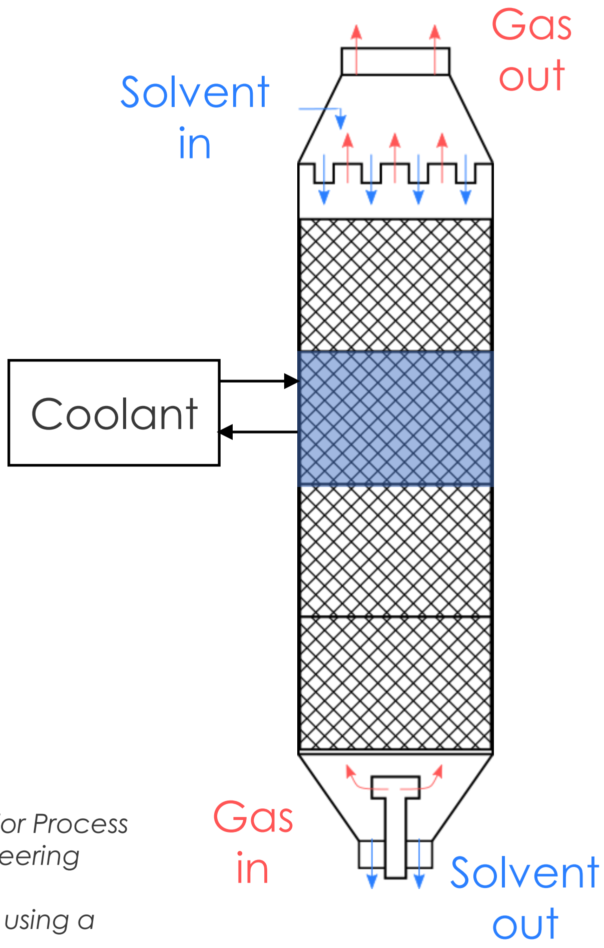


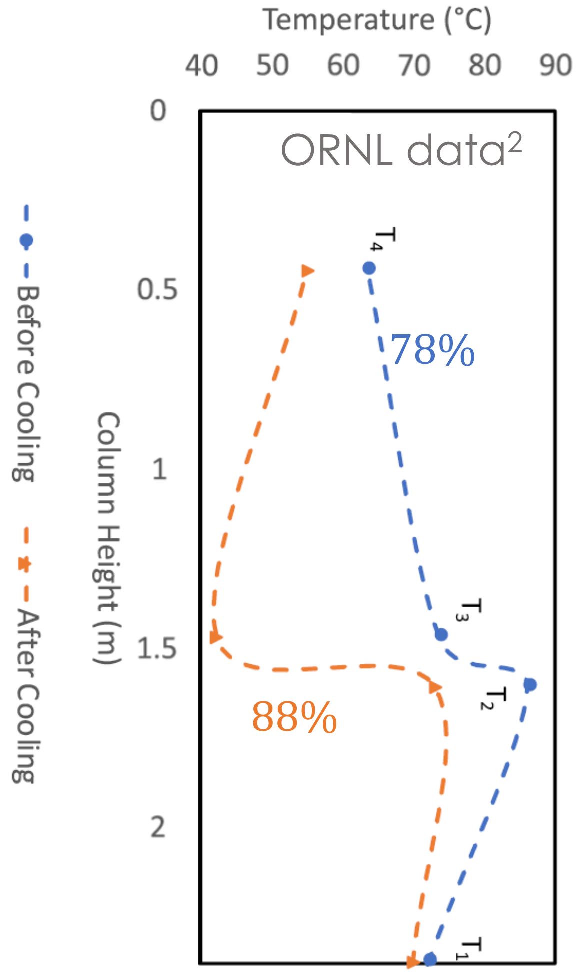
Motivation: Process Intensification of Packed Columns

- Temperature rise ⇒ Reduced reactivity and CO_2 absorption
- Process intensification can potentially mitigate these effects



Intensified packing and coolant channels.[1]



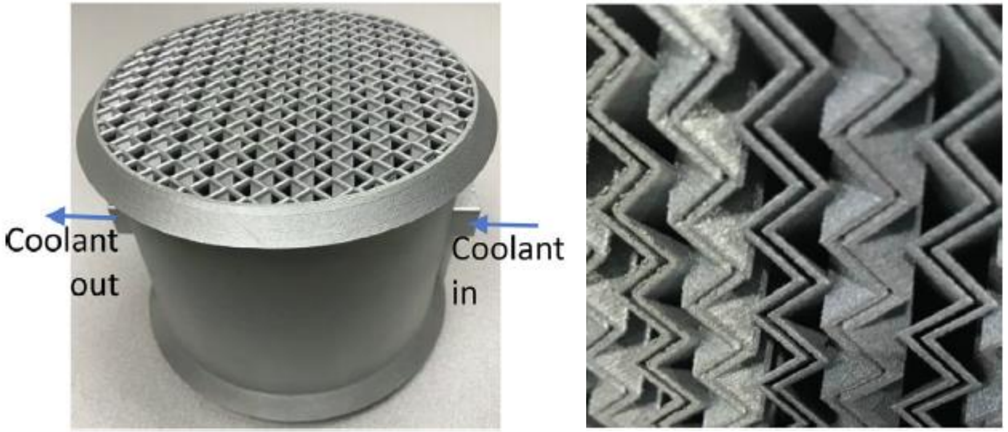


[1] Miramontes, Love, Lai, Sun, Tsouris "Additively Manufactured Packed Bed Device for Process Intensification of CO2 Absorption and Other Chemical Processes." Chemical Engineering Journal, 388, p. 124092. https://doi.org/10.1016/j.cej.2020.124092

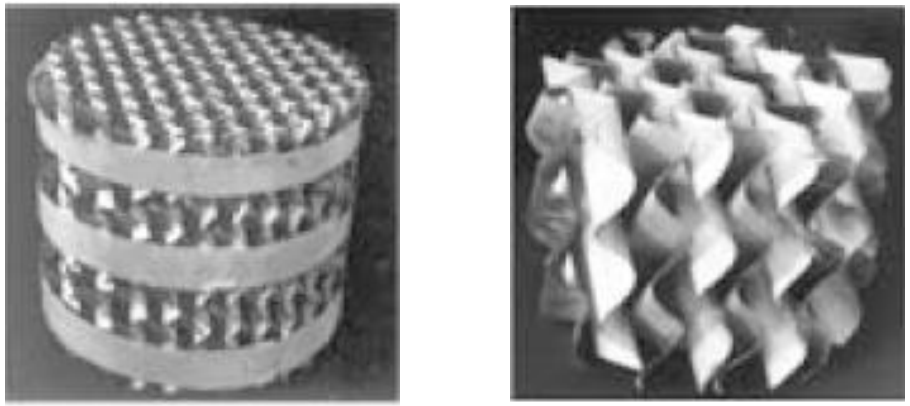
[2] Miramontes, Jiang, Love, Lai, Sun, Tsouris "Process intensification of CO_2 absorption using a 3D printed intensified packing device." AIChE J. 2020; 66:e16285. https://doi.org/10.1002/aic.16285

Motivation: Modeling for Process Optimization

- Additive manufacturing ⇒ increased flexibility with device geometries
- What is the optimal geometry of the intensified device for effective heat removal and absorption performance?
- Computational Fluid Dynamics (CFD) is a powerful tool to effectively resolve the solvent-flue gas interface and obtain detailed calculations for the following as a function of the column design.
    - Wetted area (packing-solvent interface)
    - Interfacial area (solvent-flue gas interface)
    - Liquid holdup
    - Pressure drop



Miramontes et al., Chemical Engineering Journal 388 (2020): 124092.

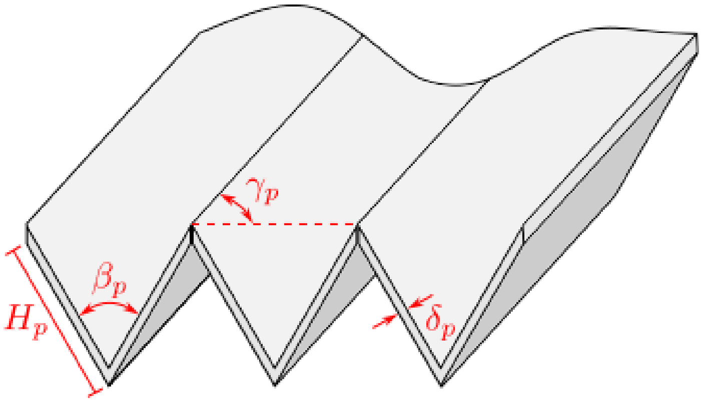


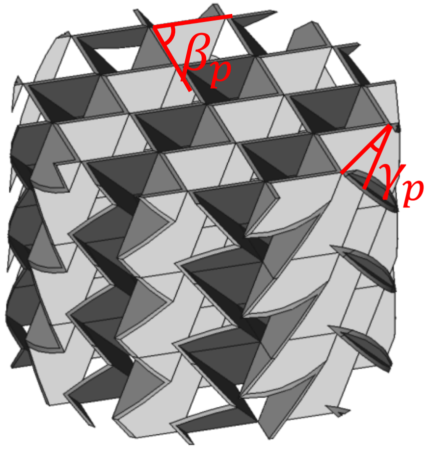
Mackowiak, Jerzy. "Fluid dynamics of packed columns." Chemische Technik. Verfahrenstechnik. Springer-Verlag Berlin Heidelberg (2010).

