Modeling Mass Transfer Performance of Packings

Di Song

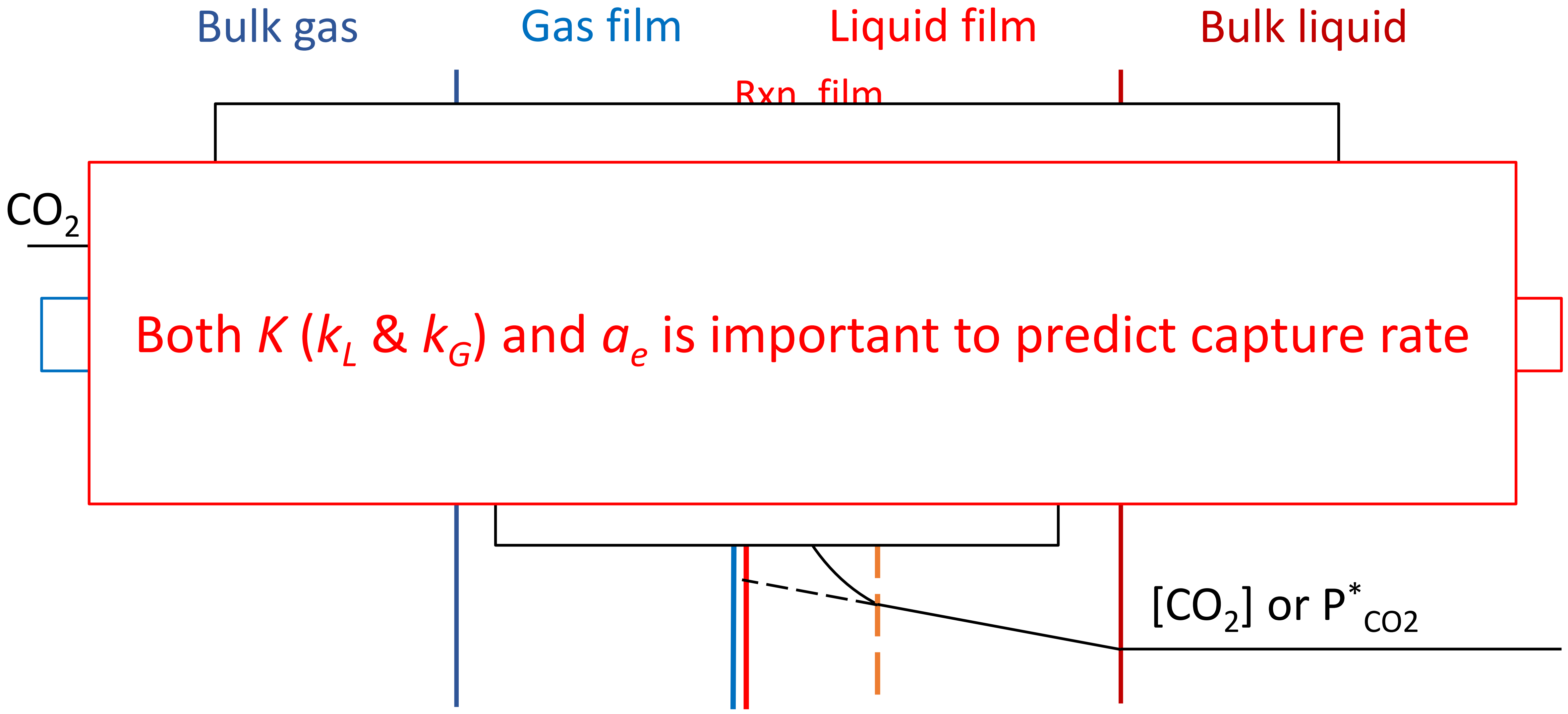
Gary Rochelle & Frank Seibert

University of Texas at Austin

Contents

Introduction

Two-film theory

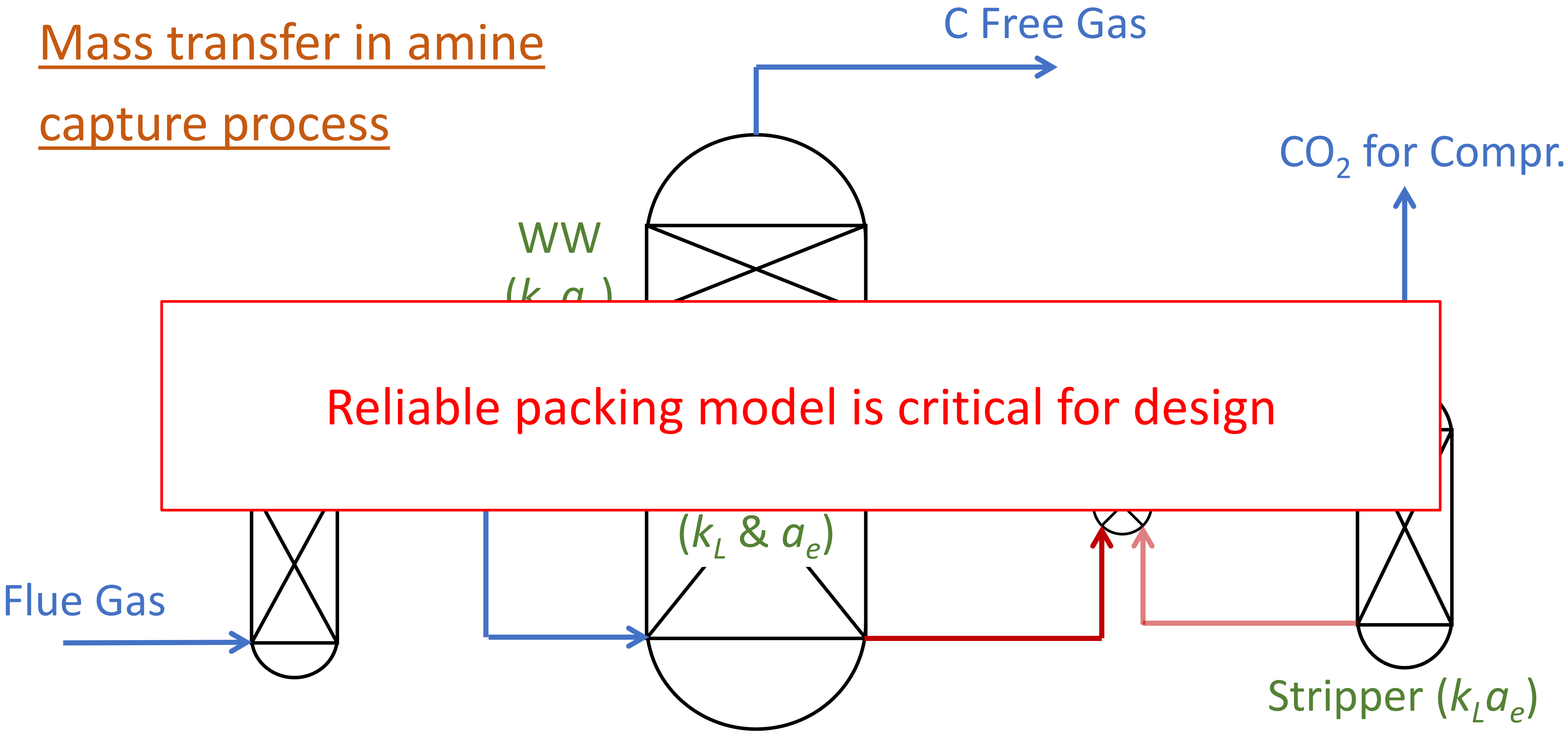


Both K (k_L & k_G) and a_e is important to predict capture rate

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



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?)

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

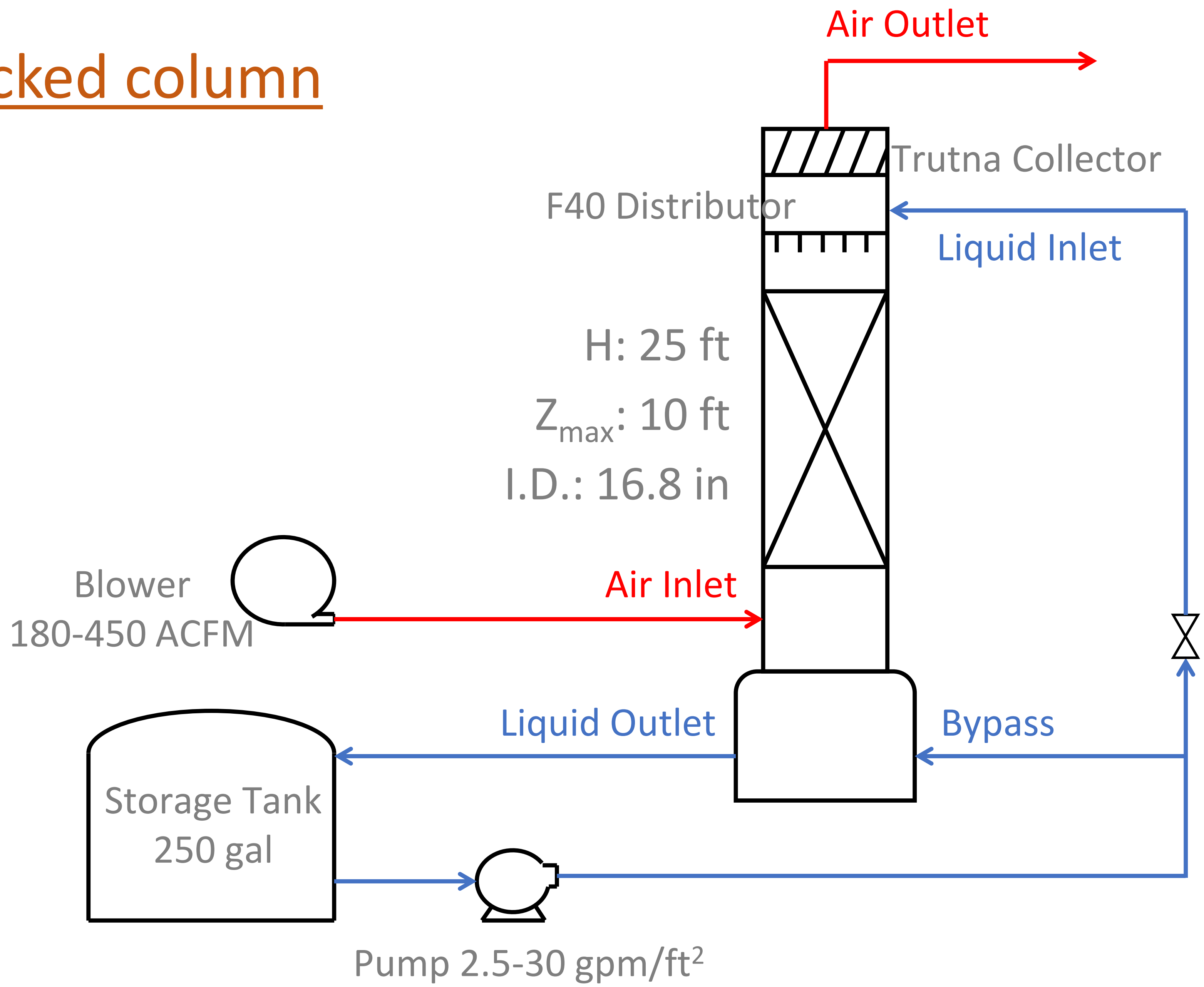
$$D = C_2 \cdot \mu^{\gamma}$$

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

- ❑ 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 + glycerol (1–70 cP)
- a_e: Ambient $CO_2/NaOH/H_2O$ + glycerol

