Carbon Capture Simulation for Industry Impact

Modeling Mass Transfer Performance of Packings

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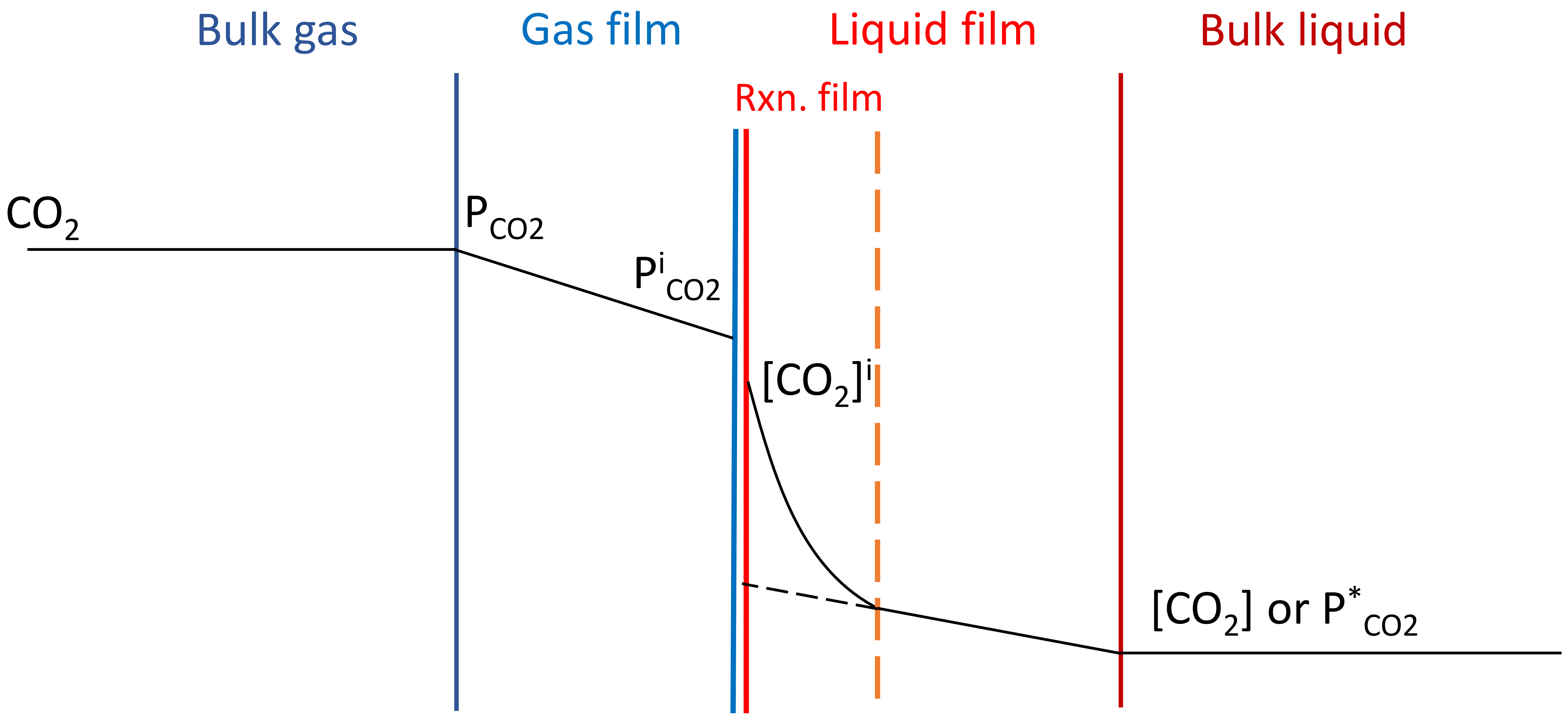
Two-film theory



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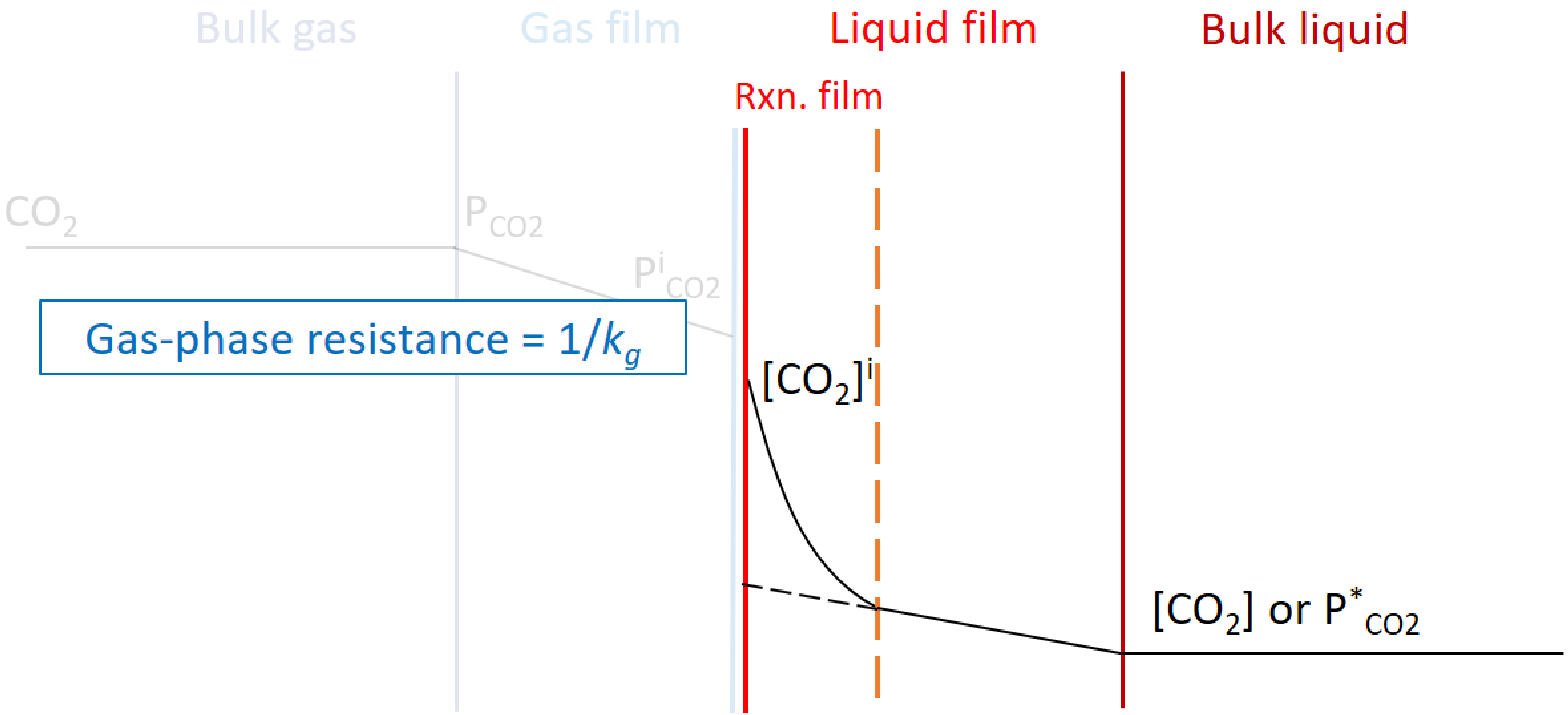

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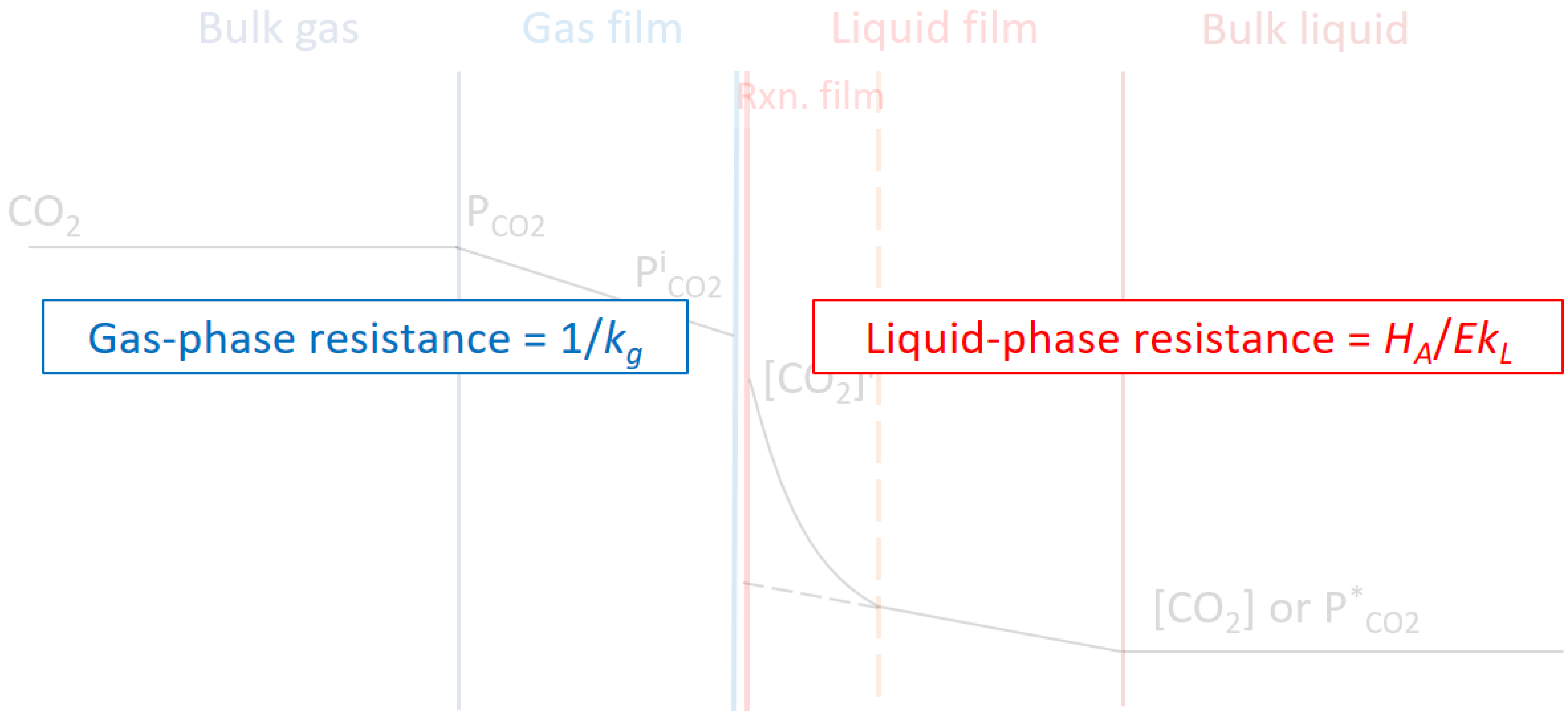
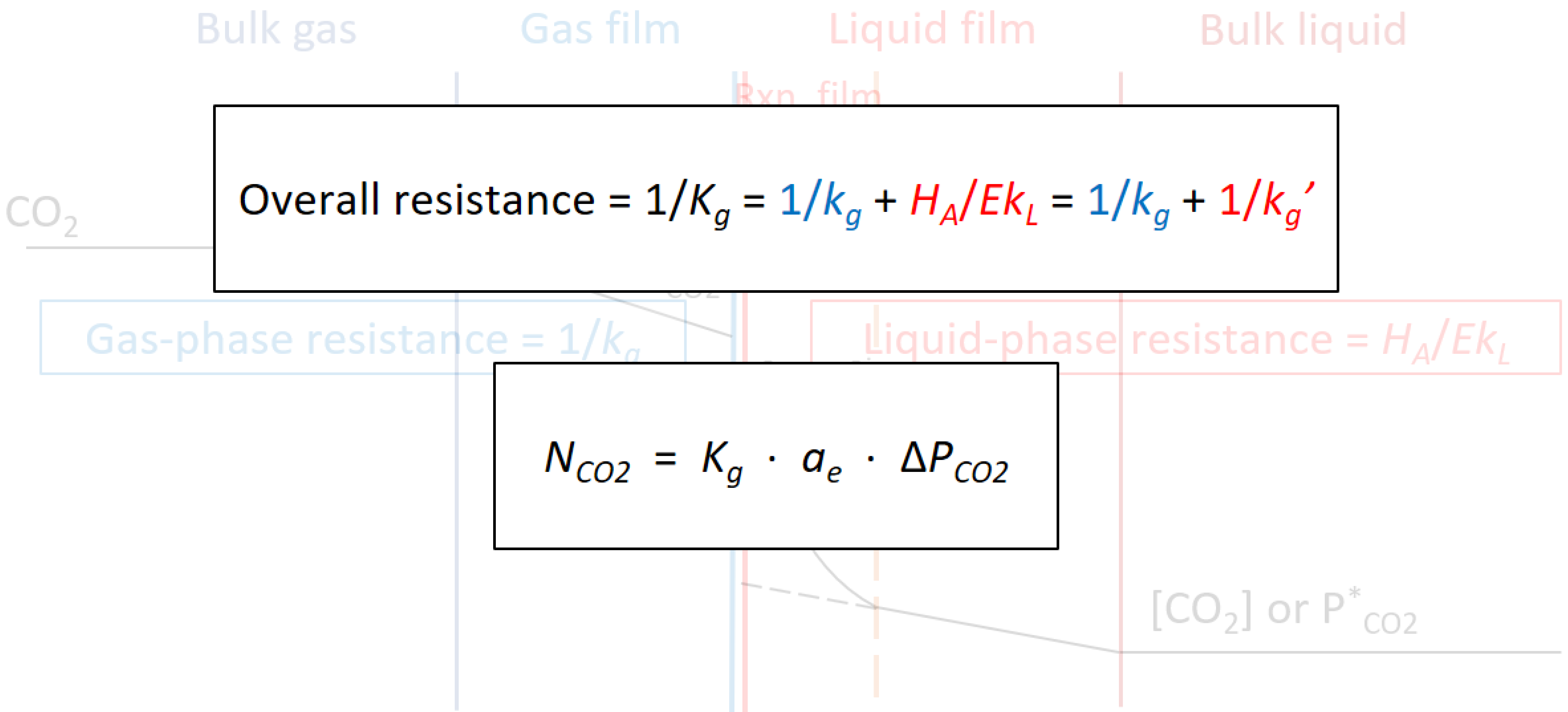