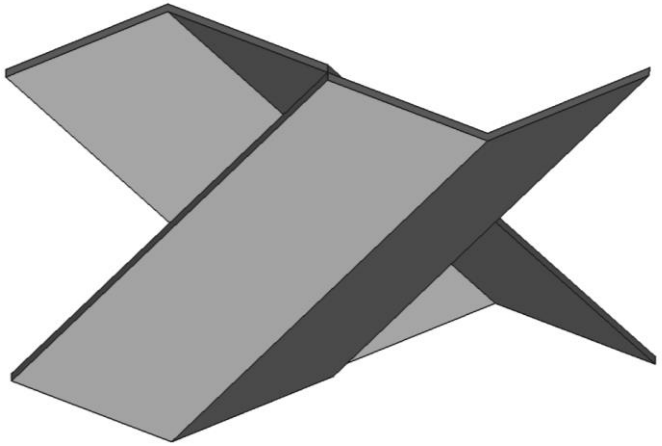
Designing Alternate Structure Packings

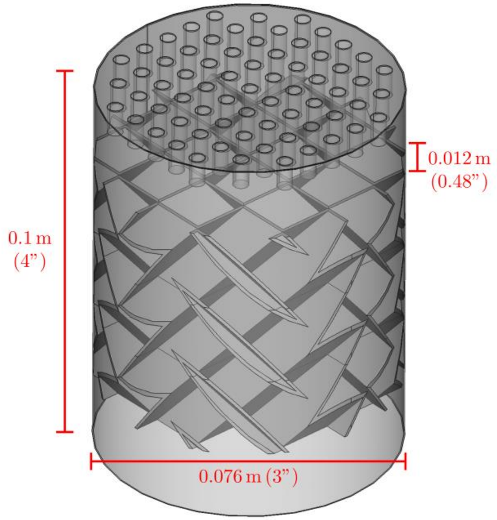
Construction of Packing Geometries

- Packing geometry is created from collocated sheets
- Each sheet is formed by patterning the repetitive elemental unit cell
- FreeCAD based Python script **automatically generates geometry** for a user-defined set of parameters
- FreeCAD supports command line execution of the script ⇒ **No GUI interface required**
- Supports saving the geometry in .STL, .STEP, and .IGES formats **suitable for CAD import in CFD software**





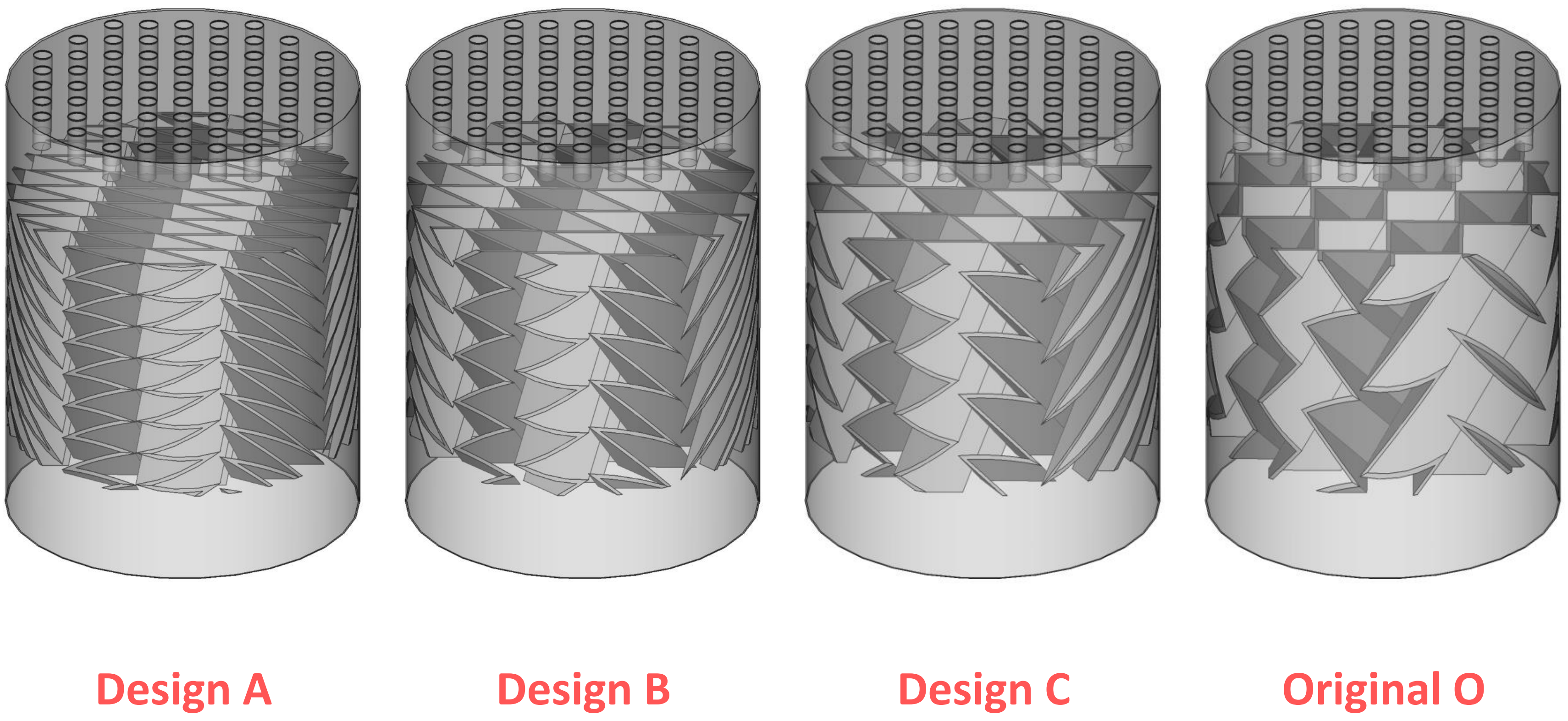




Packing Designs for Analysis

Four classes of packing designs were considered for analysis:

1. **Original Design O** derived from the angular parameters (β_p, γ_p) defining the Sulzer Mellapak 250Y
2. **Design A** obtained by modifying the crimp angle β_p to 30°
3. **Design B** obtained for $\beta_p = 60°$
4. **Design C** obtained for $\beta_p = 90°$



<u>Fixed Parameters</u>:
H = 14.75 x 10^{-3} m
t_1 = 0.891 x 10^{-3} m

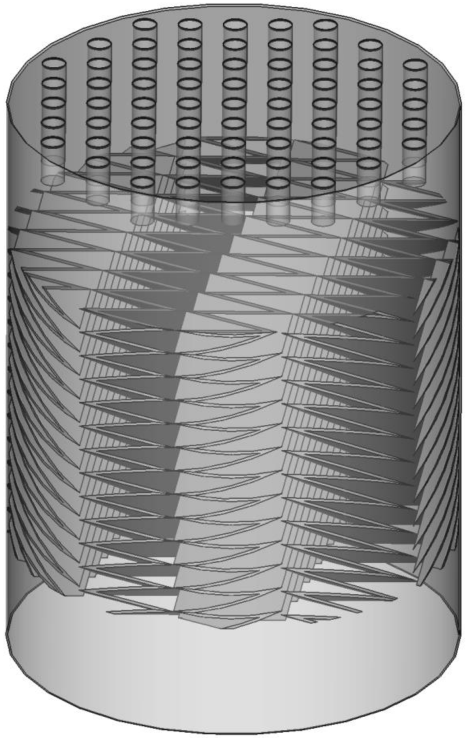
Packing Designs for Analysis

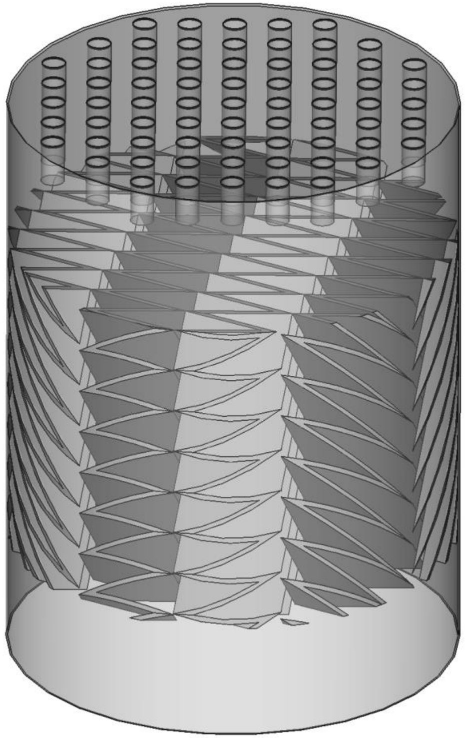
- For each design class, three different corrugation angles γ_p are considered
- Design space:

β_p, γ_p	γ_p = 30°	γ_p = 45°	γ_p = 60°
β_p = 30°	A1	A2	A3
β_p = 45°	B1	B2	B3
β_p = 60°	C1	C2	C3
β_p = 90°	O1	O2	O3

O2 → Mellapak 250.Y-like geometry

O3 → Mellapak 250.X-like geometry


A1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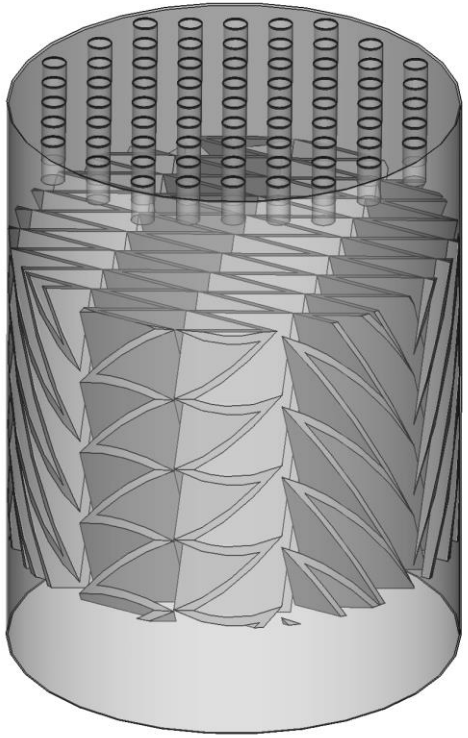
A3

Packing Designs for Analysis ($\gamma_p = 60°$)

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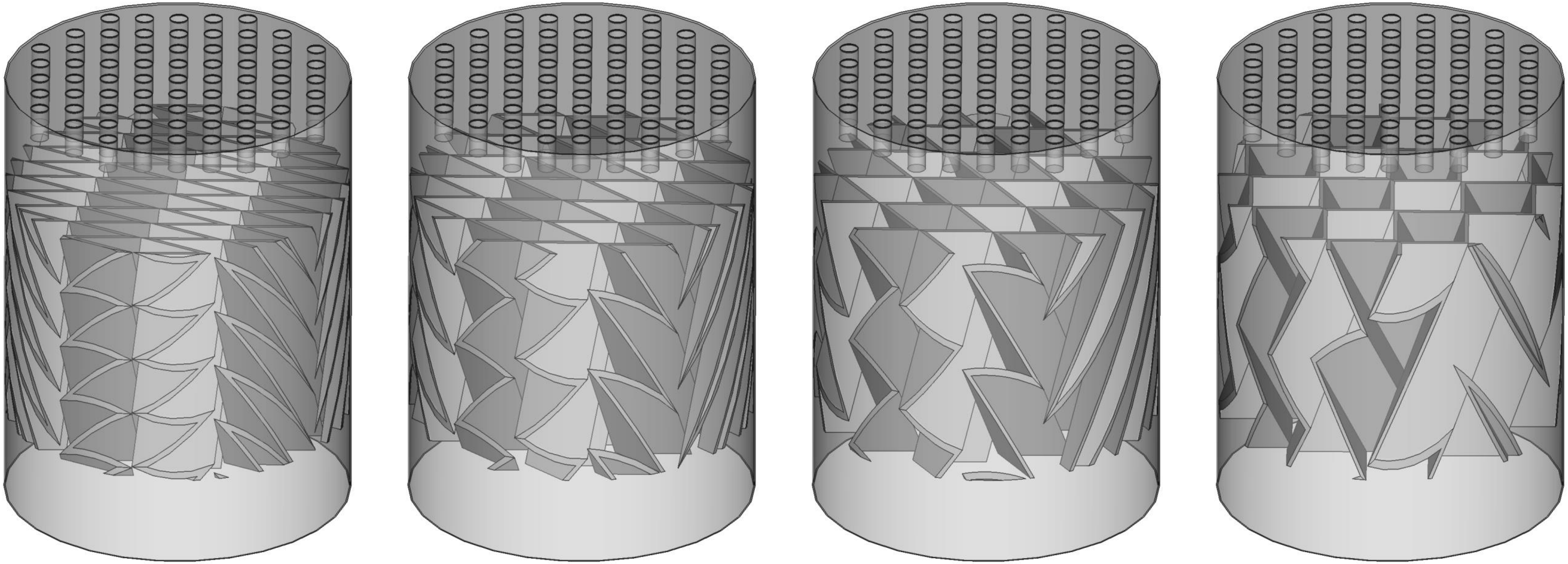
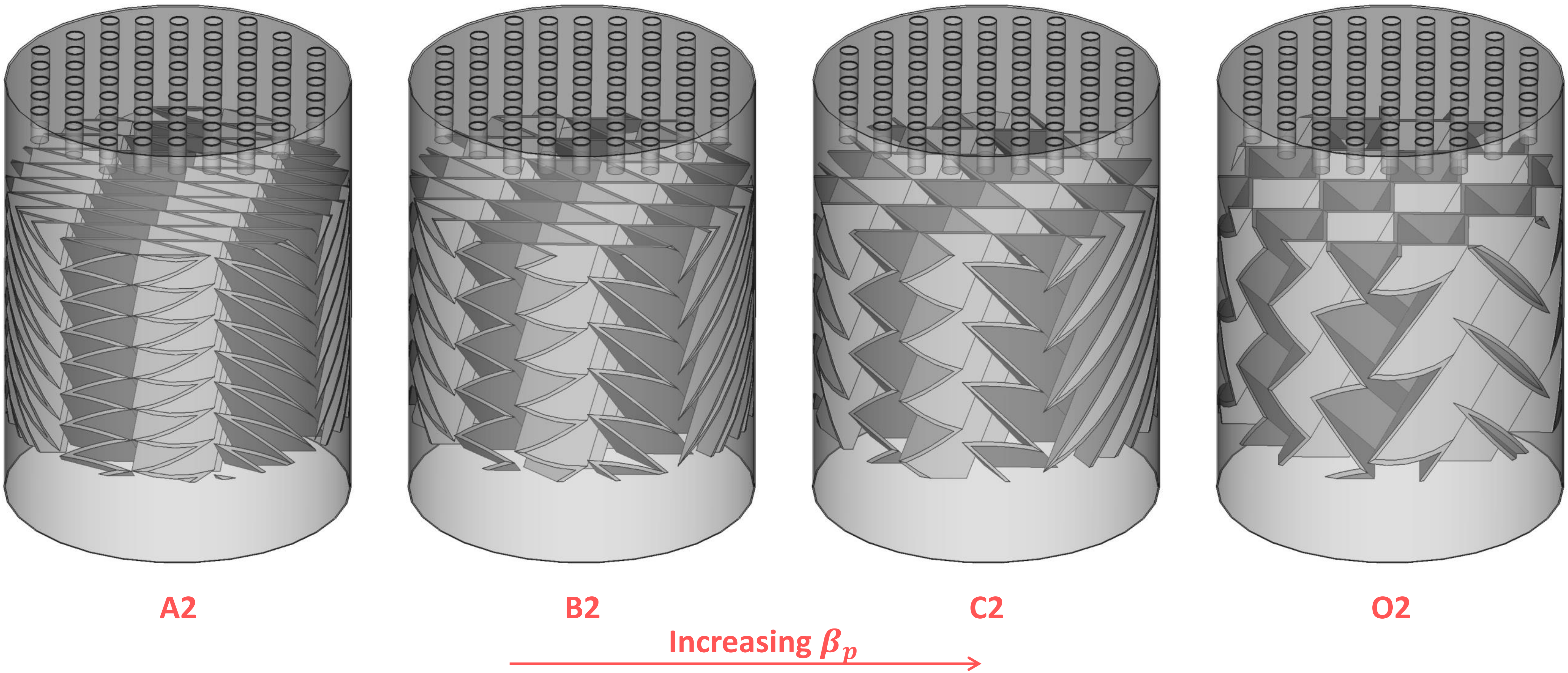