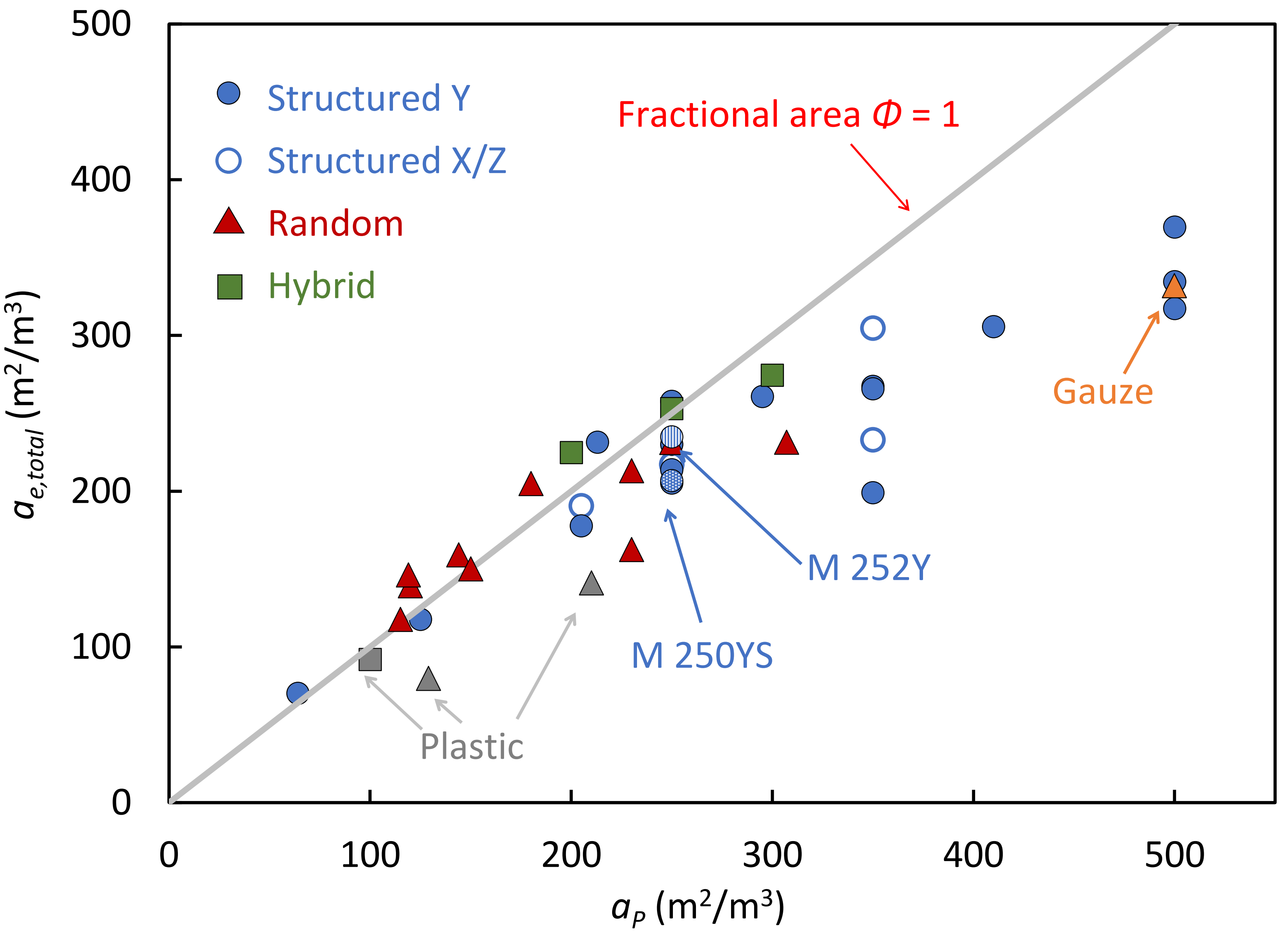
Kinetic model based on WWC exp.

SRP database

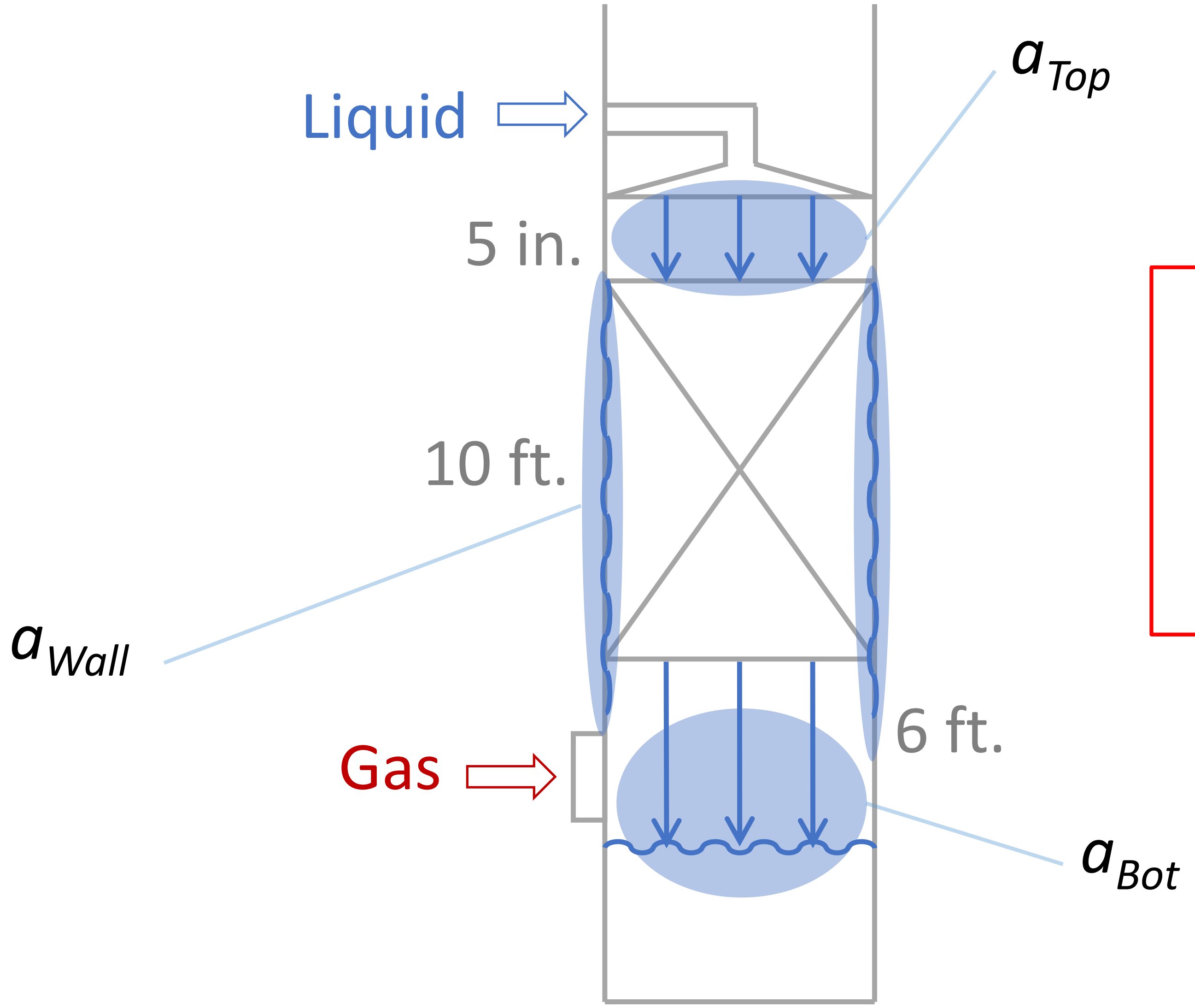
- 21 Structured Packings
  - MellaPak®, Montz-Pak®, GT-Pak®, Flexipac®, etc
- 12 Random Packings
  - Pall Ring, IMTP®, Raschig-SuperRing®, etc
- 4 Hybrid Packings
  - Raschig-SuperPak®, Hiflow Plus®
- 1 Gauze Packing