Gas-phase resistance = $1/k_g$

Liquid-phase resistance = H_A/Ek_L

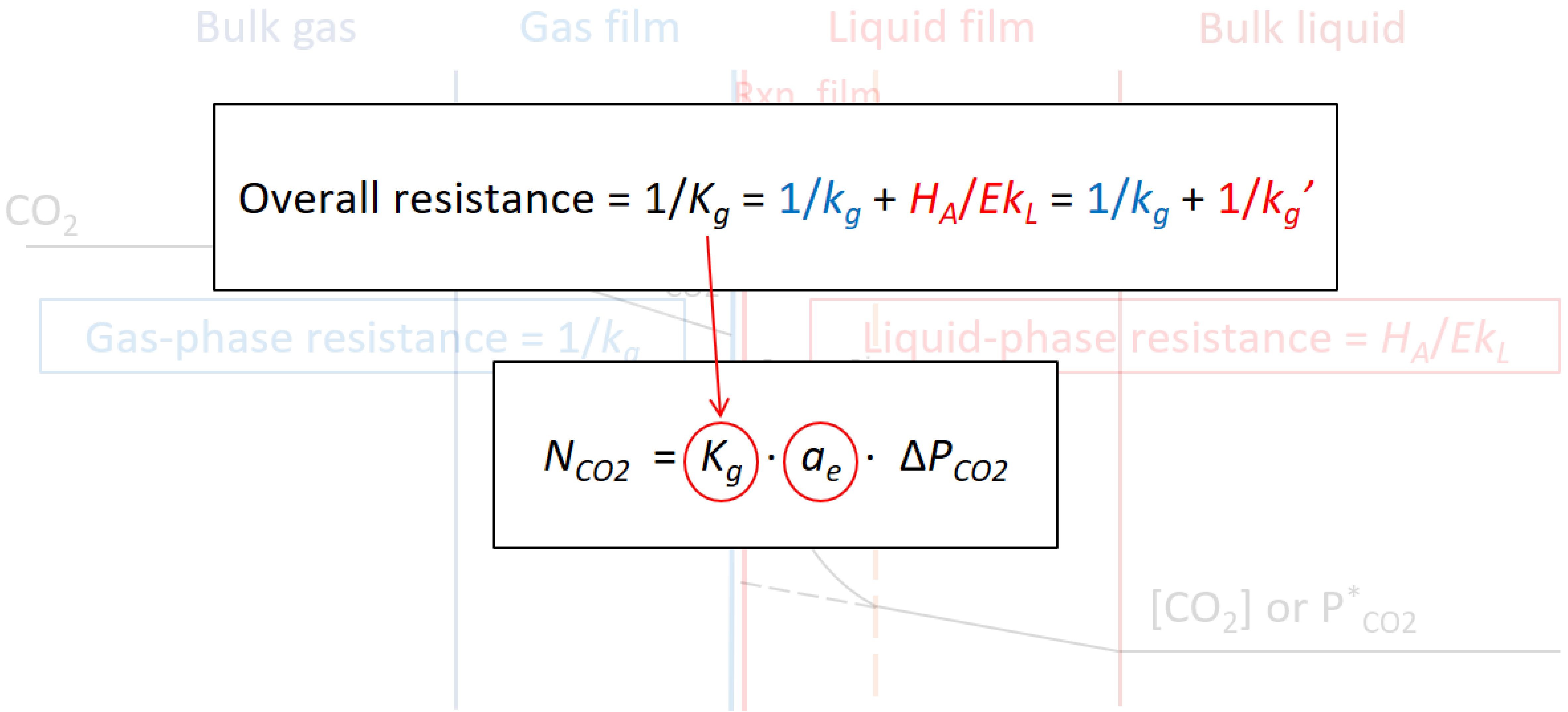
Two-film theory



$$\text{Overall resistance} = 1/K_g = 1/k_g + H_A/Ek_L = 1/k_g + 1/k_g'$$

$$N_{CO2} = K_g \cdot a_e \cdot \Delta P_{CO2}$$

Two-film theory



Overall resistance = $1/K_g = 1/k_g + H_A/Ek_L = 1/k_g + 1/k_g'$

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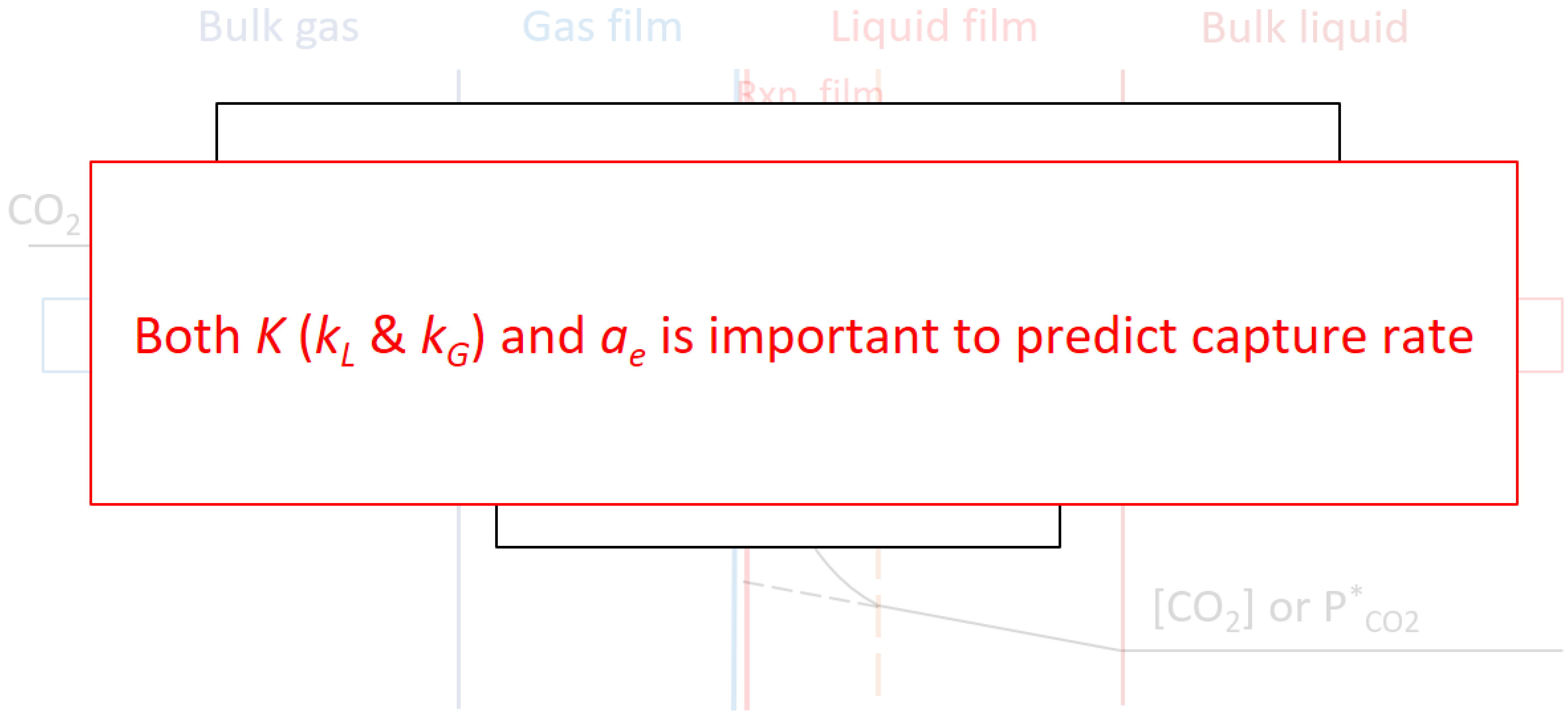
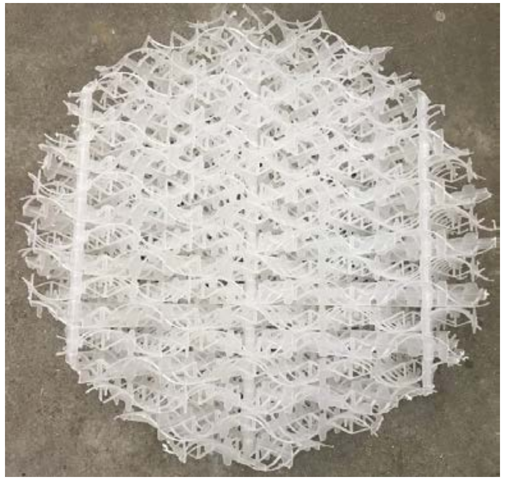
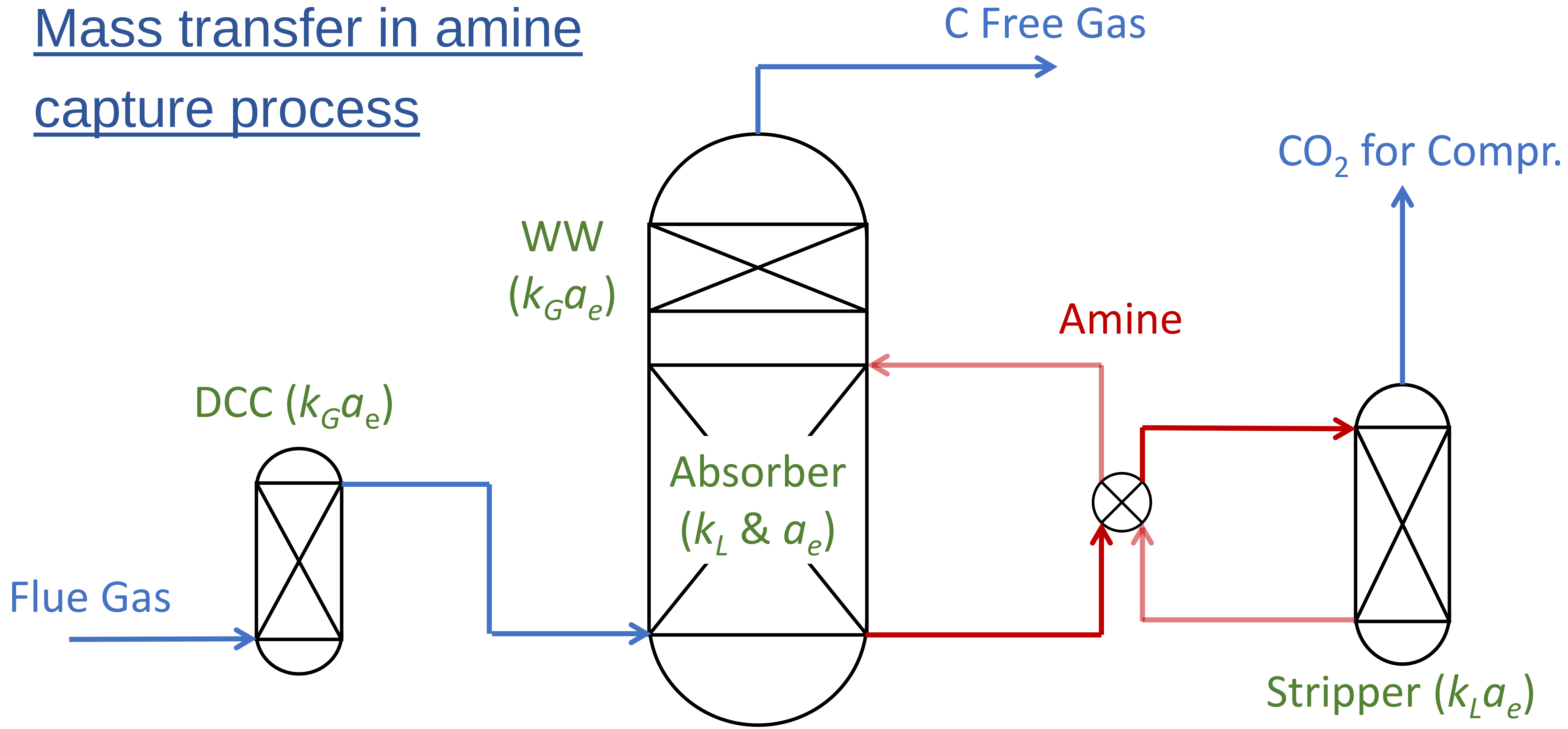