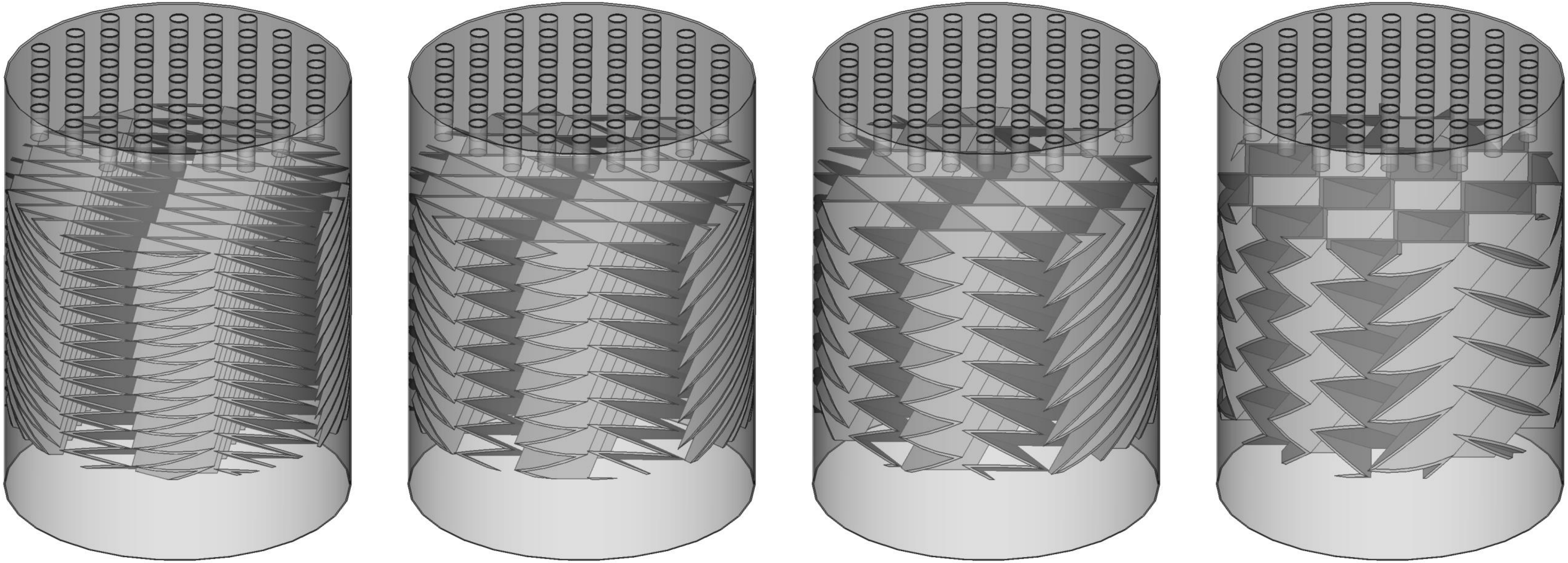
A3 B3 C3 O3

Increasing β_p →

Packing Designs for Analysis ($\gamma_p = 45°$)



Packing Designs for Analysis ($\gamma_p = 30°$)



A1 B1 C1 O1

Increasing β_p →

CFD Model and Simulation Setup

Dynamical System for Two-Phase Reacting Flows

- **Transport of liquid volume fraction (α_l):**

$$\frac{\partial(\rho_l \alpha_l)}{\partial t} + \nabla \cdot (\rho_l \alpha_l \boldsymbol{v}) = \dot{m}_l$$

$0 \le \alpha_l(\boldsymbol{x}, t) \le 1$; $\alpha_l + \alpha_g = 1$

$\dot{m}_l \Rightarrow$ Mass transfer from gas to liquid phase

- **Mass conservation:**

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0$$

$\rho = \rho_l \alpha_l + \rho_g \alpha_g$

- **Momentum conservation:**

$$\frac{\partial}{\partial t}(\rho \boldsymbol{v}) + \nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v}) = \nabla \cdot (\boldsymbol{\sigma}) + \boldsymbol{F_s} + \rho \boldsymbol{g}$$

$\boldsymbol{F}_s = \sigma_s \kappa \delta(n) \boldsymbol{n}$; $\kappa = \boldsymbol{\nabla} \cdot (\boldsymbol{n})$ and $\boldsymbol{n} = \frac{\nabla \alpha_l}{|\nabla \alpha_l|}$

$$\boldsymbol{\sigma} = -pI + 2\mu \boldsymbol{S};\ \boldsymbol{S} = \frac{1}{2}(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^{\boldsymbol{T}})$$

$\mu = \mu_l \alpha_l + \mu_g \alpha_g$

- **Species transport:**

$$\frac{\partial(\rho_i \alpha_i Y_{i,j})}{\partial t} + \nabla \cdot (\rho_i \alpha_i Y_{i,j} \boldsymbol{v}) = -\nabla \cdot \boldsymbol{J}_{i,j} + \alpha_i R_{i,j} + \sum_k \dot{m}_{k,i,j}$$

$\boldsymbol{J}_{i,j} \Rightarrow$ Species diffusion flux; $R_{i,j} \Rightarrow$ Chemical reaction rate

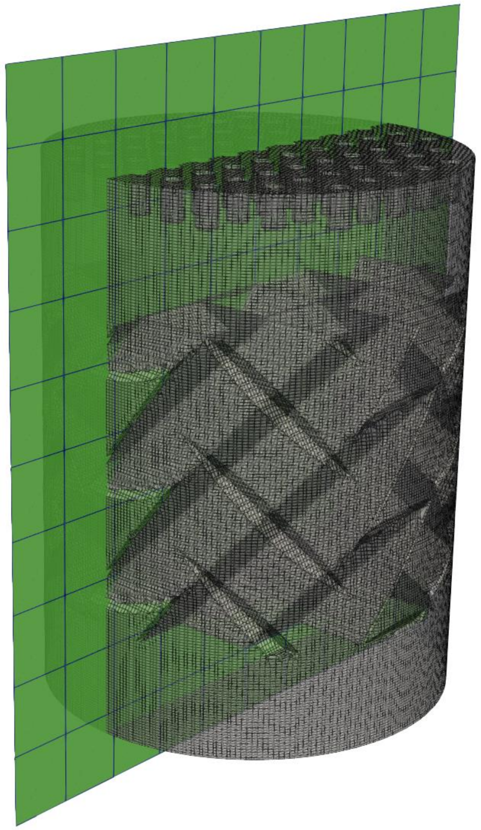
- **Energy conservation:**

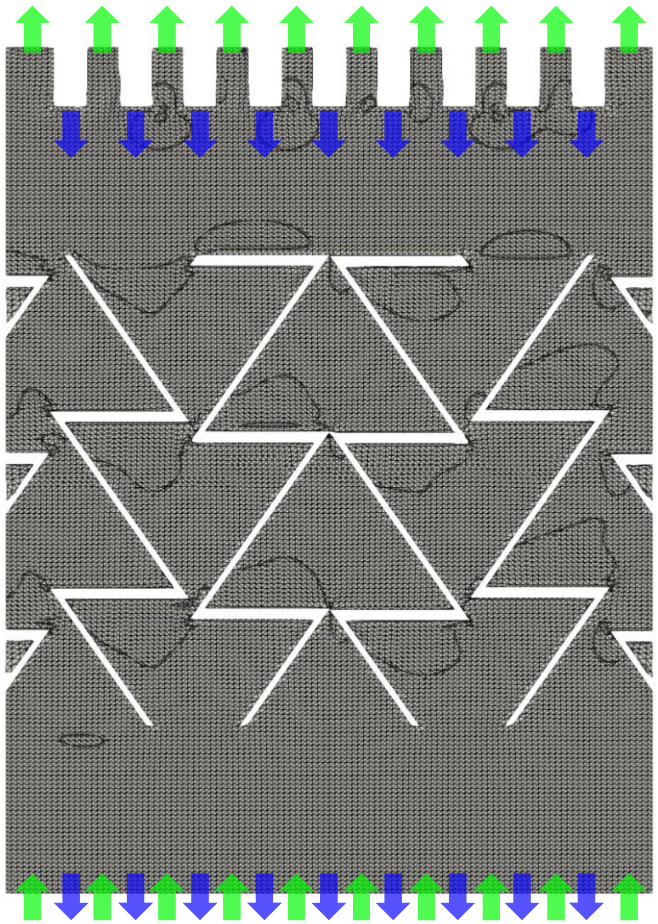
$$\frac{\partial(\rho e)}{\partial t} + \nabla \cdot ((\rho e + p)\boldsymbol{v}) = \nabla \cdot (k \nabla T + (\tau \cdot \boldsymbol{v})) - \sum_{i=1}^{N_{phases}} \sum_{j=1}^{N_{species}^i} \frac{h_j^0}{M_j} \alpha_i R_{i,j}$$