a_e model

Effective mass transfer area: a_e



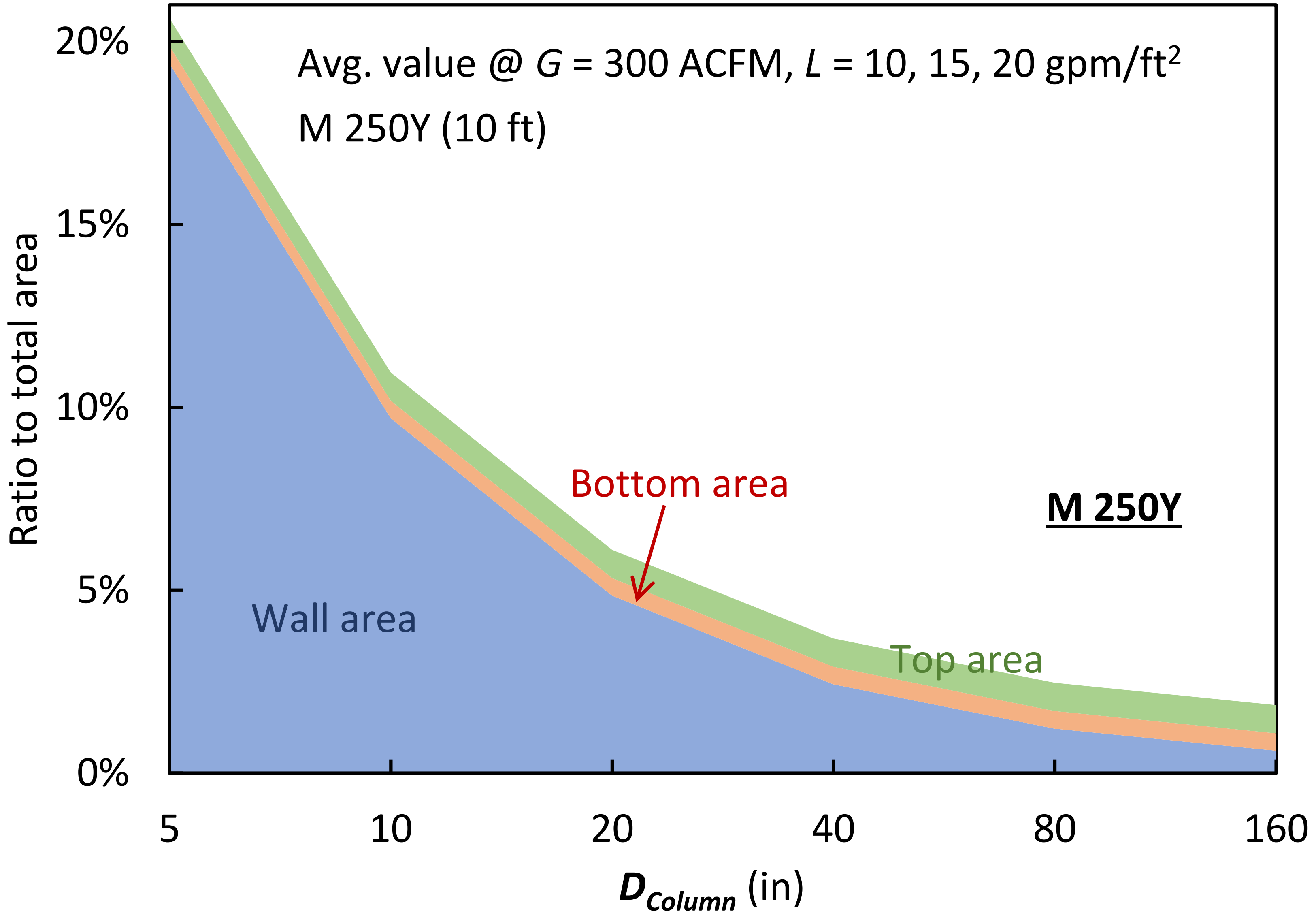
Secondary a_e



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

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

Sec. a_e is critical to scaling up



a_e Model

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

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

Random/hybrid:

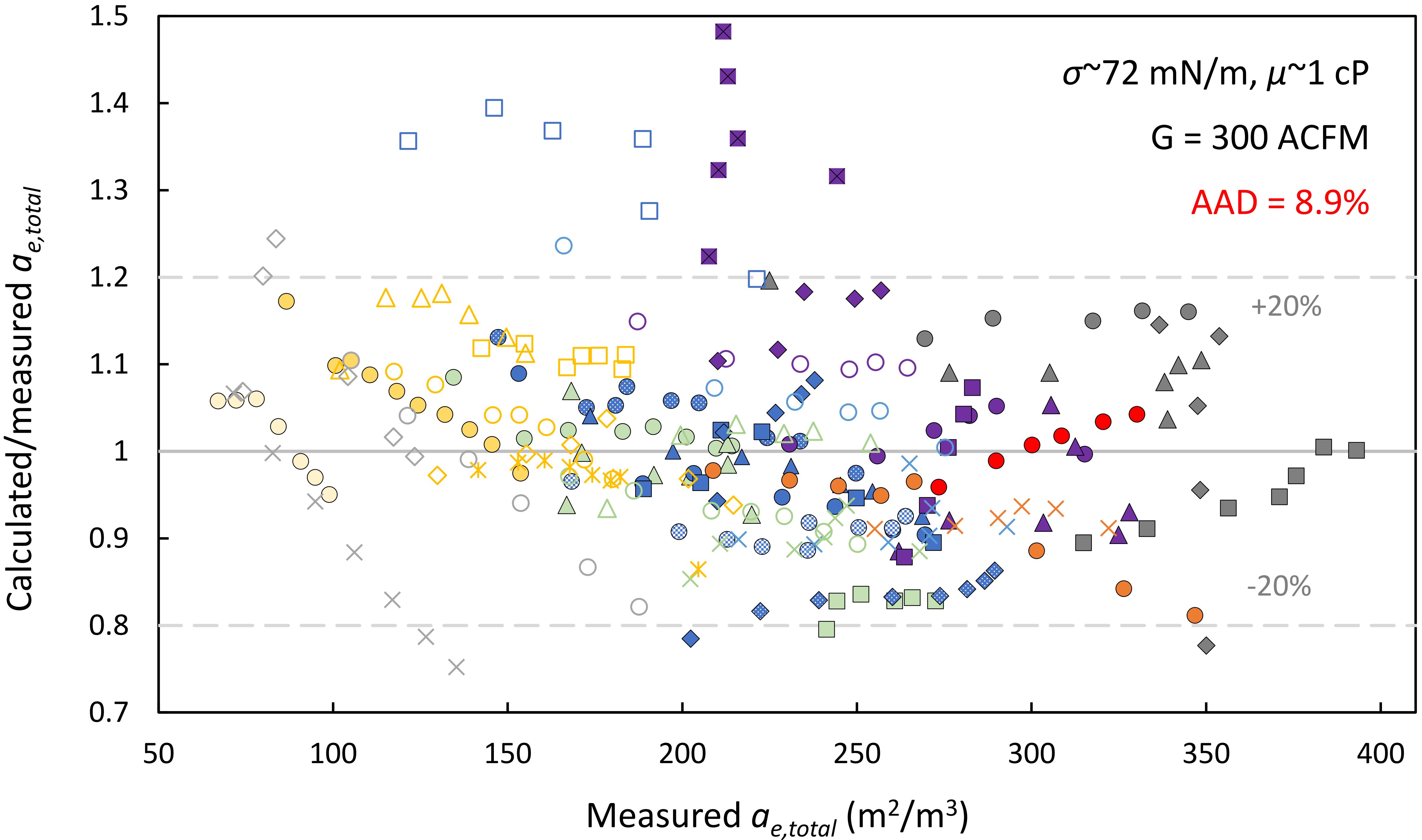
$$\eta_{type} = 1.34 - 0.26\left(\frac{a_P}{250}\right)$$

Plastic:

$\eta_{material}$ = 0.62

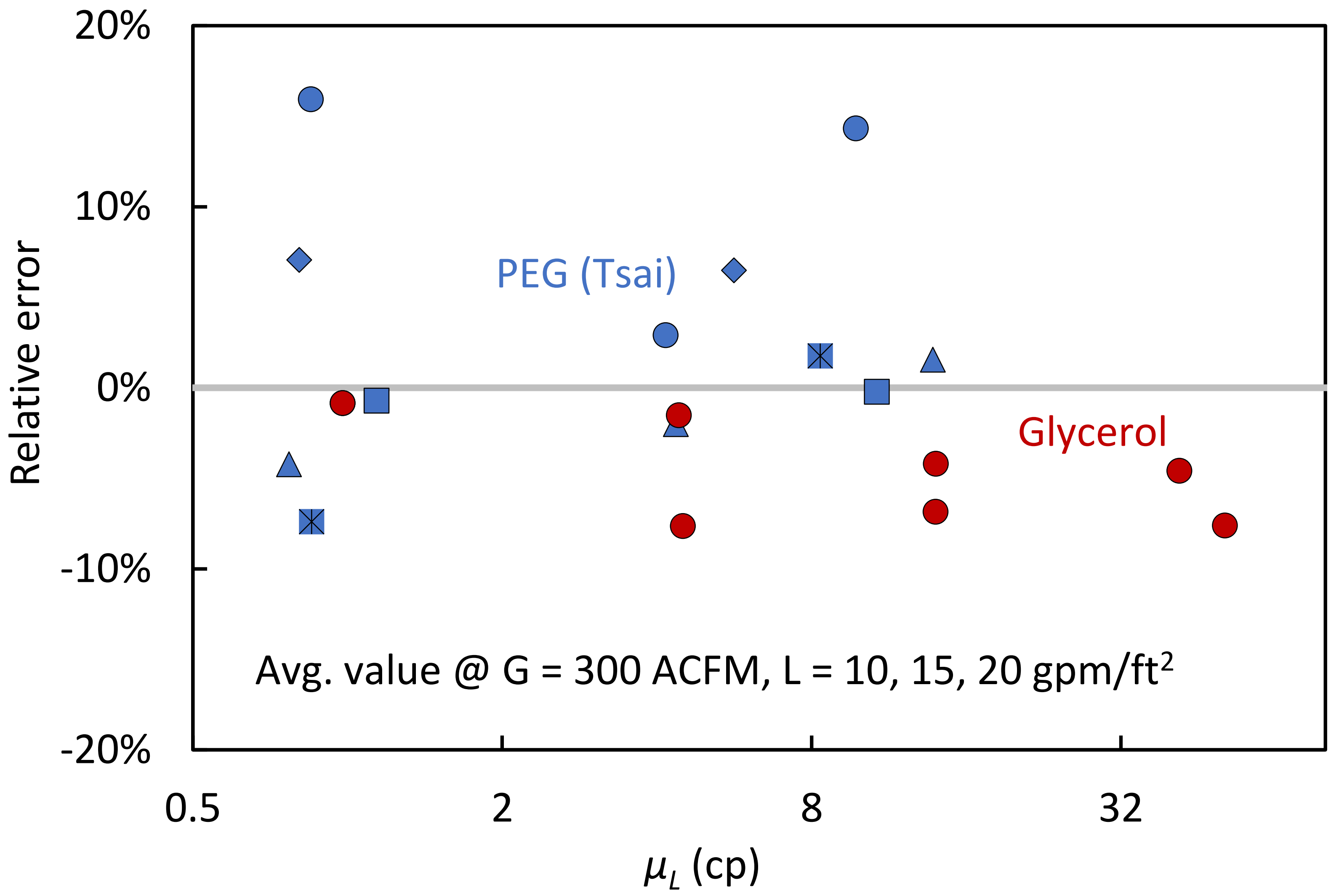
Loading zone (ΔP ≥ 400 Pa/m):