Both K (k_L & k_G) and a_e is important to predict capture rate

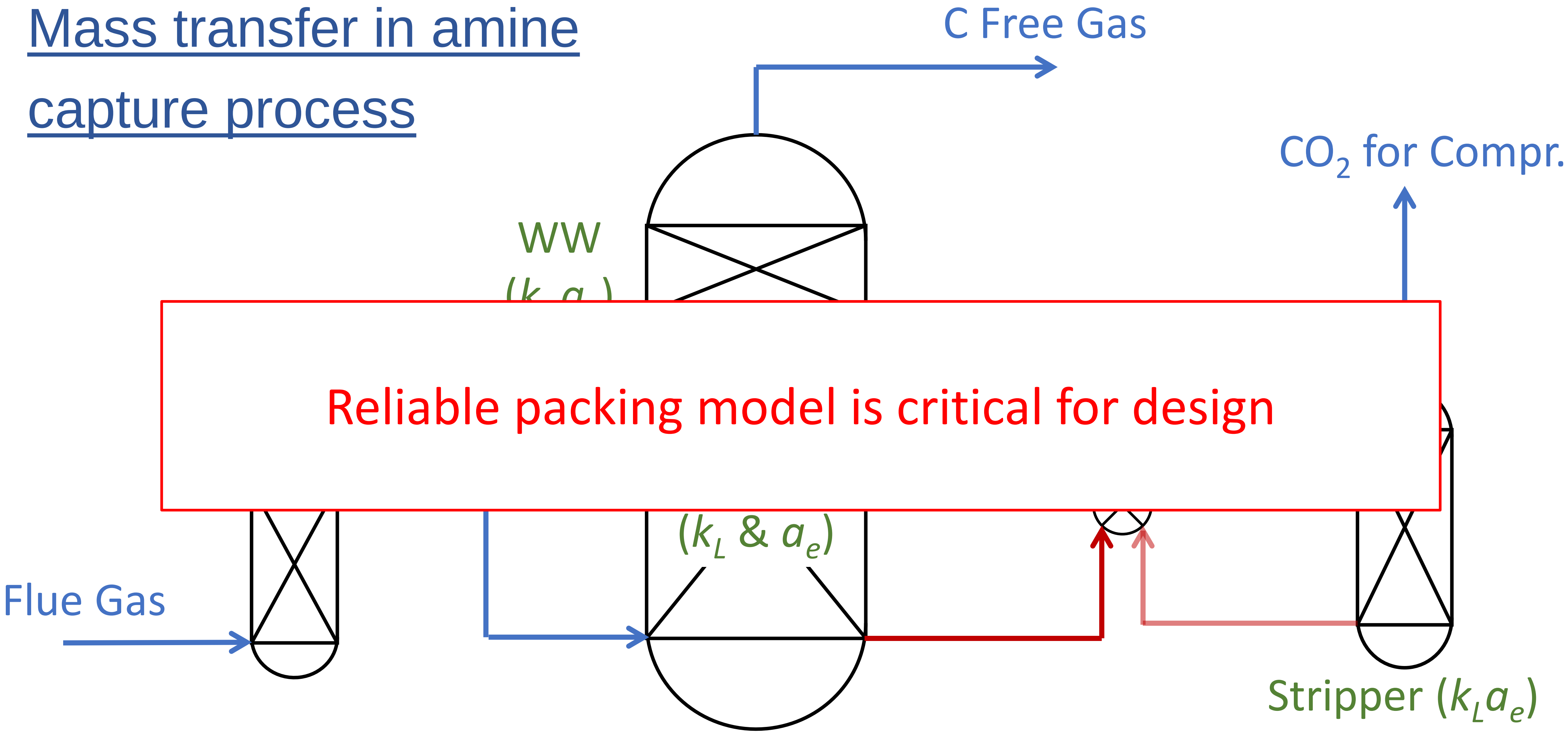
Packings

	Random	Structured	Hybrid
Since	1890s	1960s	>2000
Cost	Low	High	High
Efficiency	Moderate	High	High
Capacity	Moderate	High	Medium
Shape			

Mass transfer in amine capture process



Mass transfer in amine capture process



Reliable packing model is critical for design

μ_L is critical to solvent selection

- Heat transfer
  - *h* ↓ *Q* ↑
- Mass transfer
  - Diffusion of CO_2 through reactive layer ↓
  - Diffusion of free amine to L-G interface (surface depletion) ↓
  - Diffusion of loaded amine back to bulk liquid (P^*_{CO2}) ↓
  - Liquid turbulence ↓

$\mu_{Solvent} \gg \mu_{H2O}$

Amine soln. (α = 0.4)	H_2O	7m MEA	11m MEA	5m PZ	8m PZ
μ @ 40˚C (cP)	0.65	2.4	4.0	3.6	11.4

Water lean solvent.	Alkylcarbonates: IPADM-BOL	Switchable Carbamates: TESA	Aminosilicones: GAP-0/TEG	Nonaqueous organic amine blends: AMP/PZ + EGME + 15 wt % H_2O
μ @ 40˚C (cP)	~ 130 cP	~800 cP	~1300 cP	~30 cP

μ_L affects k_L in two ways (how much?)

$$k_L = C_1 \cdot \mu^{\alpha} \cdot D^{\beta}$$

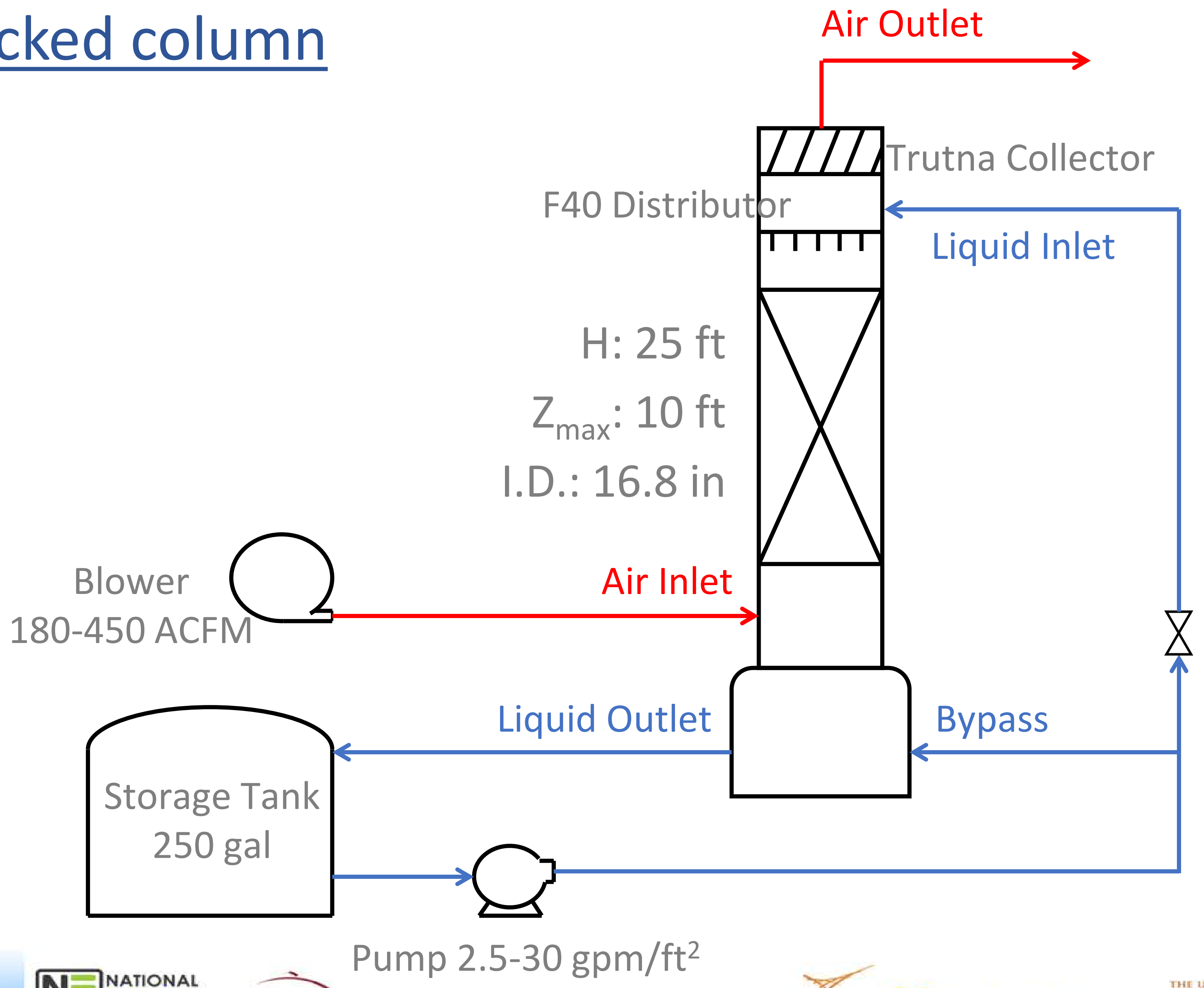
$$D = C_2 \cdot \mu^{\gamma}$$

$$k_L \ (k_L a) = C_3 \cdot \mu^{\alpha + \beta\gamma}$$

- α – Direct influence via the turbulence of liquid
- βγ – Indirect influence via *D* of mass transfer species

μ_L affects a_e?

Pilot packed column



Chemical systems

- k_G: Trace SO_2/NaOH/H_2O
- k_L: Air/Toluene/H_2O
- a_e: Ambient CO_2/NaOH/H_2O

Chemical systems

- k_G: Trace SO_2/NaOH/H_2O
- k_L: Air/Toluene/H_2O + glycerol (1–70 cP)
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Chemical systems

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Kinetic model based on WWC exp.