Problem Setup and Numerical Details

Numerical solver and algorithm:
- Multiphase flow solver: OpenFOAM
- Interface tracking: Explicit Volume of Fluid (VOF) method
- Second-order discretization for velocity and pressure

Simulation conditions:
- Liquid and gas phase in counter-current flow configuration
- Solvent: **30% MEA, 70% H_2O** (by mass)
- Flue gas: **10% CO_2, 1.5% H_2O, 88.5% N_2** (by mass)
- Constant static contact angle of **57.5°** between interface and packing walls
- RANS SST $k-\omega$ turbulence model





Problem Setup and Numerical Details

Simulation details:

- Constant gas mass velocity of **0.1 m/s** at the outlet
- Two different liquid inflow velocities are considered for each case: $v_{in} =$ **0.1 m/s** and $v_{in} =$ **0.3 m/s**
- Adjustable time step-size given by CFL < 1 is considered, which results in time-step sizes between **10^{-5} and 10^{-4}** seconds
- Mesh resolution: ≈**1.8 x 10^6 cells**
- Total 24 CFD simulations were performed using **128 cores** for up to **168 hours**

Packing	β_p	γ_p	$A_p/V\ [m^2/m^3]$
A1	30°	30°	1196.36
A2	30°	45°	858.4
A3	30°	60°	709.96
B1	45°	30°	800.44
B2	45°	45°	580.78
B3	45°	60°	485.13
C1	60°	30°	618.79
C2	60°	45°	456.98
C3	60°	60°	385.46
O1	90°	30°	460.7
O2	90°	45°	357.36
O3	90°	60°	315.28

Problem Setup and Numerical Details

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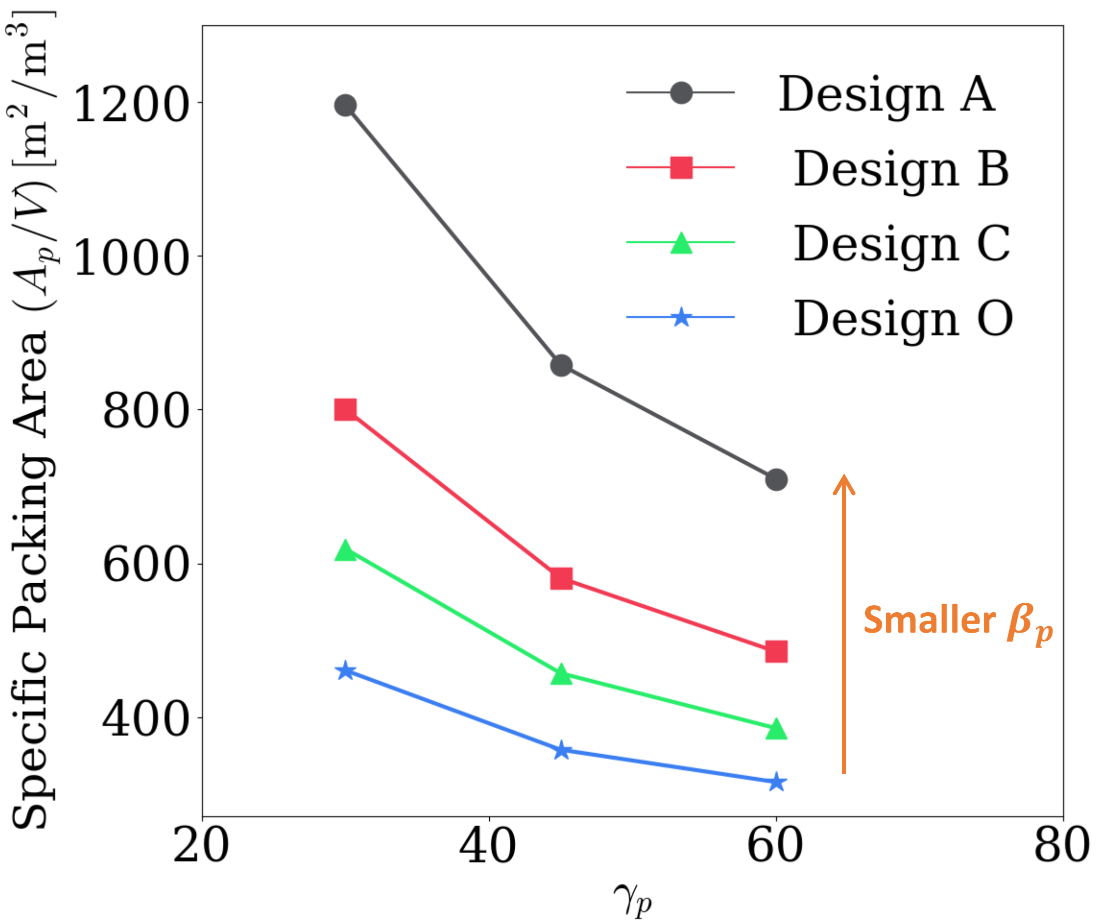
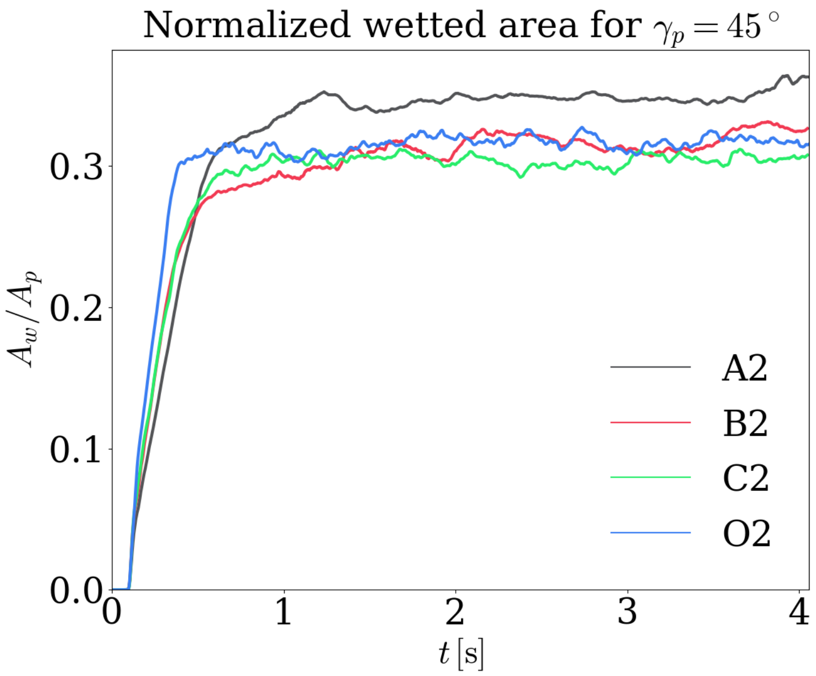
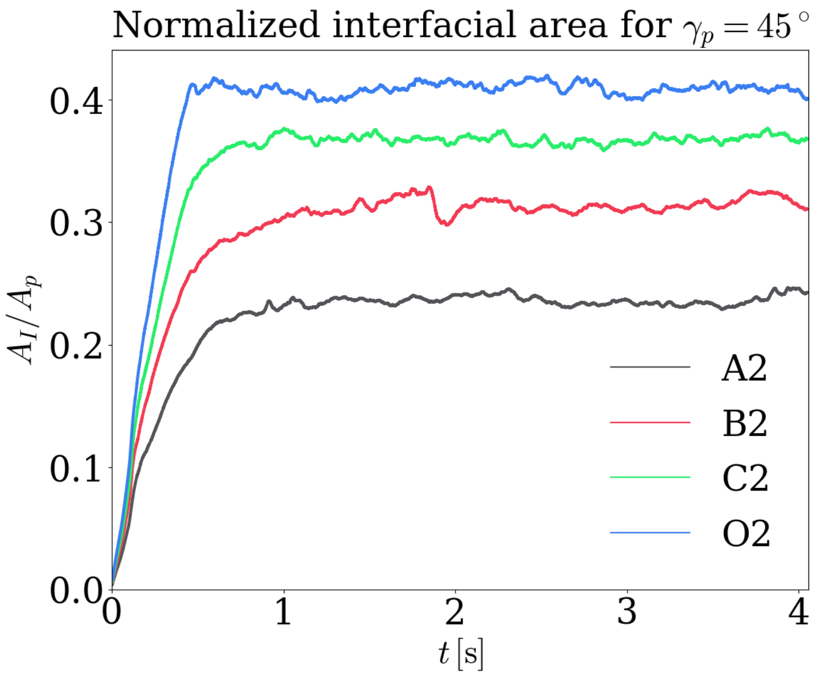
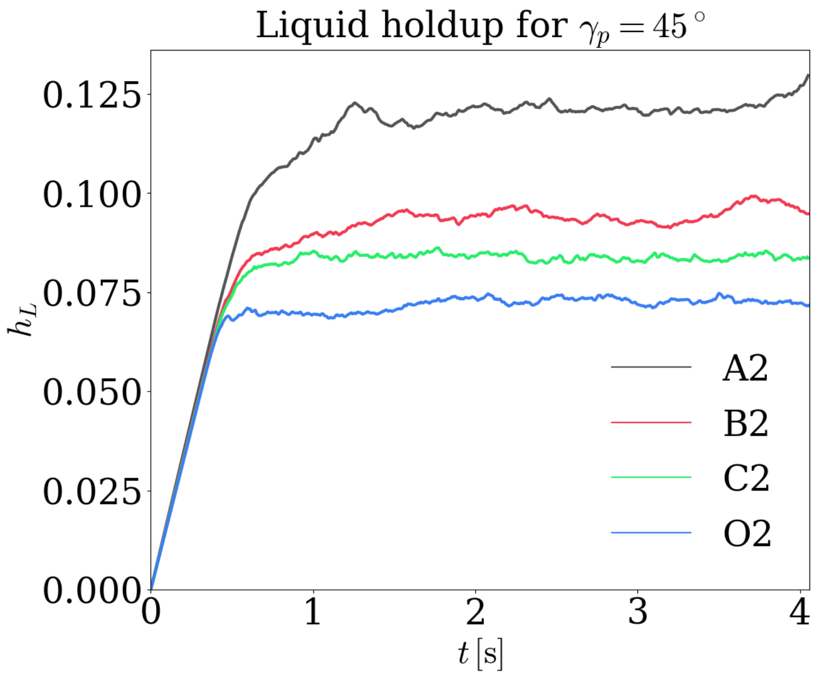