$\eta_{loading}$ = 1.15



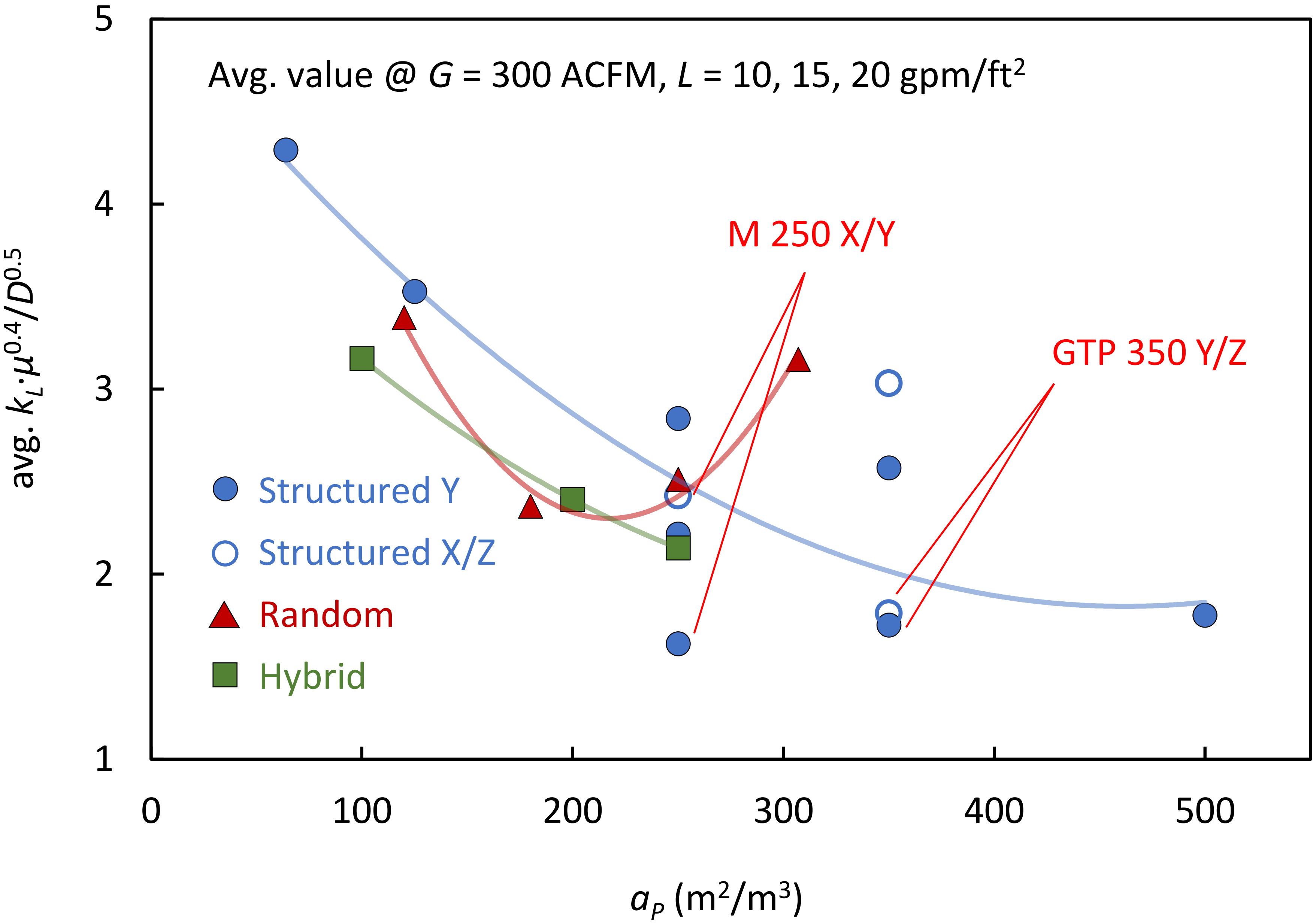
σ~72 mN/m, μ~1 cP
G = 300 ACFM
AAD = 8.9%
+20%
-20%
Calculated/measured $a_{e,total}$
Measured $a_{e,total}$ (m^2/m^3)
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
50
100
150
200
250
300
350
400