SRP database

- 21 Structured Packings

  MellaPak®, Montz-Pak®, GT-Pak®, Flexipac®, etc

- 12 Random Packings

  Pall Ring, IMTP®, Raschig-SuperRing®, etc

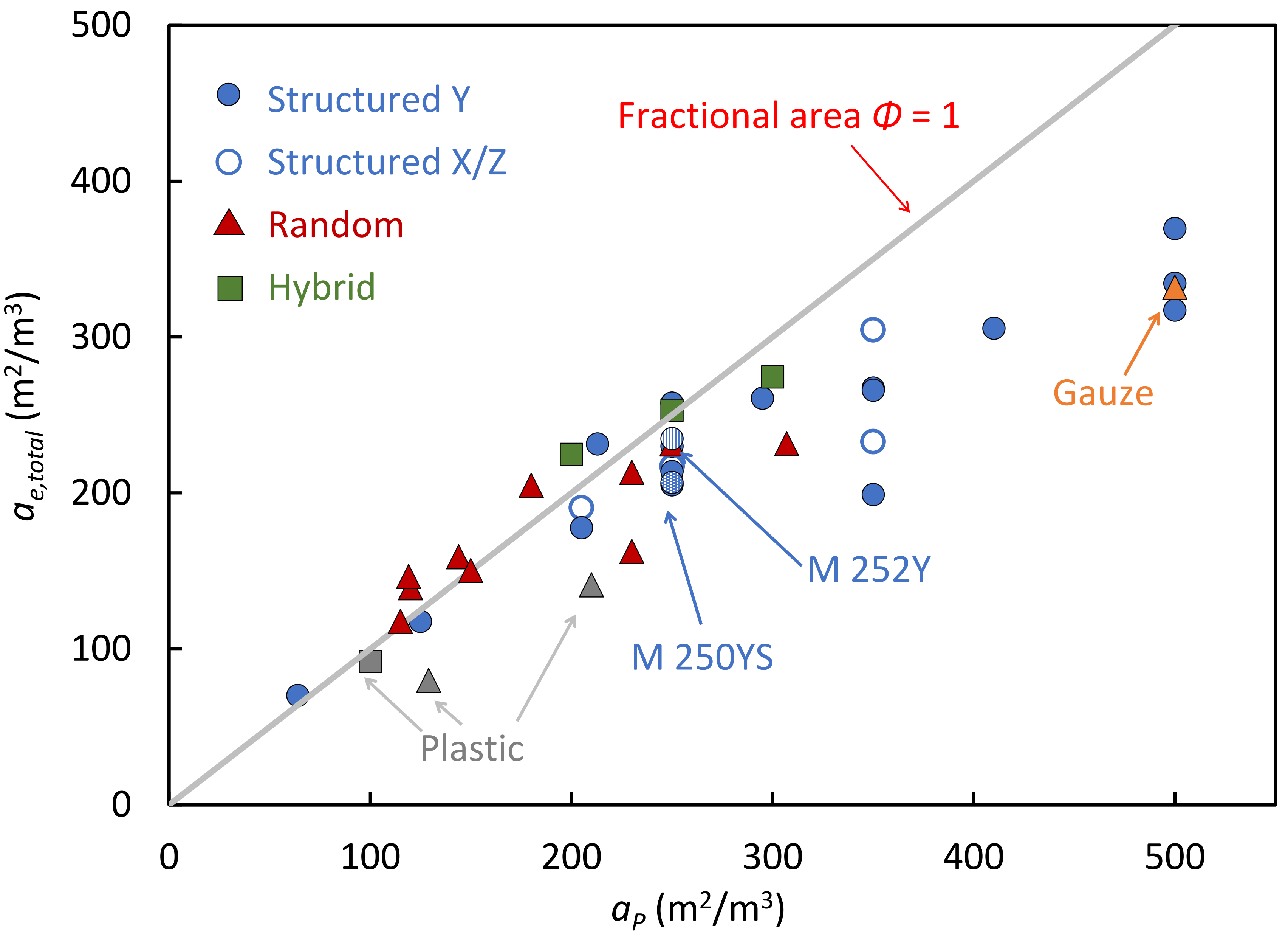
- 4 Hybrid Packings

  Raschig-SuperPak®, Hiflow Plus®

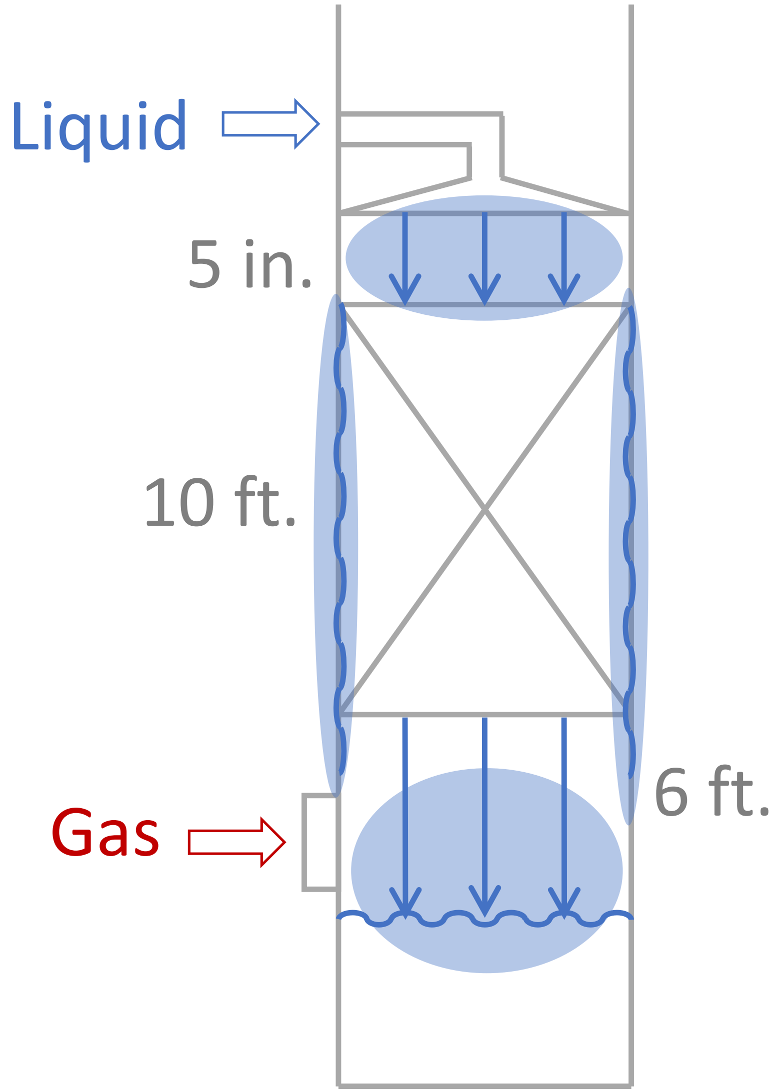
- 1 Gauze Packing

Contents

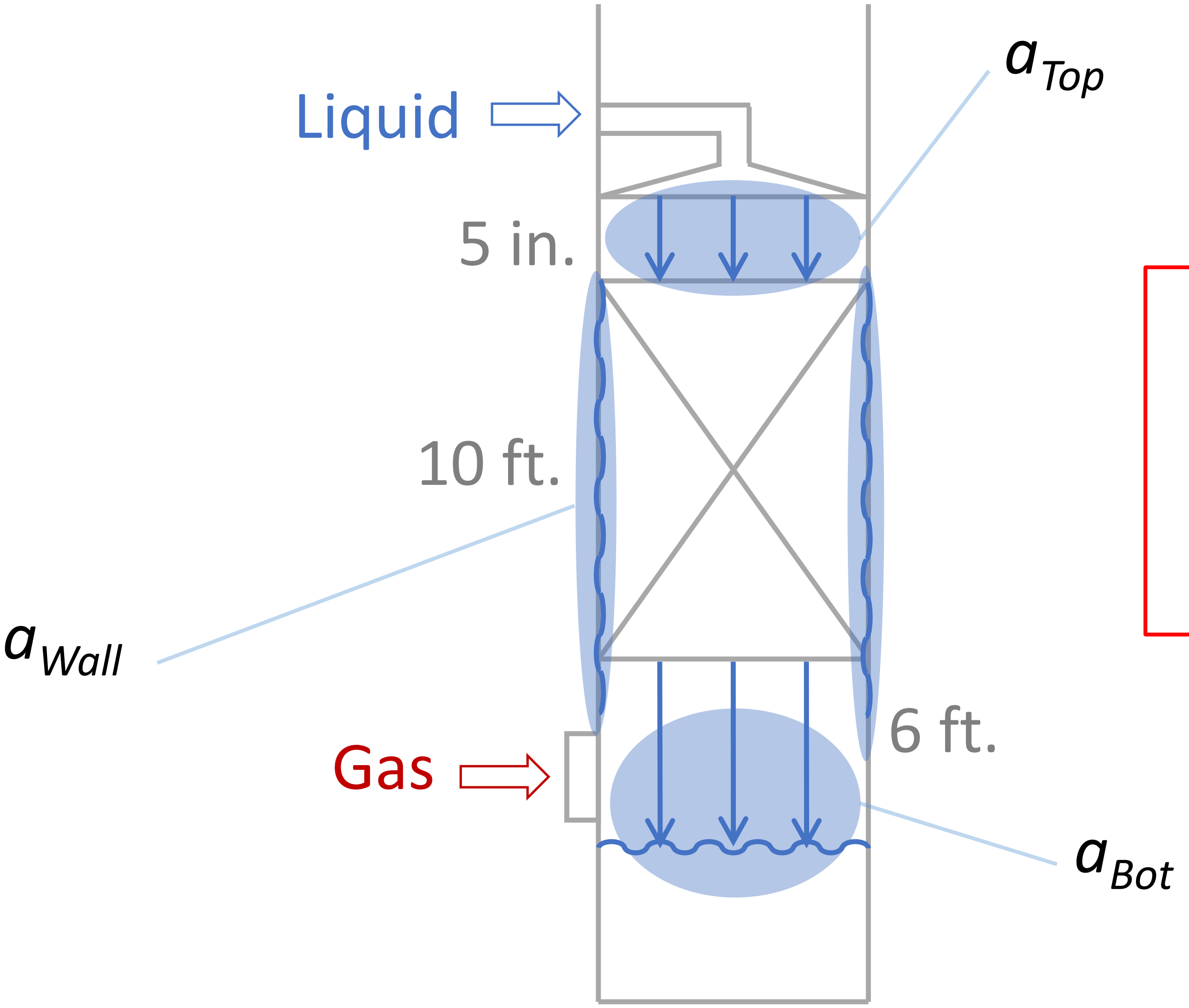
Effective mass transfer area: a_e



Secondary a_e



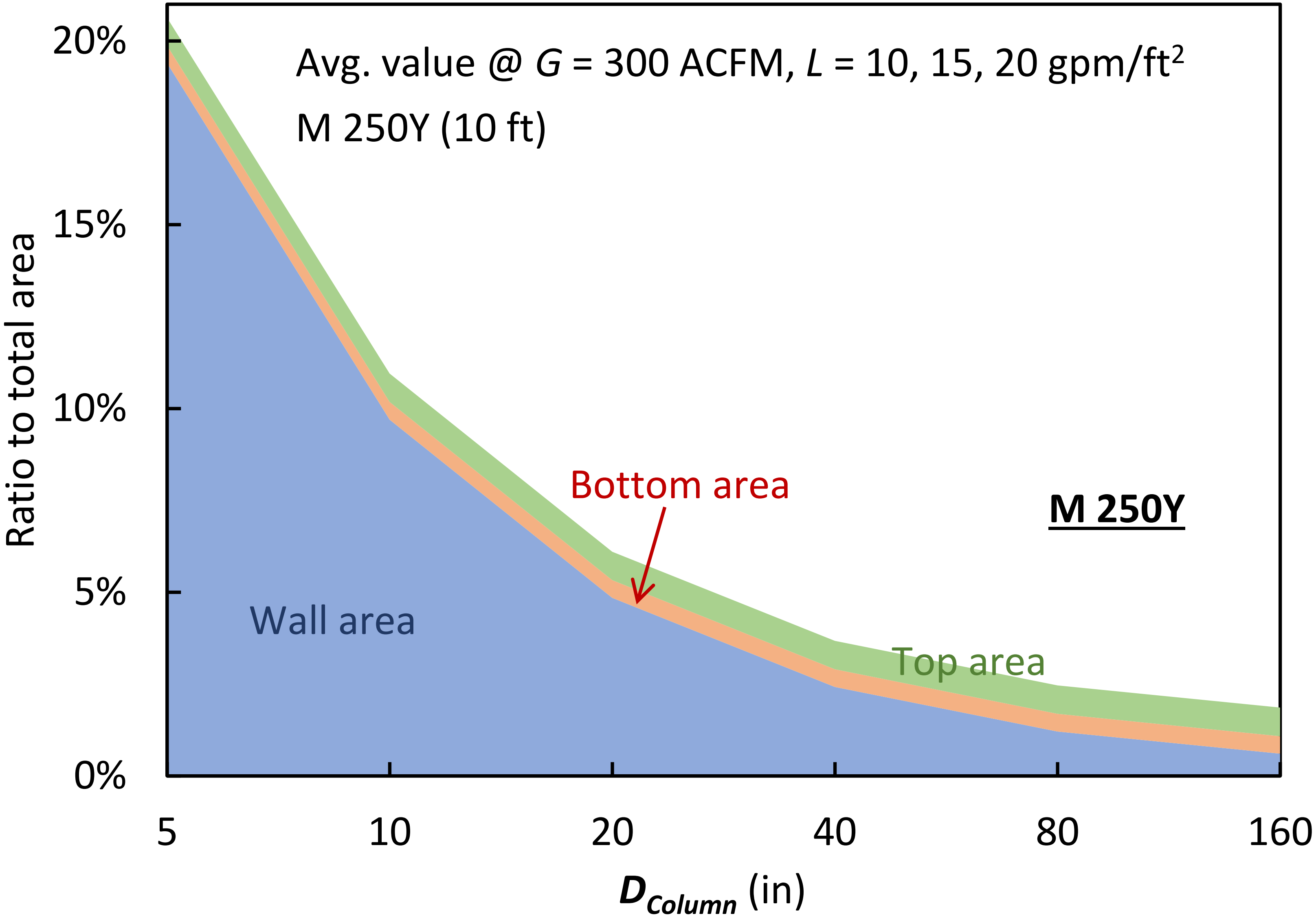
Secondary a_e



$$a_{Secondary} = a_{Top} + a_{Wall} + a_{Bot}$$

$$a_{Total} = a_{e,packing} + a_{Secondary}$$

Sec. a_e is critical to scaling up



a_e Model

$$\frac{a_{e,packing}}{a_P} = 1.16 \cdot \eta \cdot \left(We \cdot Fr^{-\frac{1}{2}}\right)^{0.138}$$

$$= 1.16 \cdot \eta_{type} \cdot \eta_{material} \cdot \eta_{loading} \cdot \left[\left(\frac{\rho_L}{\sigma}\right) \cdot g^{1/2} \cdot u_L \cdot a_P^{-3/2}\right]^{0.138} \cdot \mu_L^0$$

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Random/hybrid:

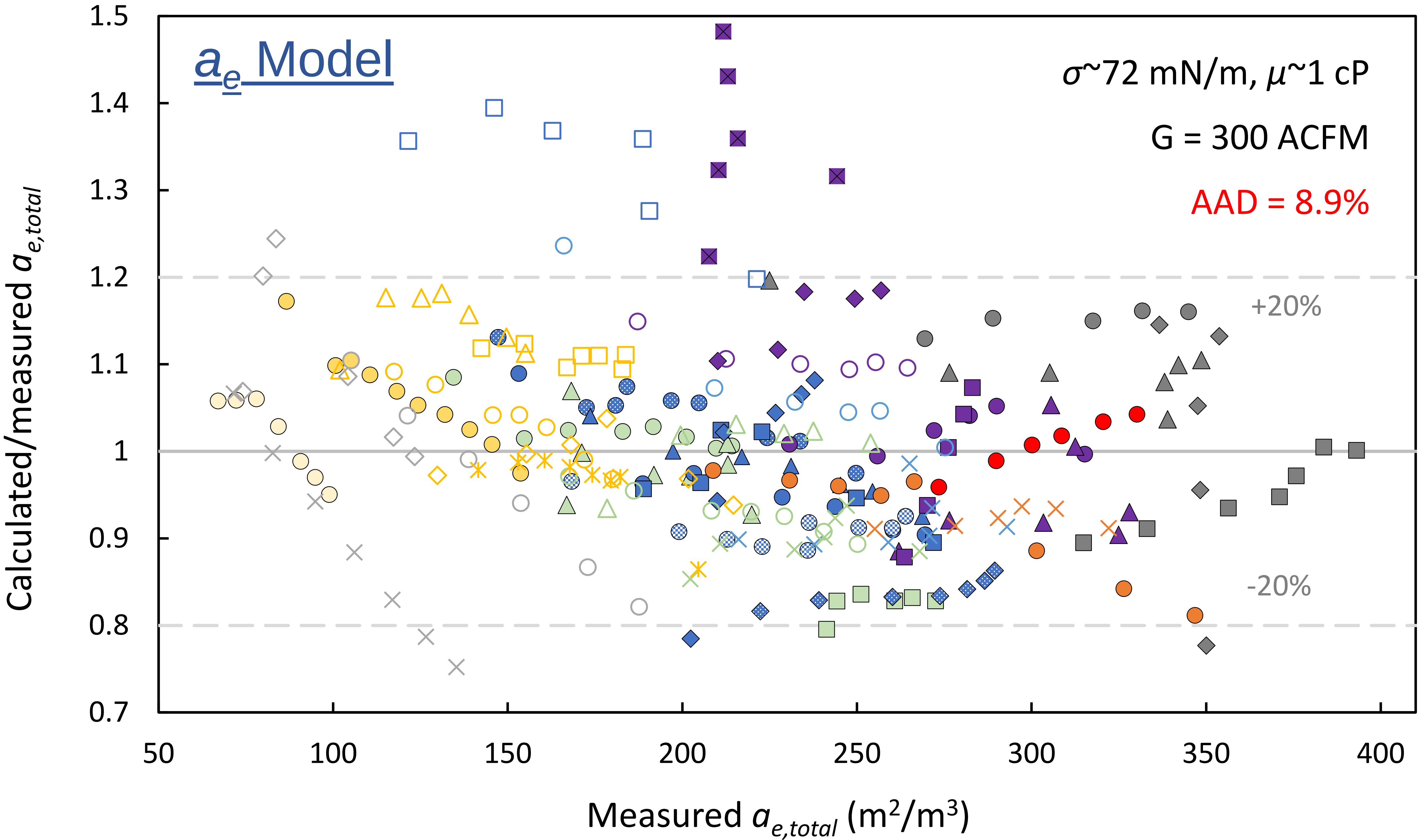
$$\eta_{type} = 1.34 - 0.26\left(\frac{a_P}{250}\right)$$

Plastic:

$\eta_{material}$ = 0.62

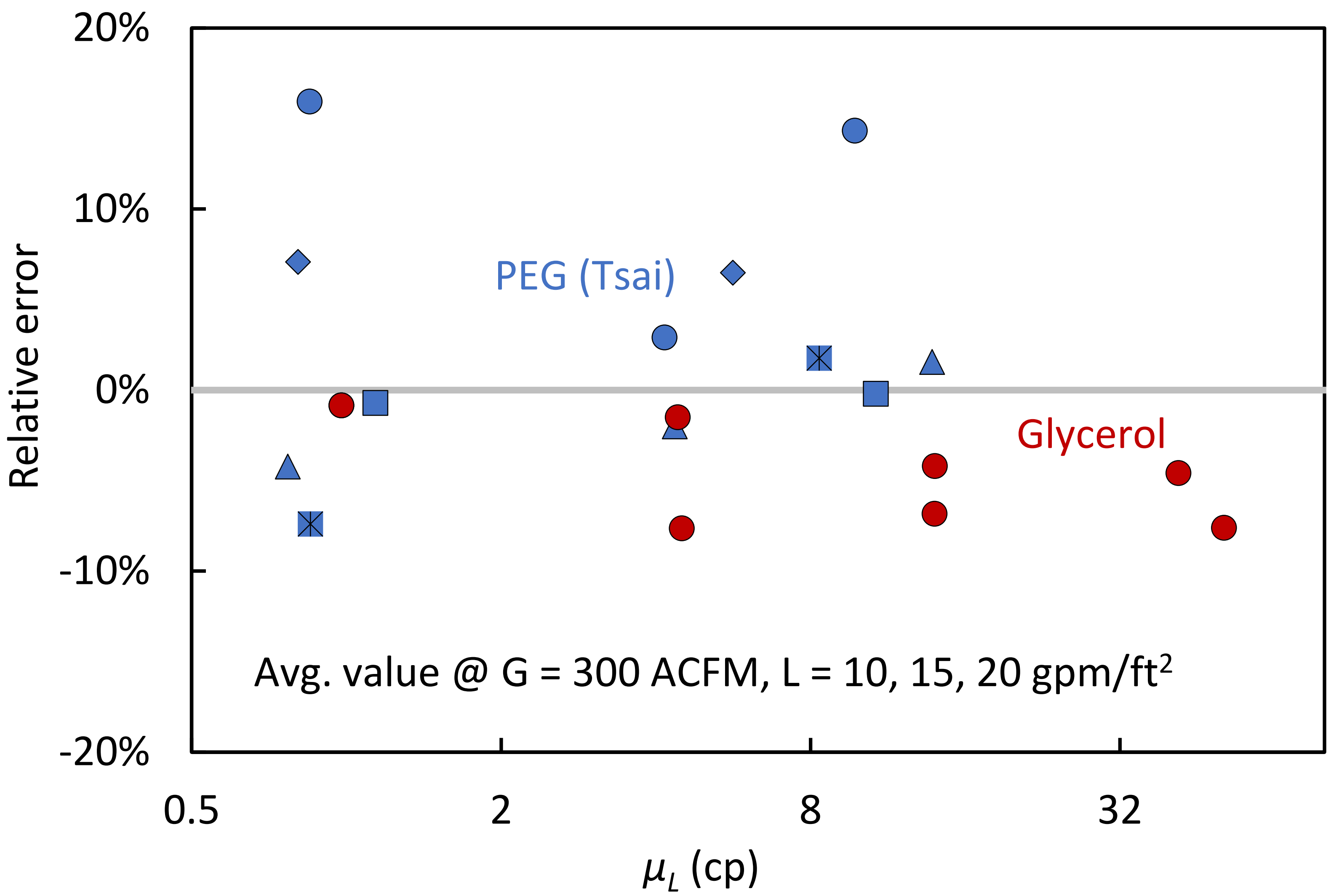
Loading zone (ΔP ≥ 400 Pa/m):

$\eta_{loading}$ = 1.15



a_e Model
σ~72 mN/m, μ~1 cP
G = 300 ACFM
AAD = 8.9%
+20%
-20%
Calculated/measured $a_{e,total}$
Measured $a_{e,total}$ (m^2/m^3)
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
50
100
150
200
250
300
350
400

a_e model w/ viscosity



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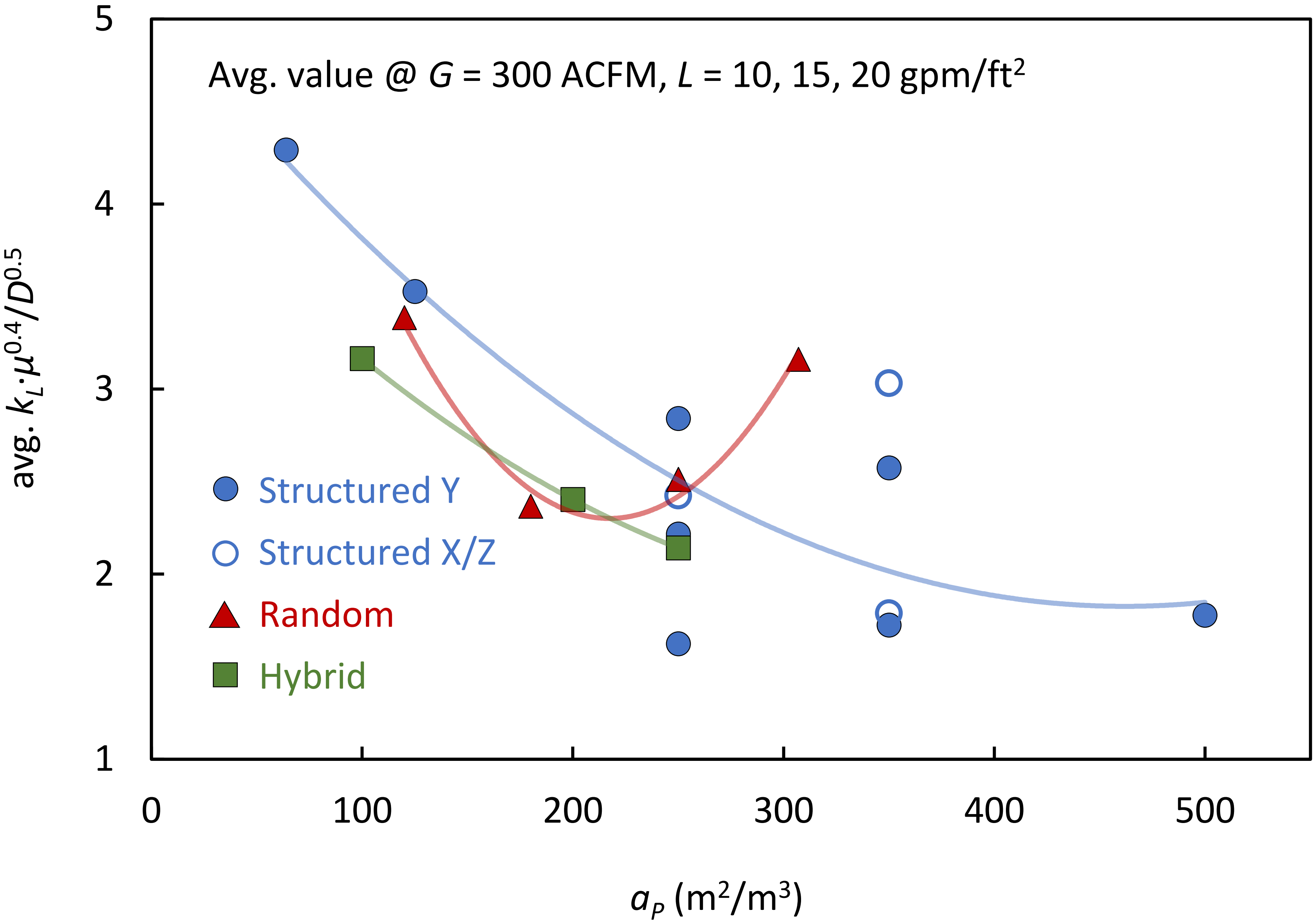
Liquid film mass transfer coefficient: k_L