Simulation Results

Key Hydrodynamic Metrics at Low Inflow Velocity ($v_{in} = 0.1$ m/s)







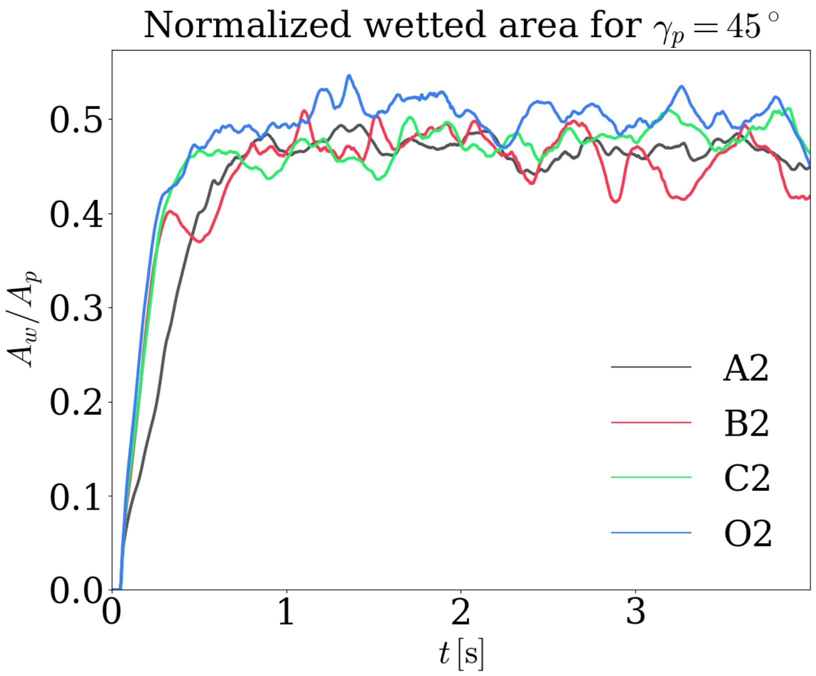
Normalized wetted area = A_w/A_p
Wetted area (A_w) = $\int_{walls} \alpha_l dA$

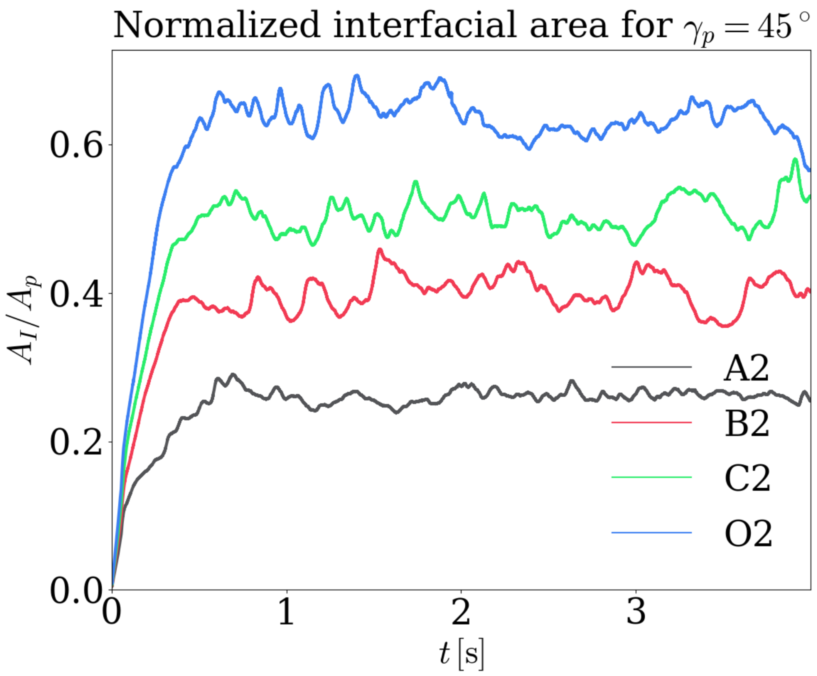
Normalized interfacial area = A_I/A_p
Interfacial area (A_I) = $\int_V \mid \nabla \alpha_l \mid d\boldsymbol{x}$

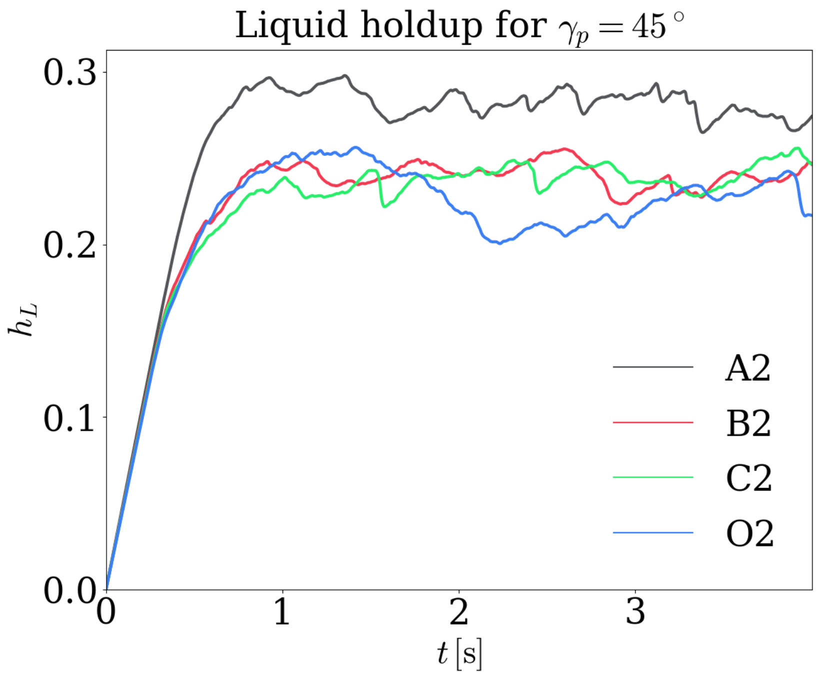
Liquid holdup (h_l) = $\frac{1}{V} \int_V \alpha_l d\boldsymbol{x}$

- Interfacial and wetted areas are generally observed to approach a statistically stationary state within 4 flow-through time intervals.