a_e model w/ viscosity

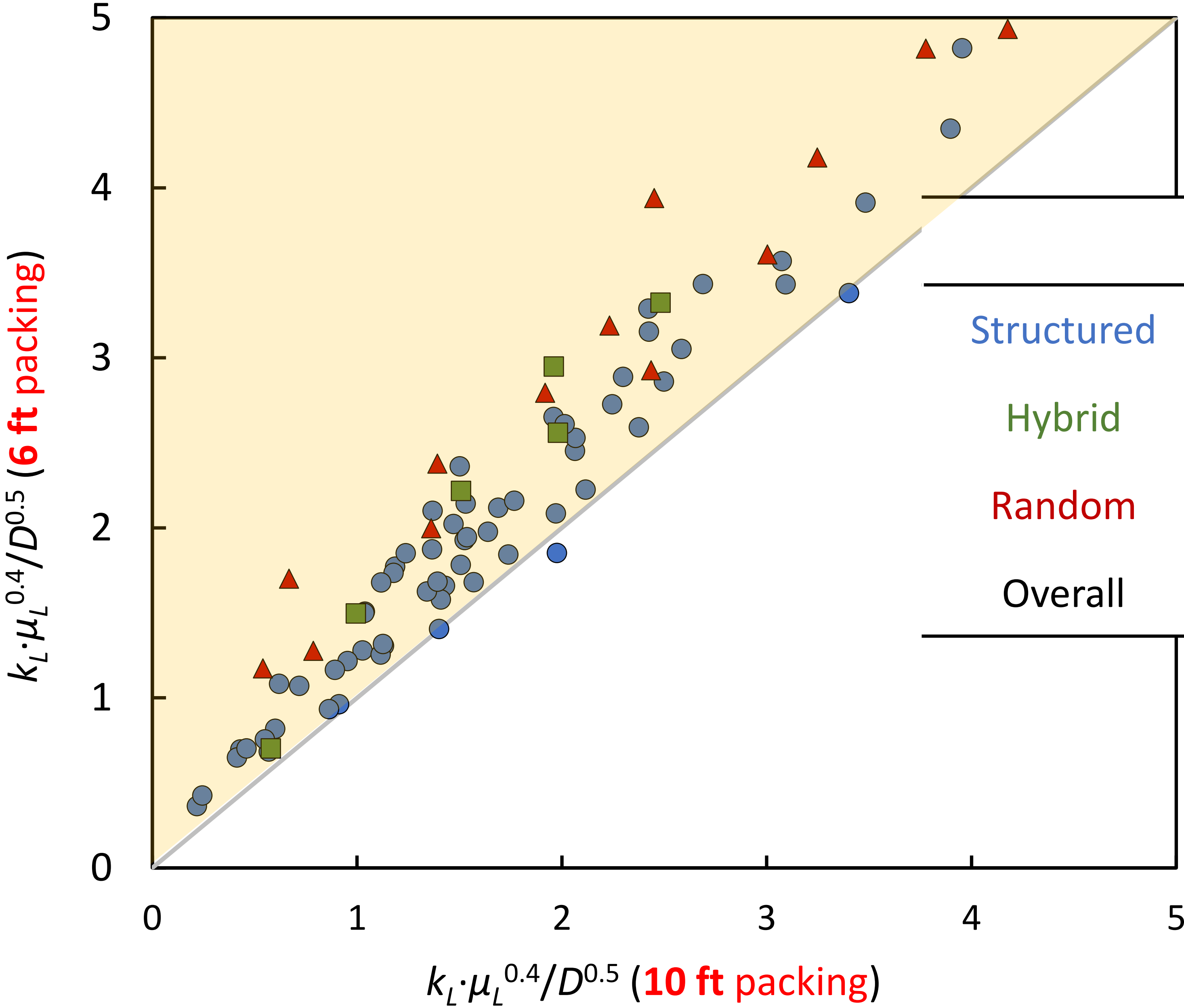


k_L model

Liquid film mass transfer coefficient: k_L



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

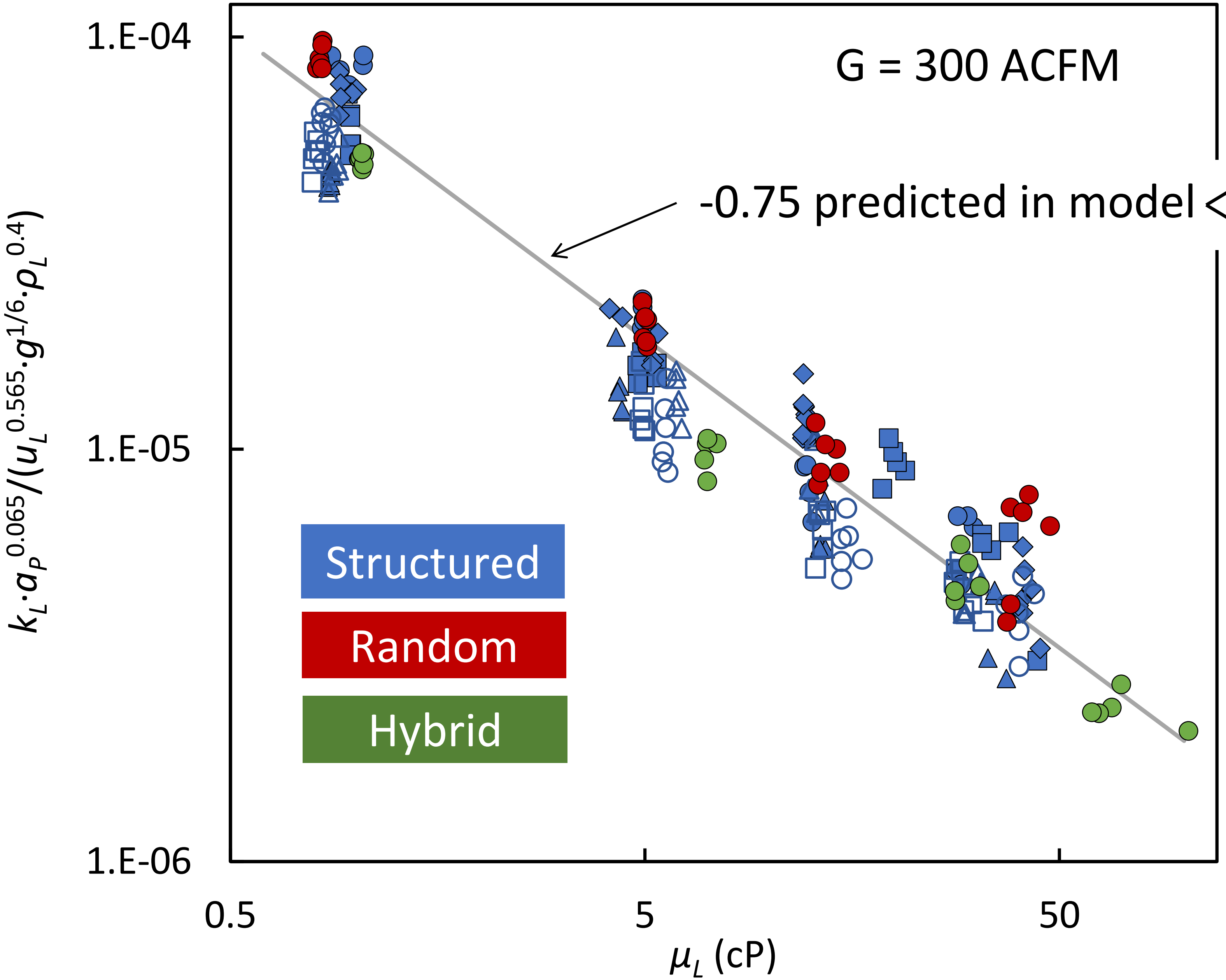
Correction = $\frac{\ln(1.32/1)}{\ln(6/10)} = -0.54$

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



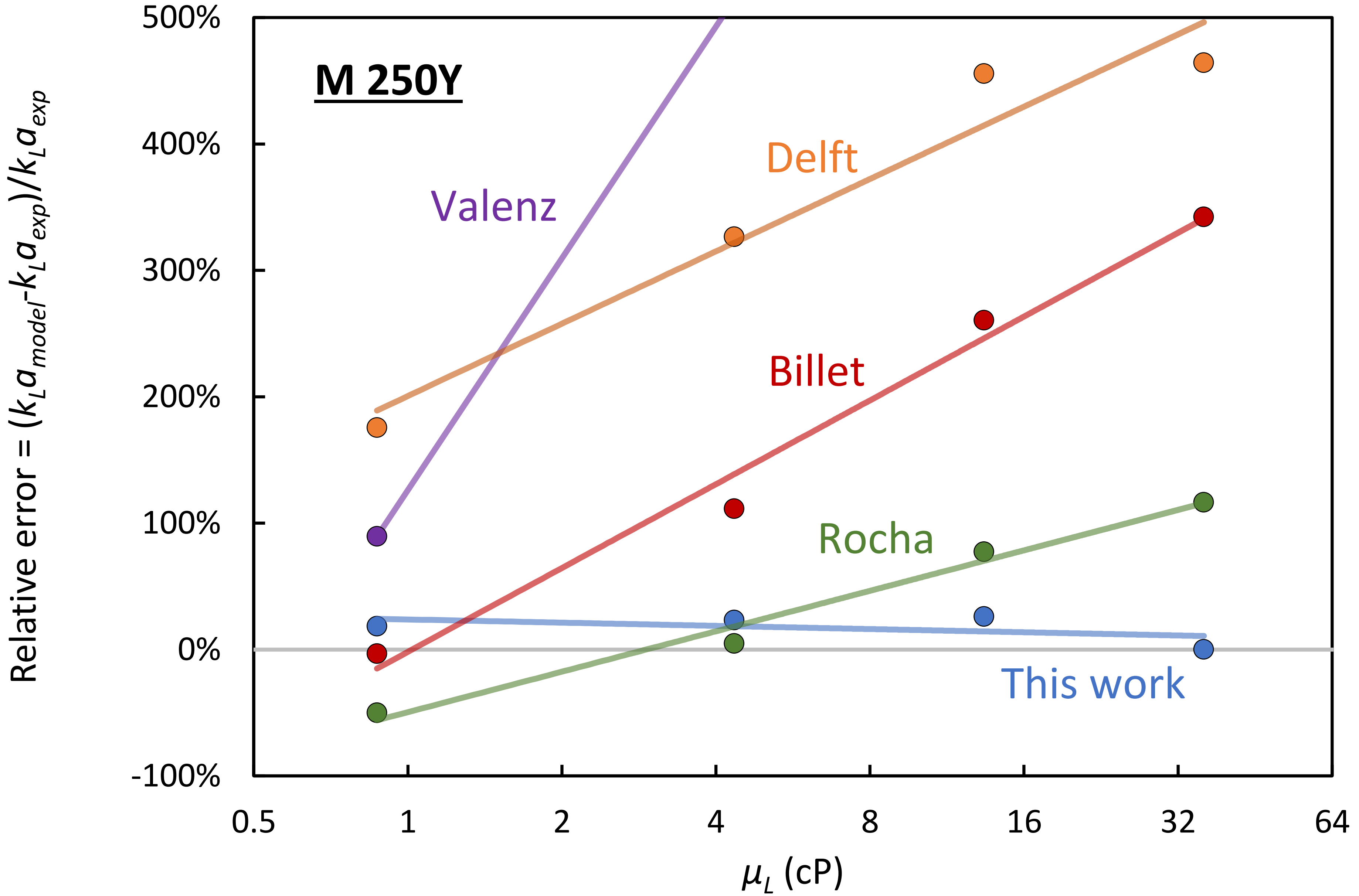
Universally applicable

Direct = -0.40

Indirect = -0.35

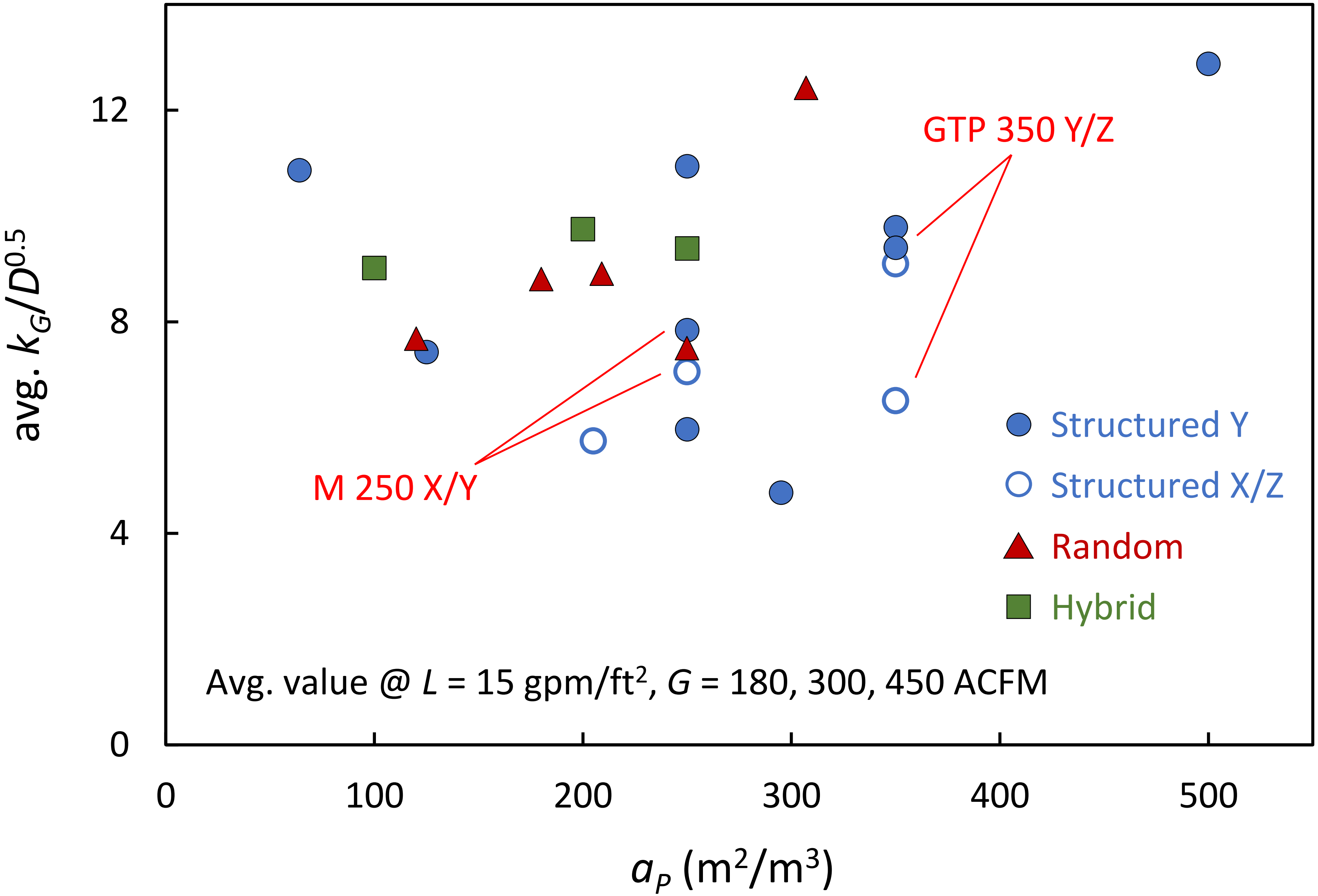
System-specific based on *D*-*μ* relationship