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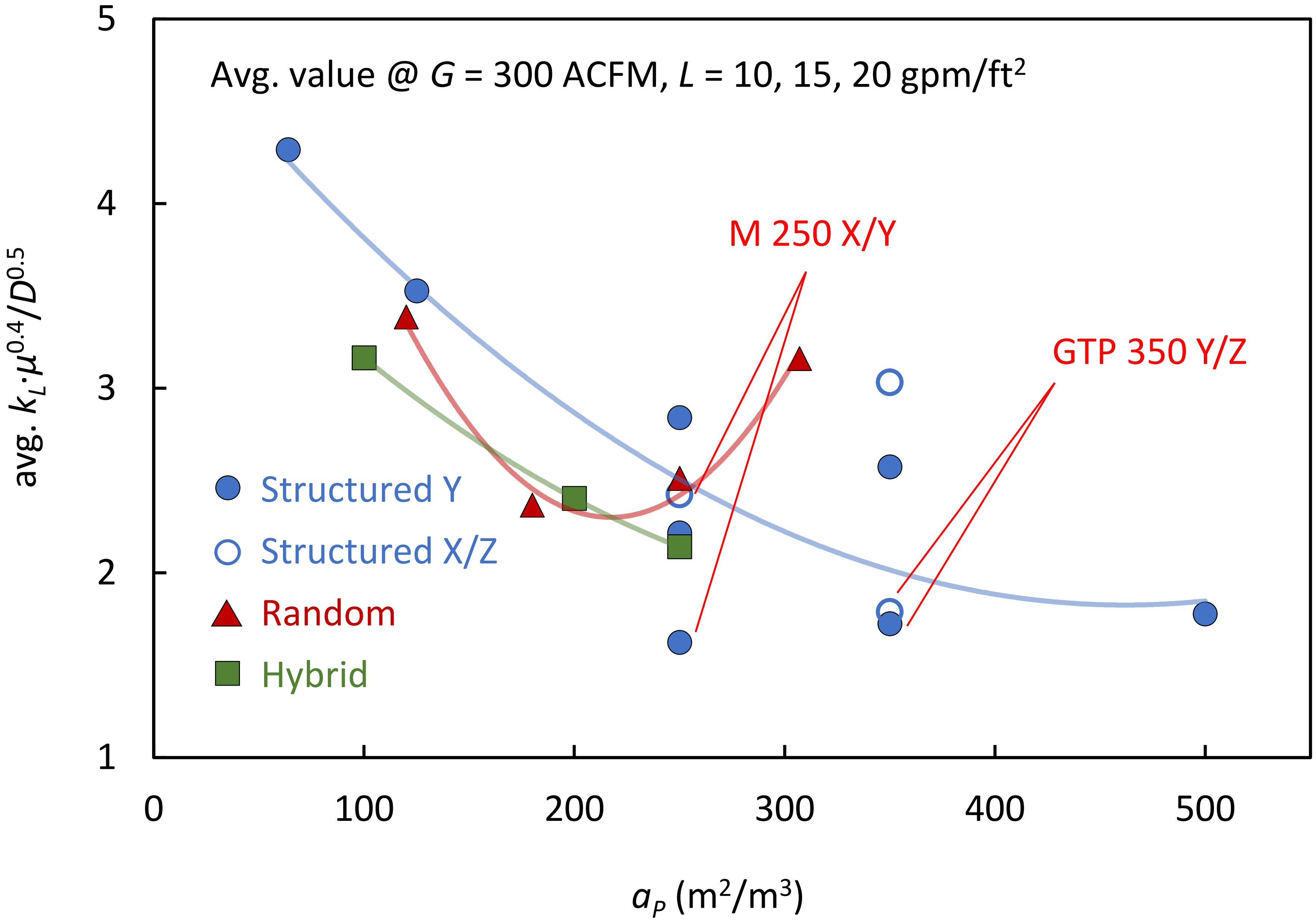
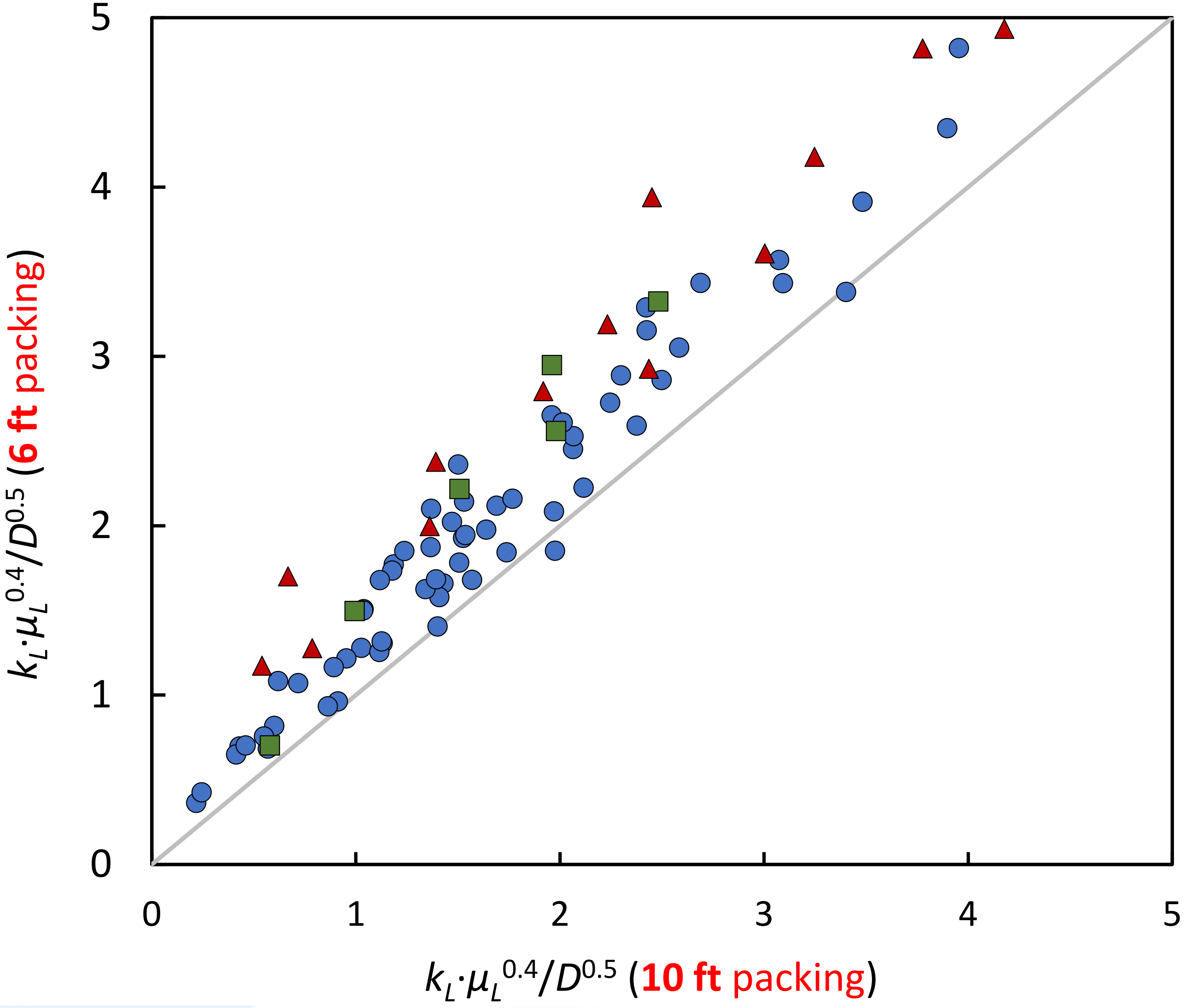


Scaling packing height (k_L)



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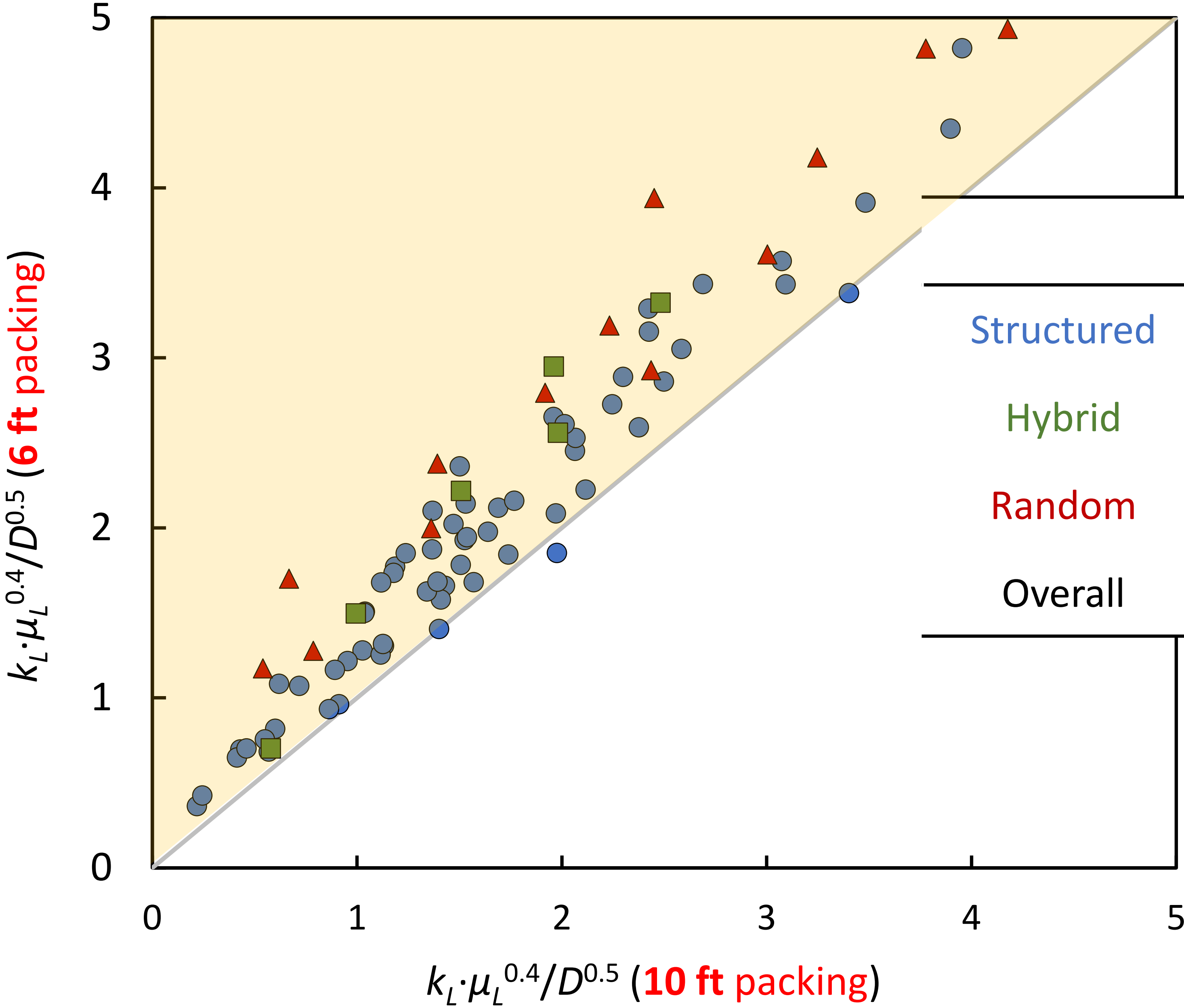
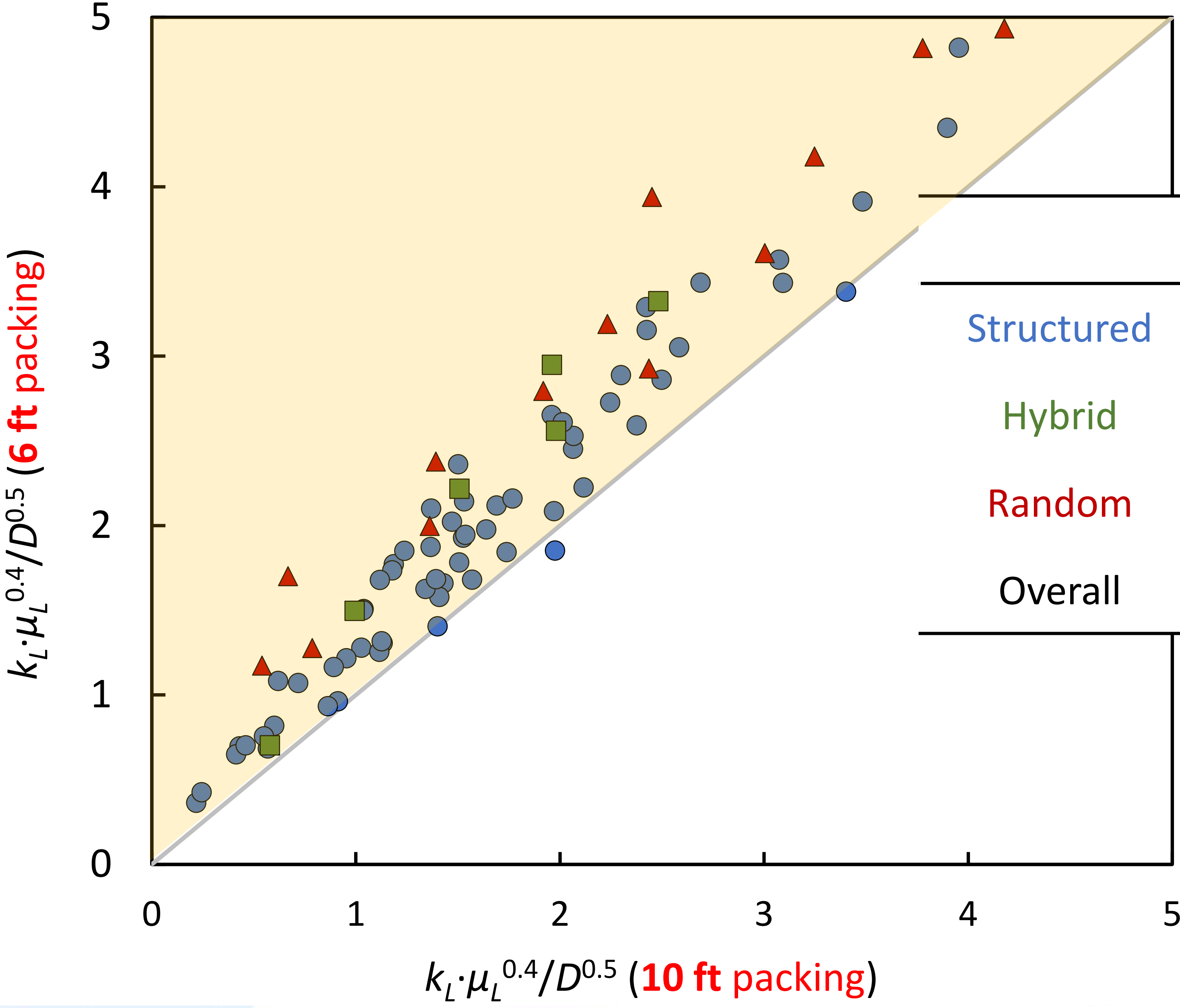