Key Hydrodynamic Metrics at Low Inflow Velocity ($v_{in} = 0.3$ m/s)







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Wetted area (A_w) = $\int_{walls} \alpha_l dA$

Normalized interfacial area = A_I/A_p
Interfacial area (A_I) = $\int_V | \nabla\alpha_l | d\boldsymbol{x}$

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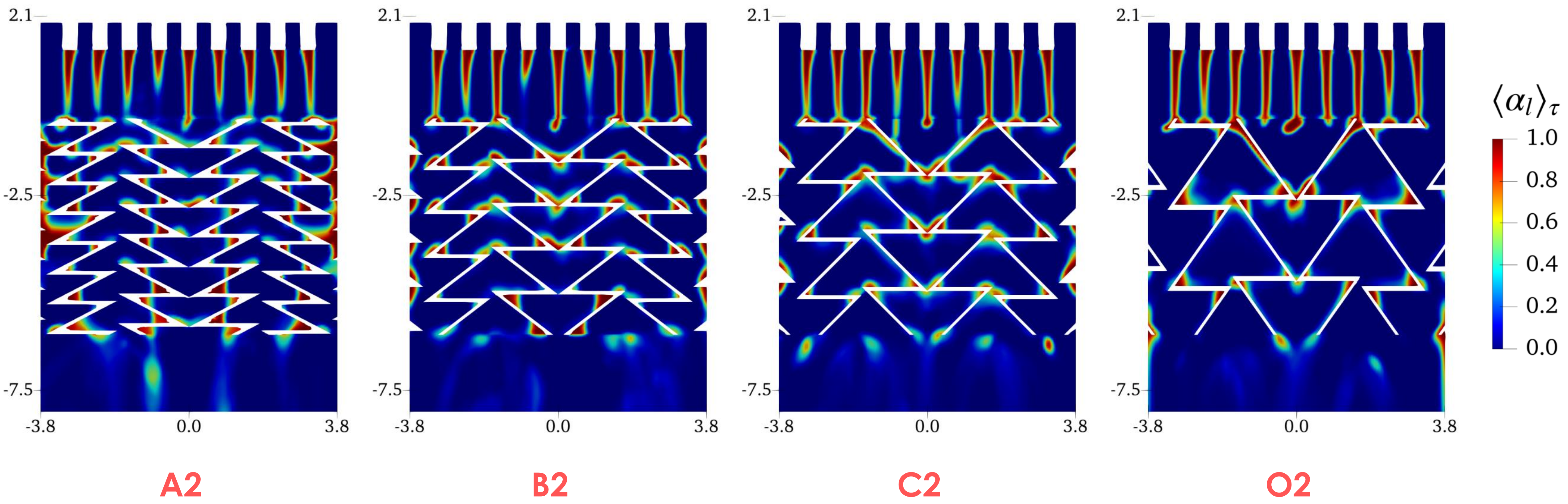
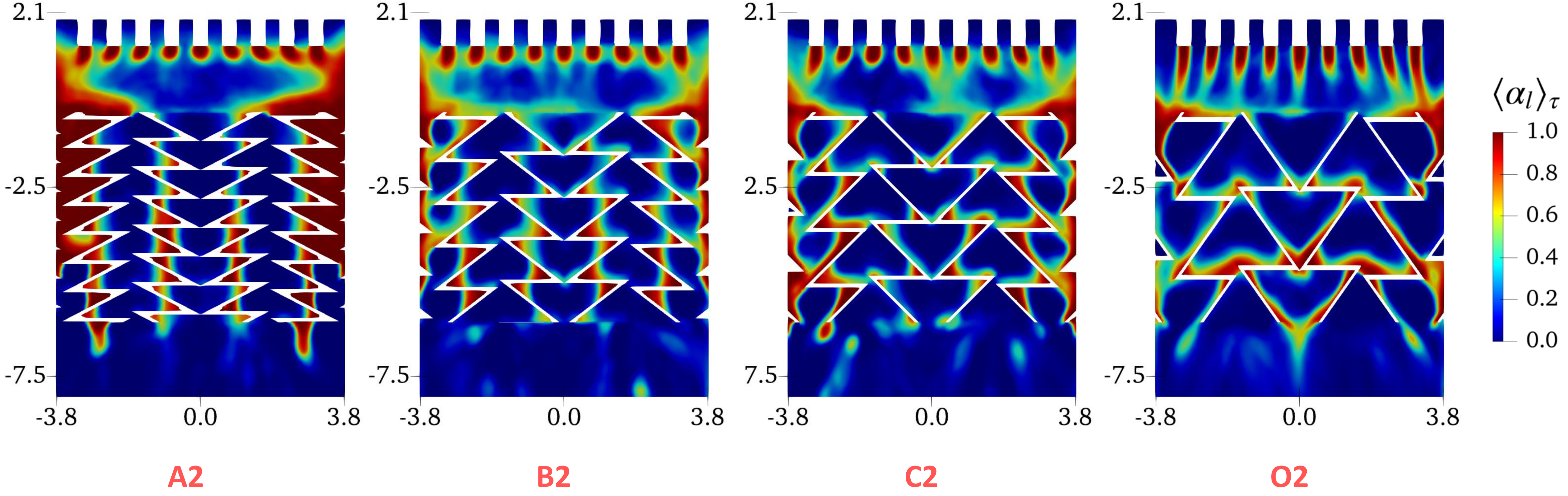
Effects of Geometry Modifications: Solvent Distribution



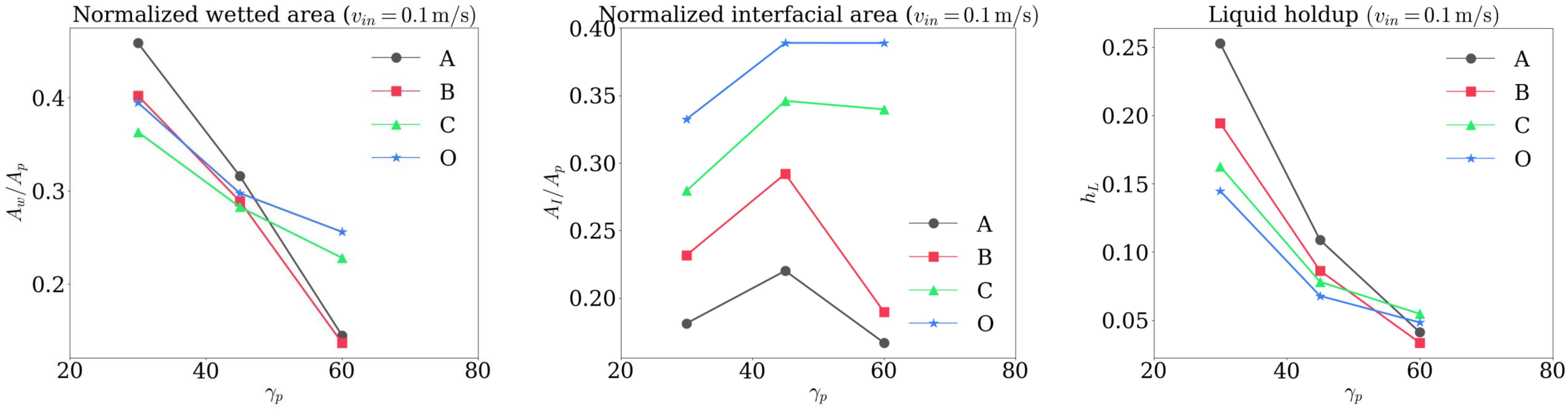
- Distribution of time-averaged liquid volume fraction $< \alpha_l >_\tau$ on XZ planar slice at v_{in} = 0.1 m/s at steady-state.