Comparison to other work: μ_L



k_G model

Gas film mass transfer coefficient: k_G



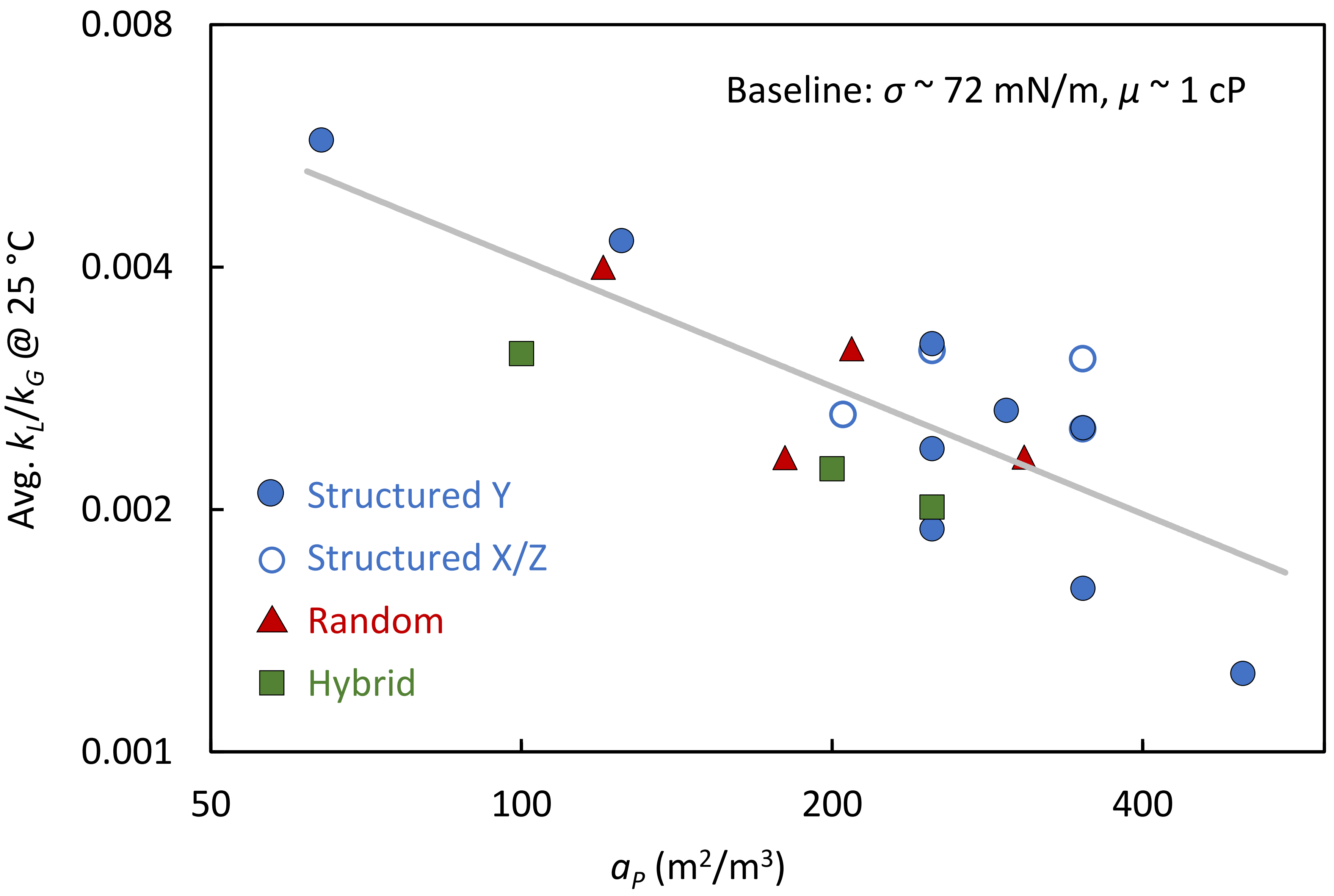
Model of k_G

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

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

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

Finer packings are more controlled by k_L



Conclusions

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
  - μ_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!

University of Texas at Austin

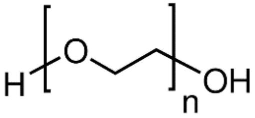
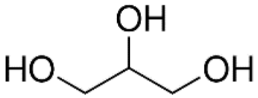
Di Song (Graduating 10/2017)

dsong@utexas.edu

512-750-1480

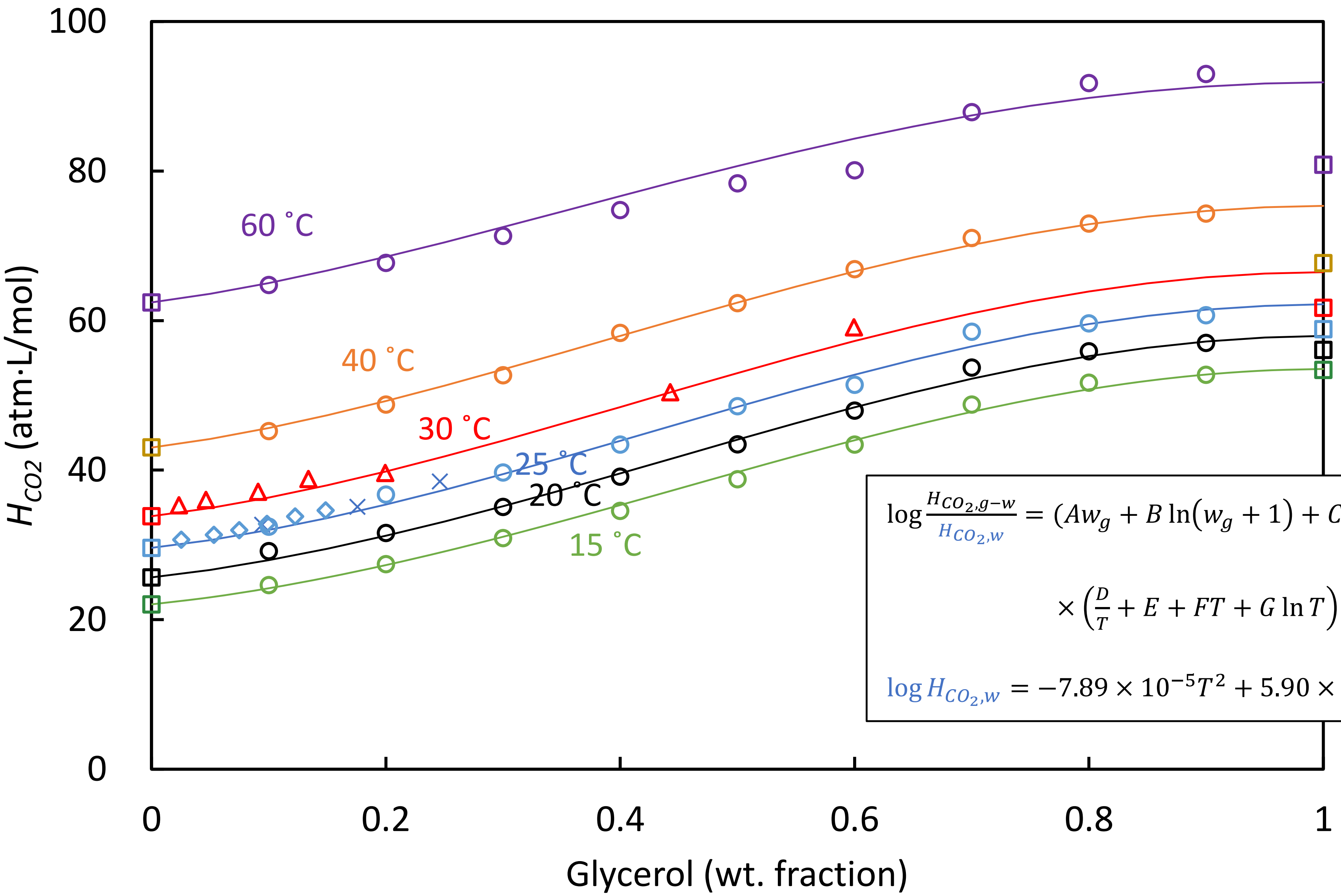
Back-up slides

Why glycerol?

	Structure	M_w	wt % to 100 cP (20 ˚C)	Tested ?	Dissolve in H_2O	Newtonian ?	Affect *D*?	Affect kinetics?	Hazardous?
PEG		0.4 M	2.2	Yes	Hard	No	No	No	No
Glycerol		92.1	88	No	Easy	Yes	Yes	Yes	No