	6-10 ft Ratio
Structured	1.29
Hybrid	1.39
Random	1.54
Overall	1.32

Scaling packing height (k_L)



	6-10 ft Ratio
Structured	1.29
Hybrid	1.39
Random	1.54
Overall	1.32

Maldistribution is worse for taller bed

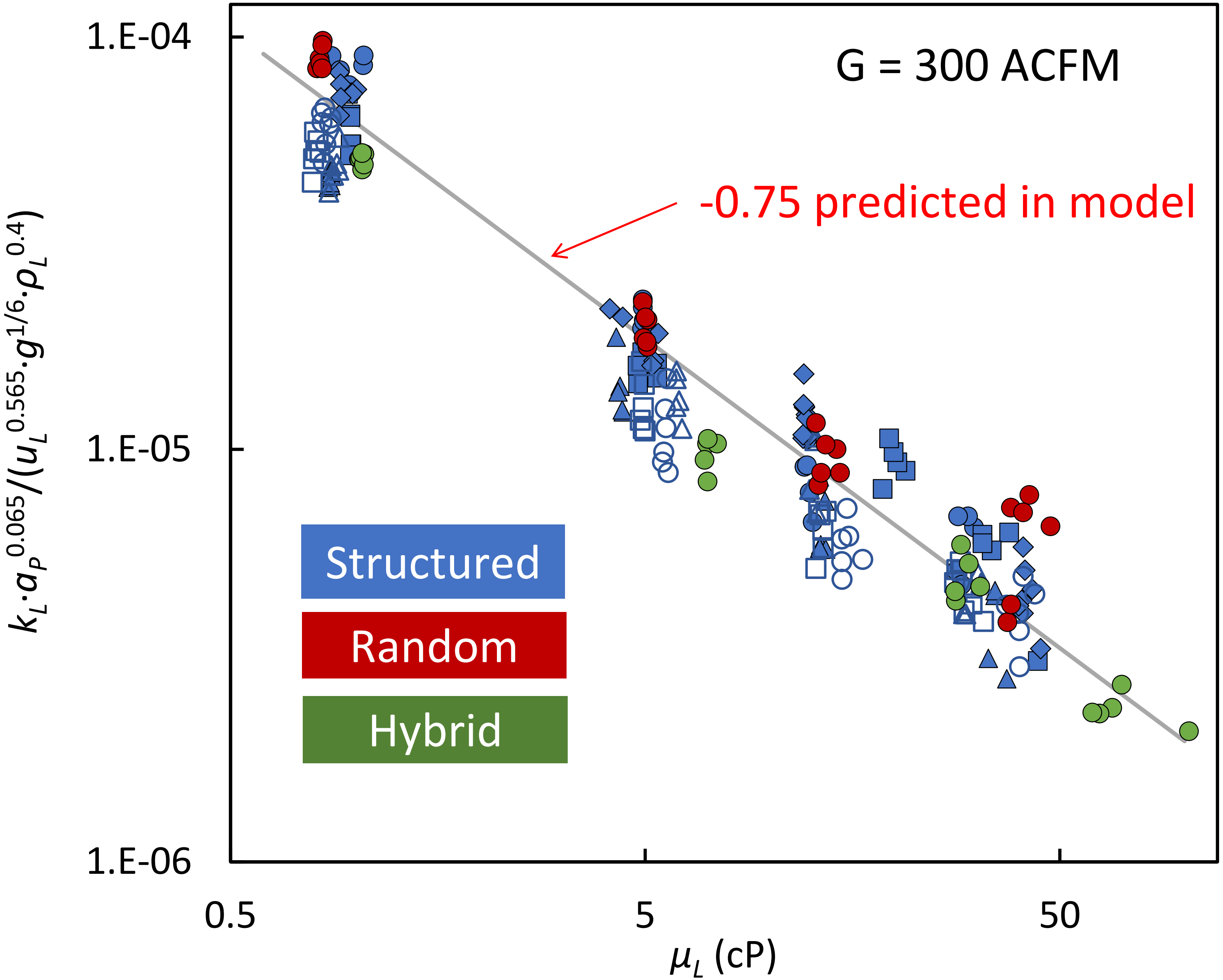
$$\text{Correction} = \frac{\ln(1.32/1)}{\ln(6/10)} = -0.54$$

k_L Model

$$Sh_L = 0.12 \cdot Sc_L^{0.5} \cdot Re_L^{0.565} \cdot Ga_L^{1/6} \cdot \left(\frac{Z}{1.8}\right)^{-0.54}$$

$$k_L = 0.12 \cdot u_L^{0.565} \cdot \left(\frac{\mu_L}{\rho_L}\right)^{-0.4} \cdot D_L^{0.5} \cdot g^{1/6} \cdot a_P^{-0.065} \cdot \left(\frac{Z}{1.8}\right)^{-0.54}$$

Dependence on μ_L of k_L



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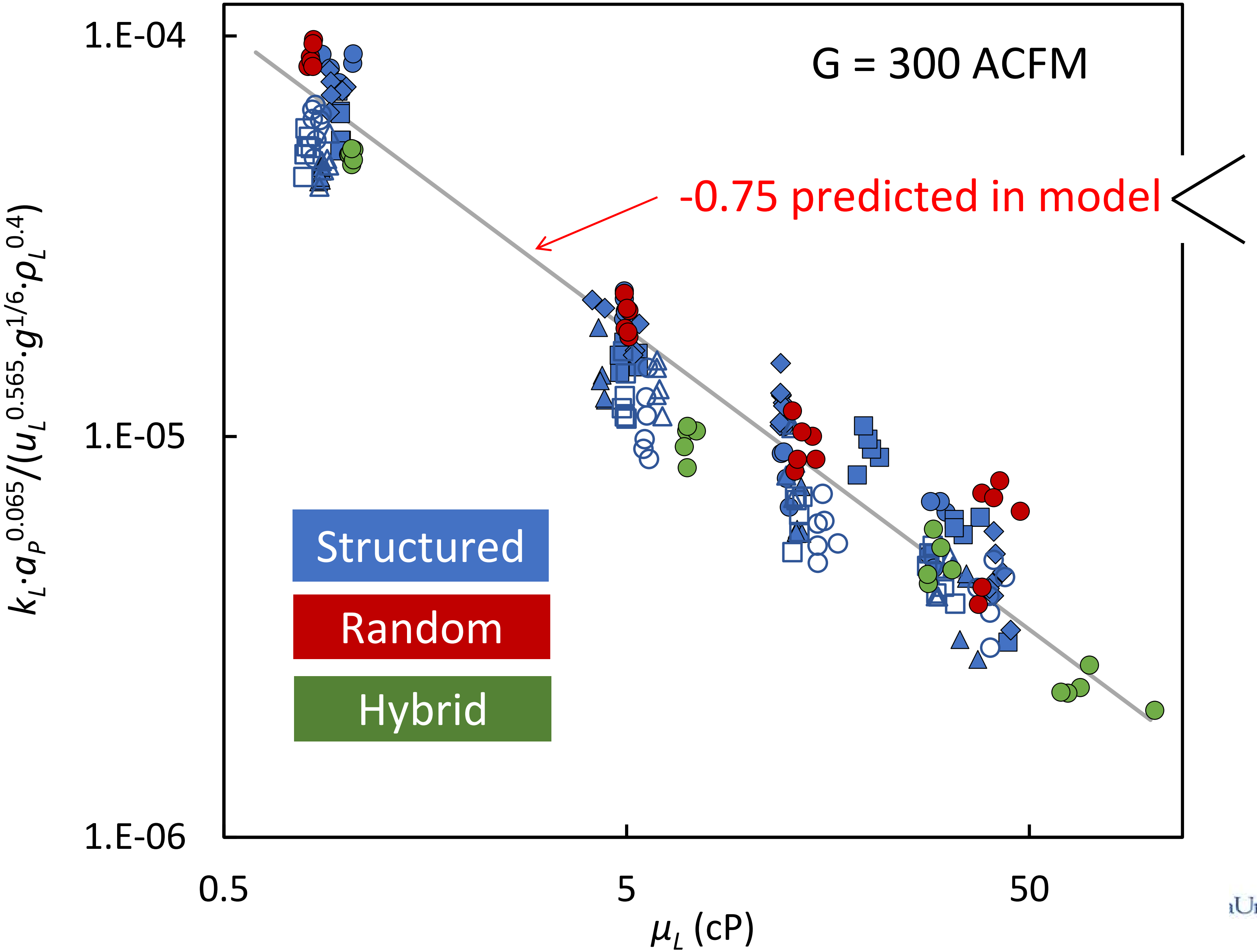
Dependence on μ_L of k_L