Effects of Geometry Modifications: Solvent Distribution



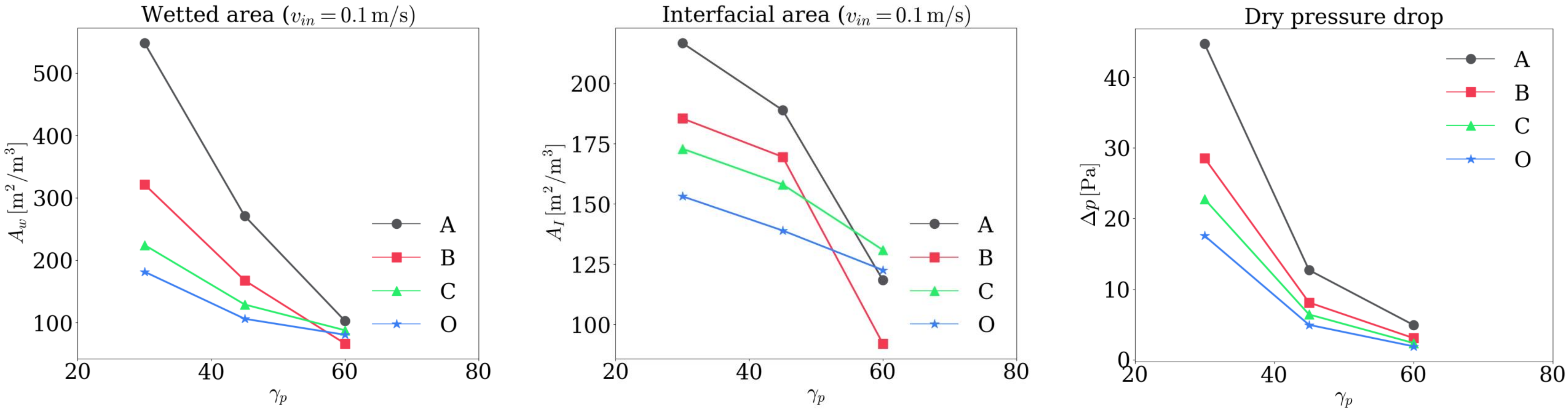
- Distribution of time-averaged liquid volume fraction $< \alpha_l >_\tau$ on XZ planar slice at v_{in} = 0.3 m/s at steady-state.

Effects of Geometry Modifications



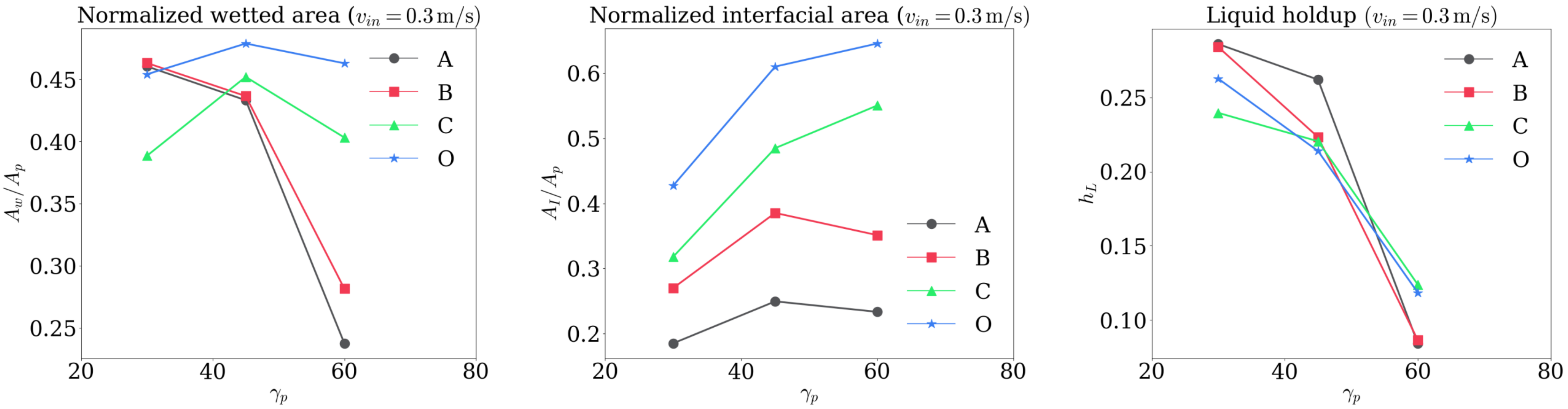
- Relative to A_p, packings with smaller crimping and corrugation angles have a higher normalized wetted area.
- For each β_p, packings with γ_p = 45° are observed to be optimal in terms of normalized interfacial area. The normalized interfacial area is observed to increase with β_p indicating that the Mellapak 250Y-like geometry is optimal (among the cases considered) for normalized interfacial area.
- Liquid holdup is up to 66% higher for packings with lower β_p at lower angles.

Effects of Geometry Modifications



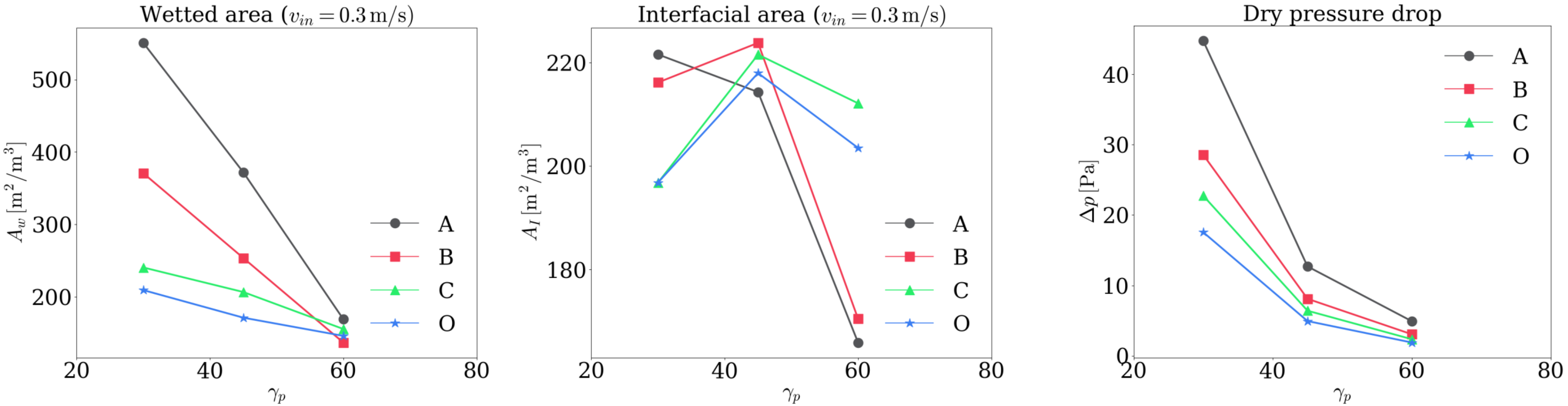
- The absolute wetted area per unit volume, A_w, is higher for packings with smaller corrugation and crimping angles. Compared to $\beta_p = 90°$, the wetted area is up to 3 times higher for $\beta_p = 30°$.
- The absolute interfacial area per unit volume, A_I, is generally higher for packings with smaller corrugation and crimping angles. Compared to $\beta_p = 90°$, the interfacial area is up to 1.4 times higher for $\beta_p = 30°$.
- The dry pressure drop is higher for packings with smaller corrugation angles. Compared to $\beta_p = 90°$, the pressure drop is up to 2.6 times higher for $\beta_p = 30°$.

Effects of Geometry Modifications



- For higher β_p, packings with $\gamma_p = 60°$ are generally observed to be optimal in terms of normalized interfacial area. The normalized interfacial area is observed to increase with β_p indicating that the Mellapak 250X-like geometry is optimal (among the cases considered) for normalized interfacial area.
- For each γ_p, liquid holdup is generally similar across packings with different β_p.

Effects of Geometry Modifications



- The absolute wetted area per unit volume, A_w, is higher for packings with smaller corrugation and crimping angles. Compared to $\beta_p = 90°$, the wetted area is up to 2.63 times higher for $\beta_p = 30°$.
- The absolute interfacial area per unit volume, A_I, is generally higher for packings with smaller corrugation and crimping angles. The highest interfacial area is observed for packing B2, i.e., with $\beta_p = \gamma_p = 45°$.

Summary and Conclusions

- Hydrodynamics of columns equipped with different packing designs ranging from more compact to less compact structures relative to the Mellapak Y series packing structure (packing O2) were analyzed using CFD.
- Among the packings tested, those with corrugation and crimp angles of 30° were shown to achieve highest wetted areas, with up to 2.6 and 3 times more wetted areas than Mellapak Y series packing structures for similar-sized columns under similar operating conditions.
- A trade-off is observed between dry pressure drop and observed wetted area. While packings with smaller β_p and γ_p show higher wetted areas, these packings produce even higher pressure drop. In this regard, packings with $\gamma_p = 60°$ show the lowest liquid holdup and dry pressure drop per unit wetted area. This suggests that such packings are also capable of supporting higher liquid load without causing the column to be flooded.
- Considering this trade-off, packing C3 ($\beta_p = 60°$ and $\gamma_p = 60°$) is observed to be more effective than Mellapak Y (O2) or X (O3) series packing structures, as it packs 7.8% more specific area than O2, while providing 52.6% more interfacial area at a higher liquid load and reducing the dry pressure drop by 52.2%.

Thank you

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