Blue – preferable; Red – undesirable

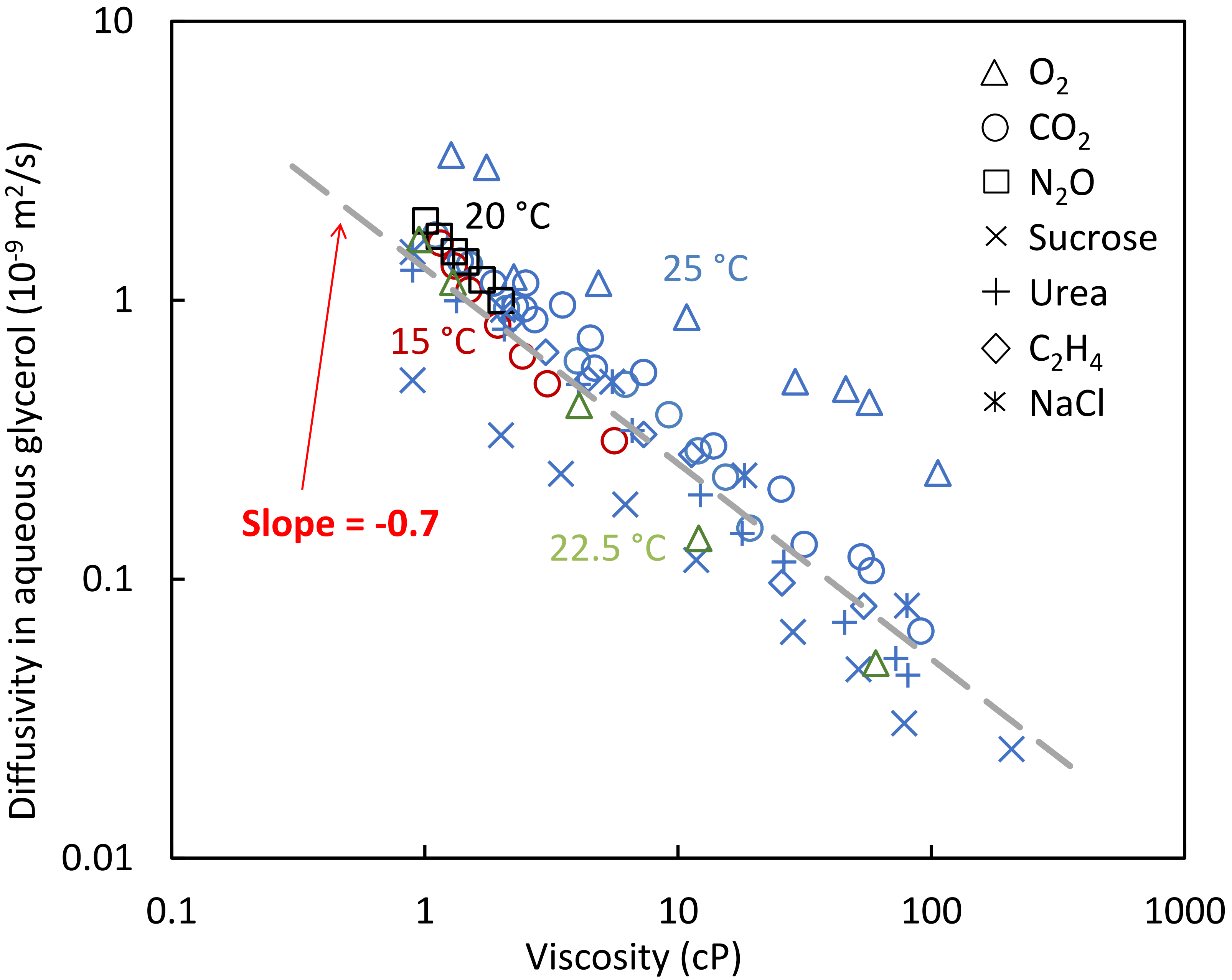
Henry constant of CO_2



$$\log \frac{H_{CO_2,g-w}}{H_{CO_2,w}} = \left(Aw_g + B\ln(w_g+1) + C\ln^2(w_g+1)\right) \times \left(\frac{D}{T} + E + FT + G\ln T\right)$$