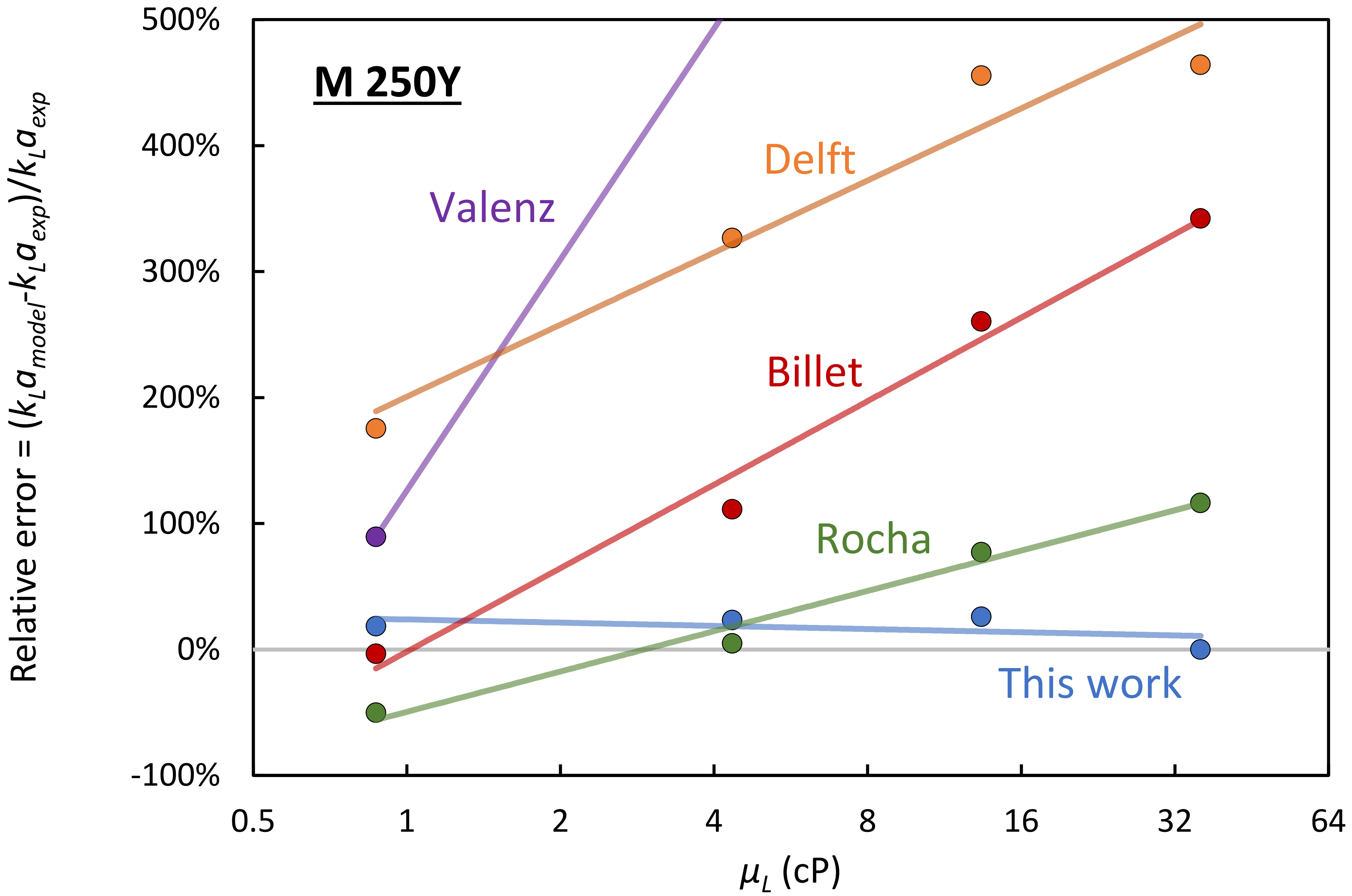
Universally applicable

Direct = -0.40

Indirect = -0.35

System-specific based on *D*-*μ* relationship

Comparison to other work: μ_L



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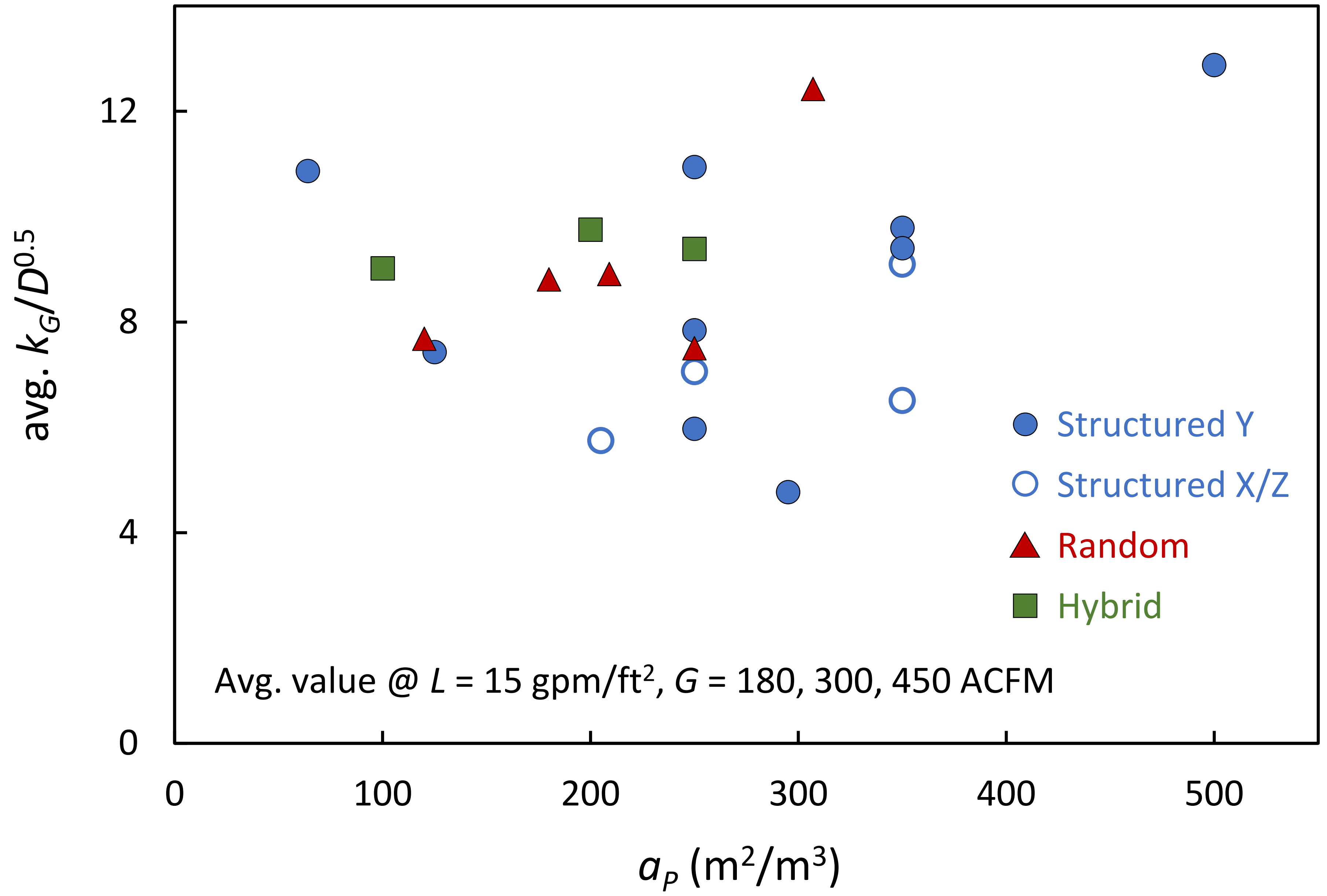
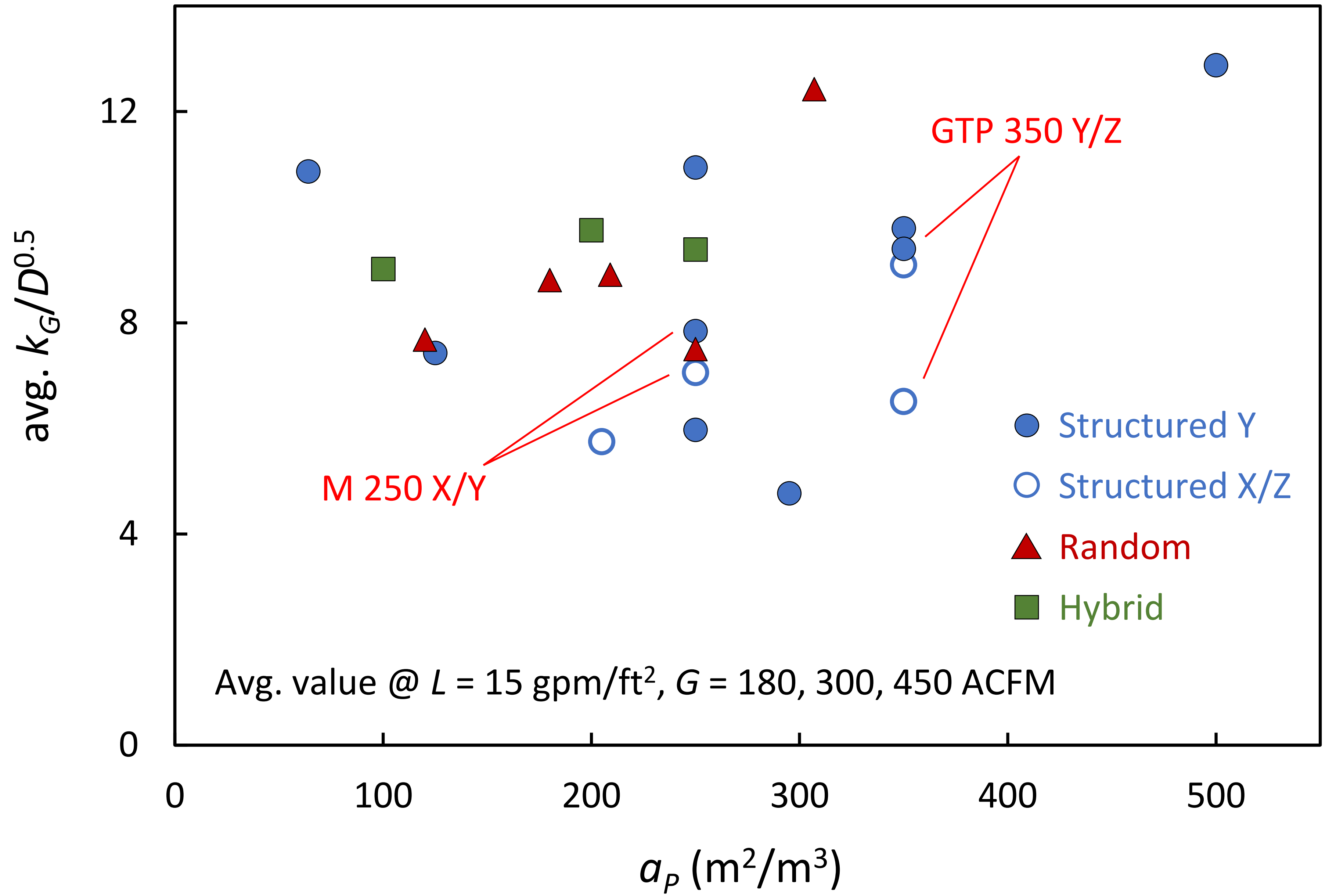
Gas film mass transfer coefficient: k_G



Gas film mass transfer coefficient: k_G



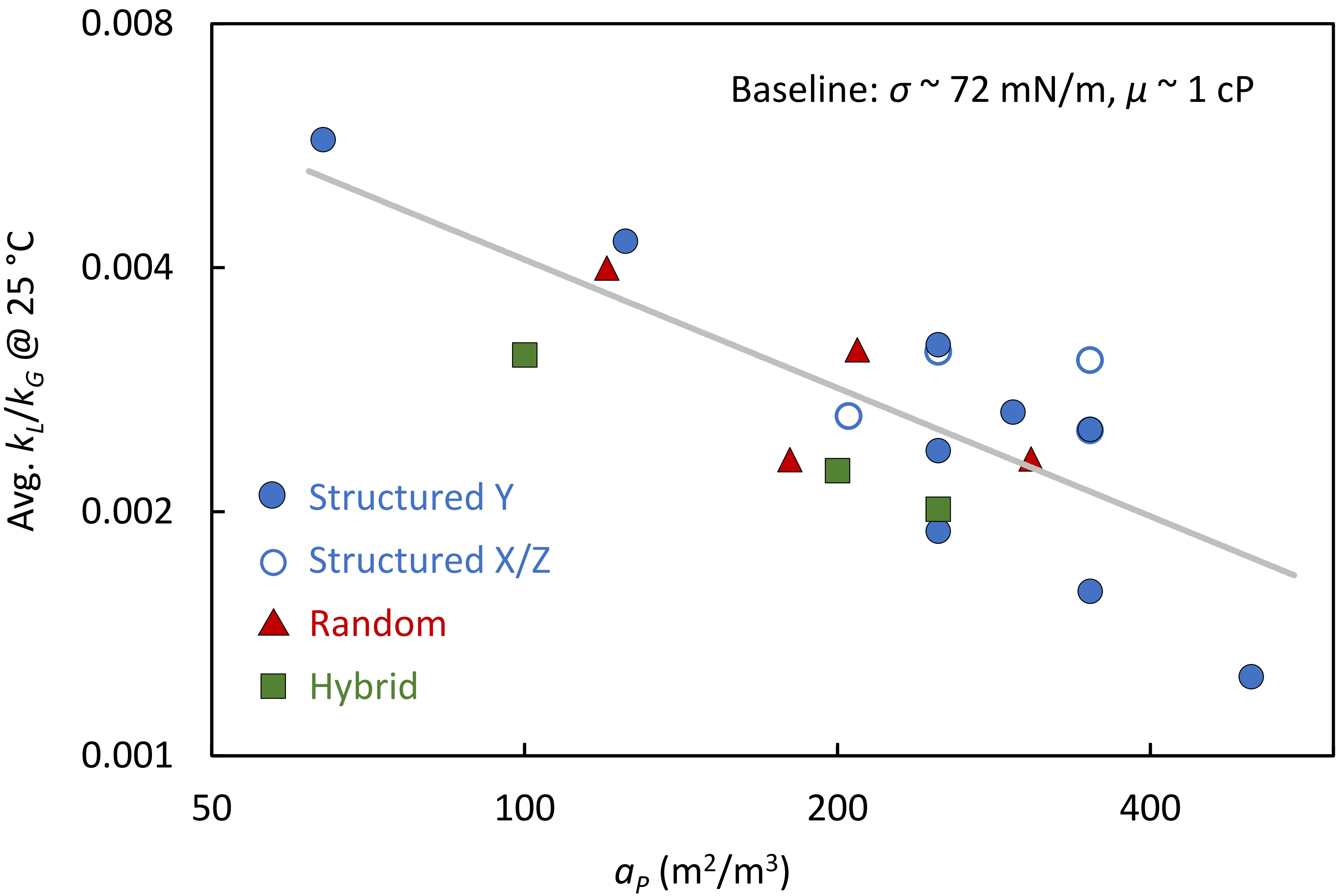
Model of k_G

$$Sh_G = 0.28 \cdot {Sc_G}^{0.5} \cdot {Re_G}^{0.62} \cdot \left(\frac{\sin 2\alpha}{\sin(2 \times 45°)}\right)^{0.65}$$

$$k_G = 0.28 \cdot u_G^{0.62} \cdot \left(\frac{\mu_G}{\rho_G}\right)^{-0.12} \cdot D_G^{0.5} \cdot a_P^{0.38} \cdot (\sin 2\alpha)^{0.65}$$

$\alpha_{effective}$ = 45° (for random/hybrid packings)

Finer packings are more controlled by k_L



Contents

Significance of this work

- Reliable & simple mass transfer models
  - Large database & column size, variance of μ_L
  - No packing-specific parameter
- $$\frac{a_{e,packing}}{a_P} = 1.16 \cdot \eta \cdot \left(We \cdot Fr^{-\frac{1}{2}}\right)^{0.138}$$
- $$Sh_L = 0.12 \cdot Sc_L^{0.5} \cdot Re_L^{0.565} \cdot Ga_L^{1/6} \cdot \left(\frac{Z}{1.8}\right)^{-0.54}$$
- $$Sh_G = 0.28 \cdot Sc_G{}^{0.5} \cdot Re_G{}^{0.62} \cdot (\sin 2\alpha)^{0.65}$$

- Selection of packing
  - a_P, α, material, type
- Selection of solvent
  - $\boldsymbol{\mu_L}$, σ, ρ_L
- Selection of operating condition
  - L, G
- Scale-up of column design
  - Secondary effect, liquid maldistribution

Conclusions

- $k_L \propto \mu_L^{-0.75}$ (-0.4 & -0.35)
- $a_e \neq f(\mu_L)$
- All types of packings have similar behavior in $\Delta\mu_L$
- Z (or L/D) may strongly affect mass transfer

Recommendations

- Avoid finest packings
- Use low μ_L solvent
- Use reliable models (developed in this work)

Thanks!

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