$$\log H_{CO_2,w} = -7.89\times10^{-5}T^2 + 5.90\times10^{-2}T - 9.12$$

Diffusivity in aqueous glycerol



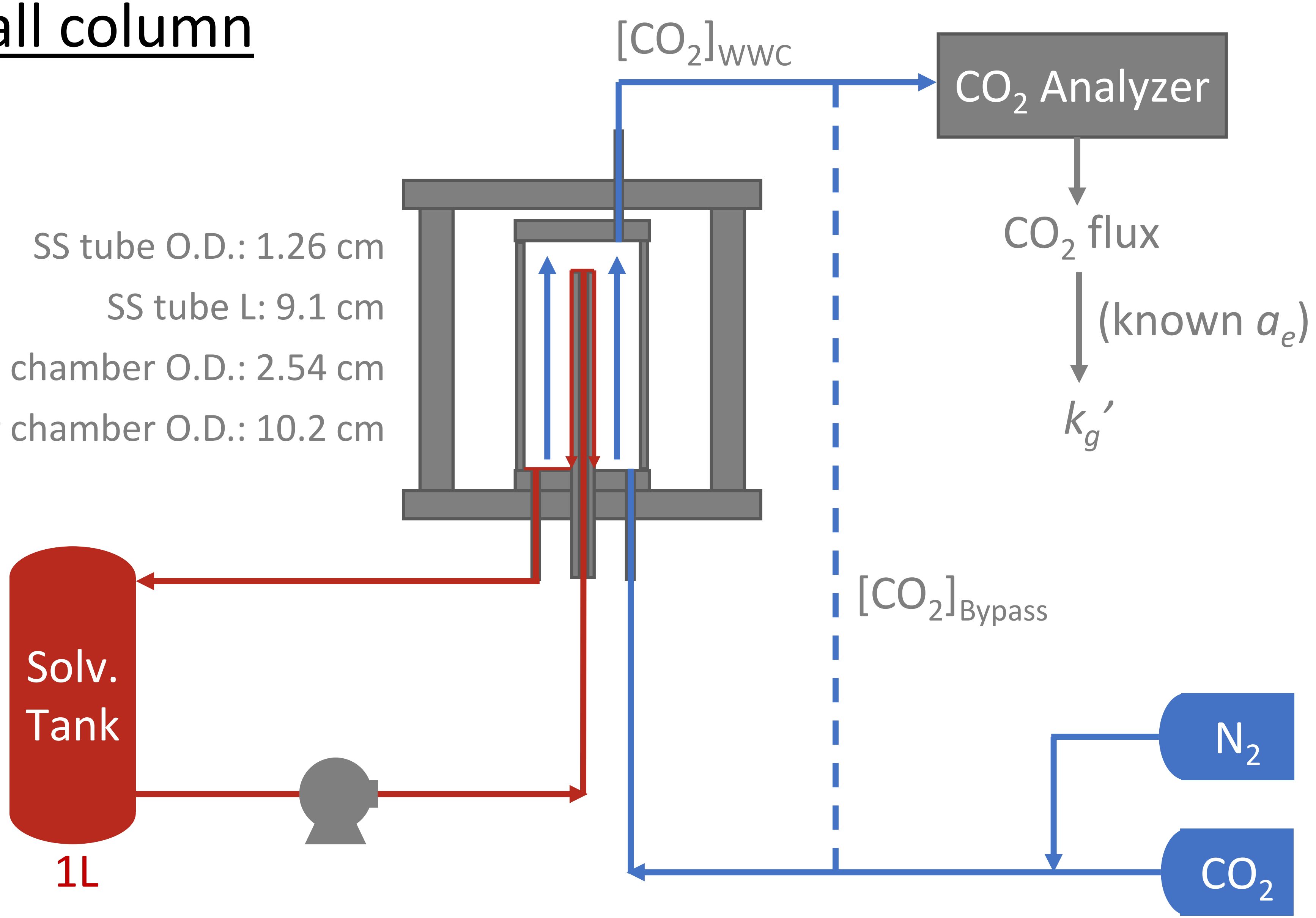
Wetted-wall column

SS tube O.D.: 1.26 cm

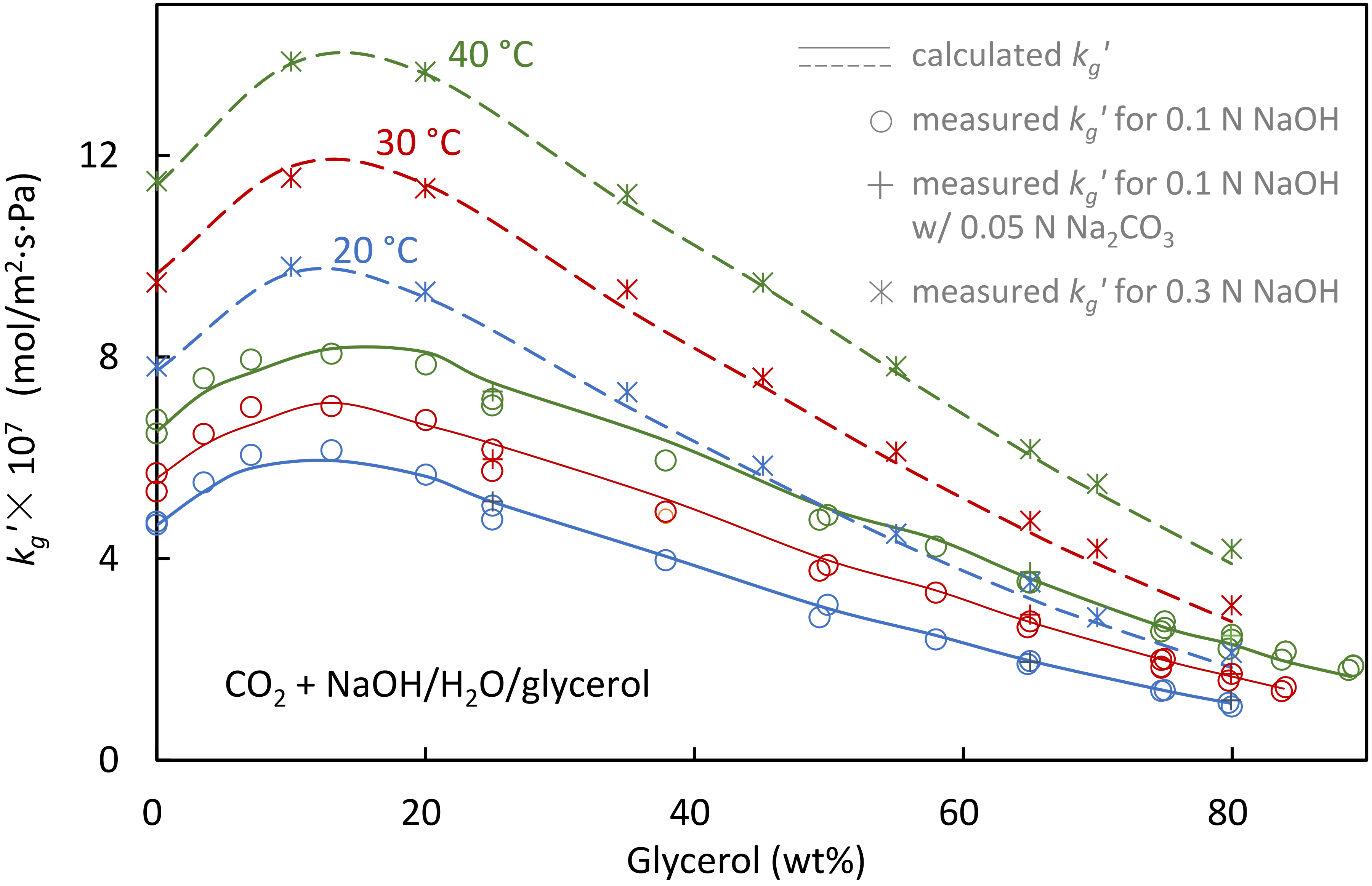
SS tube L: 9.1 cm

Rxn chamber O.D.: 2.54 cm

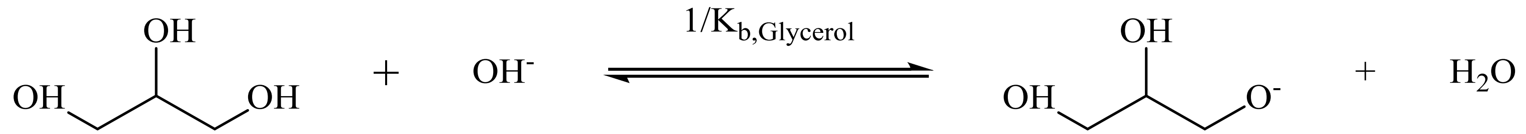
Outer chamber O.D.: 10.2 cm

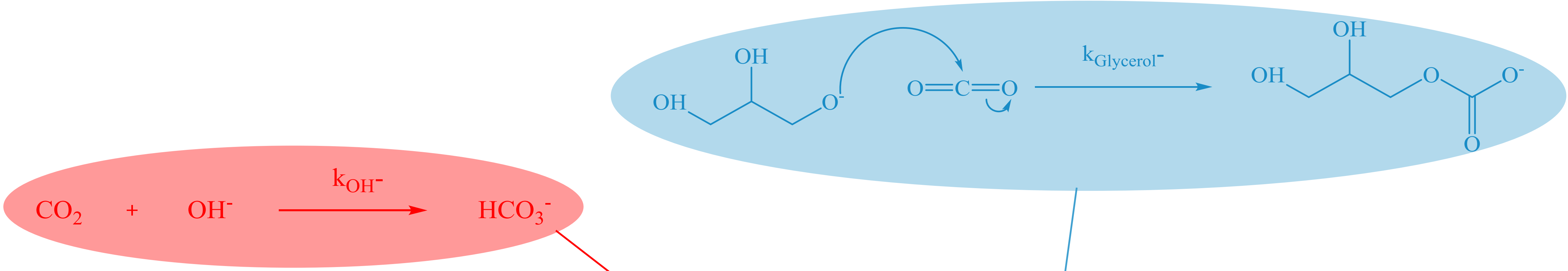


Non-monotonic trend of k_g'



Equilibrium and Rxns for CO_2/NaOH/H_2O-Glycerol

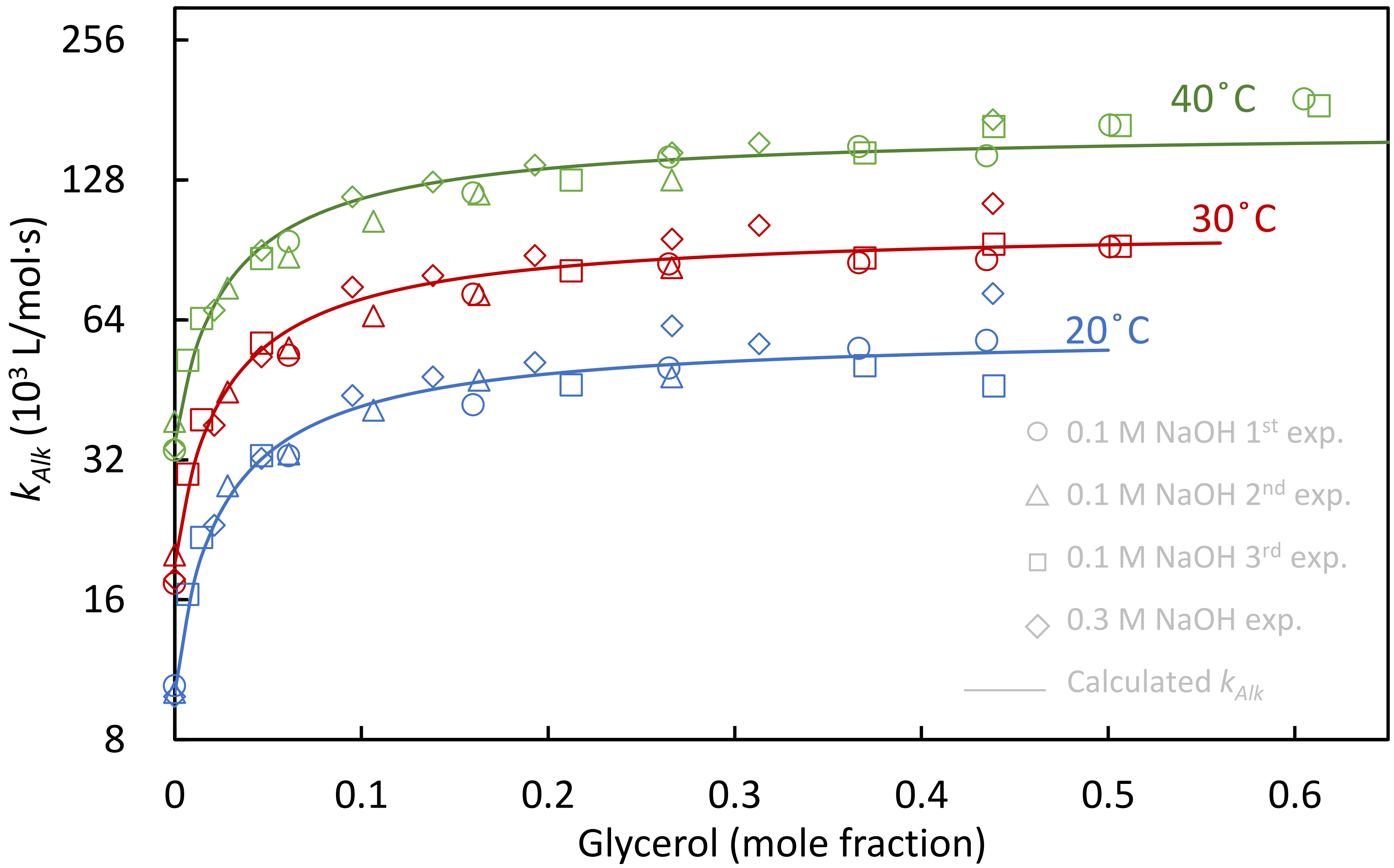




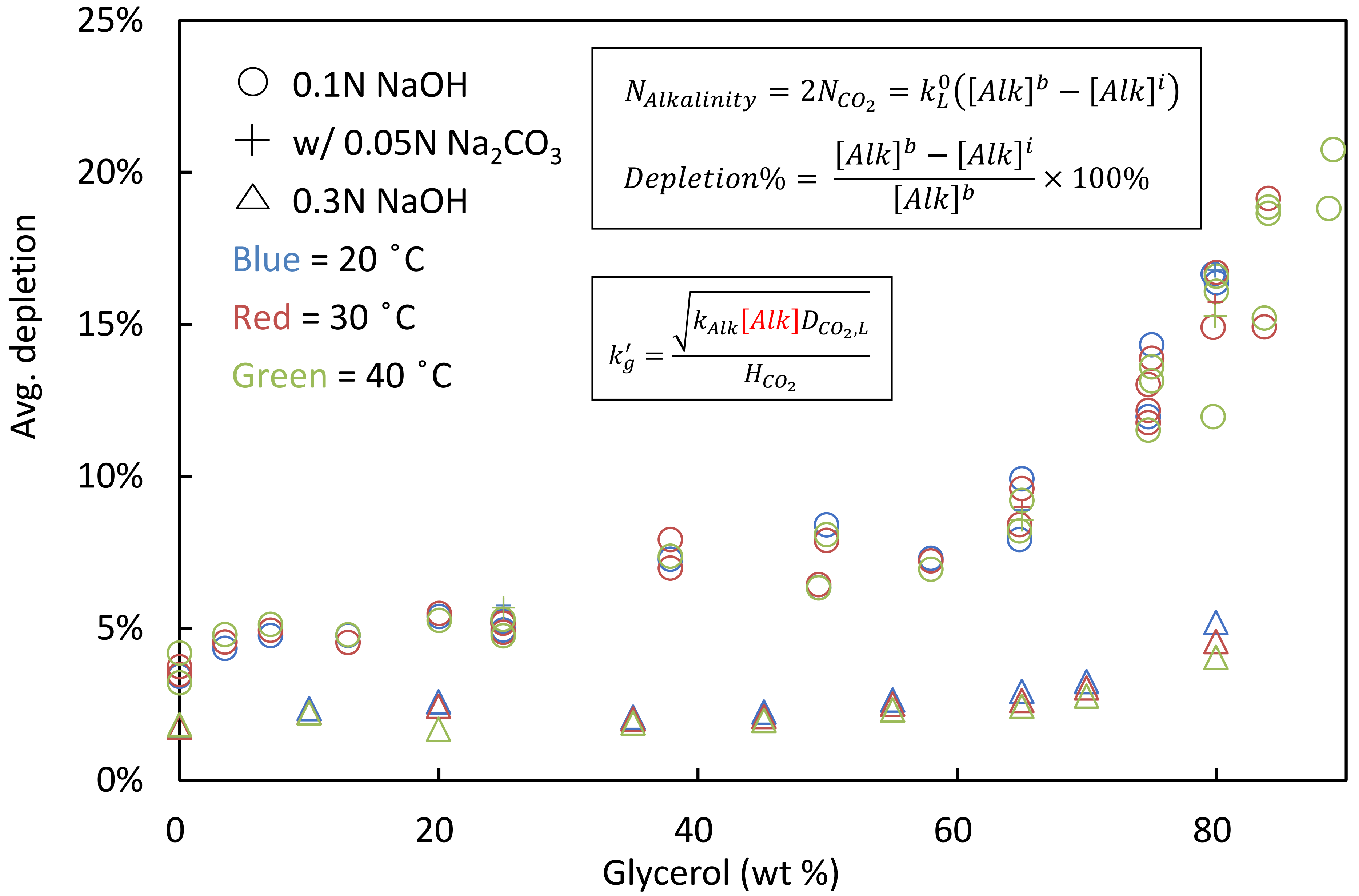
$$k_{Alk} = k_{OH^-}\left(\frac{[OH^-]}{[Alk]}\right) + k_{Glycerol^-}\left(\frac{[Glycerol^-]}{[Alk]}\right)$$

$$k_g' = \frac{\sqrt{k_{Alk}[Alk]D_{CO_2,L}}}{H_{CO_2}}$$

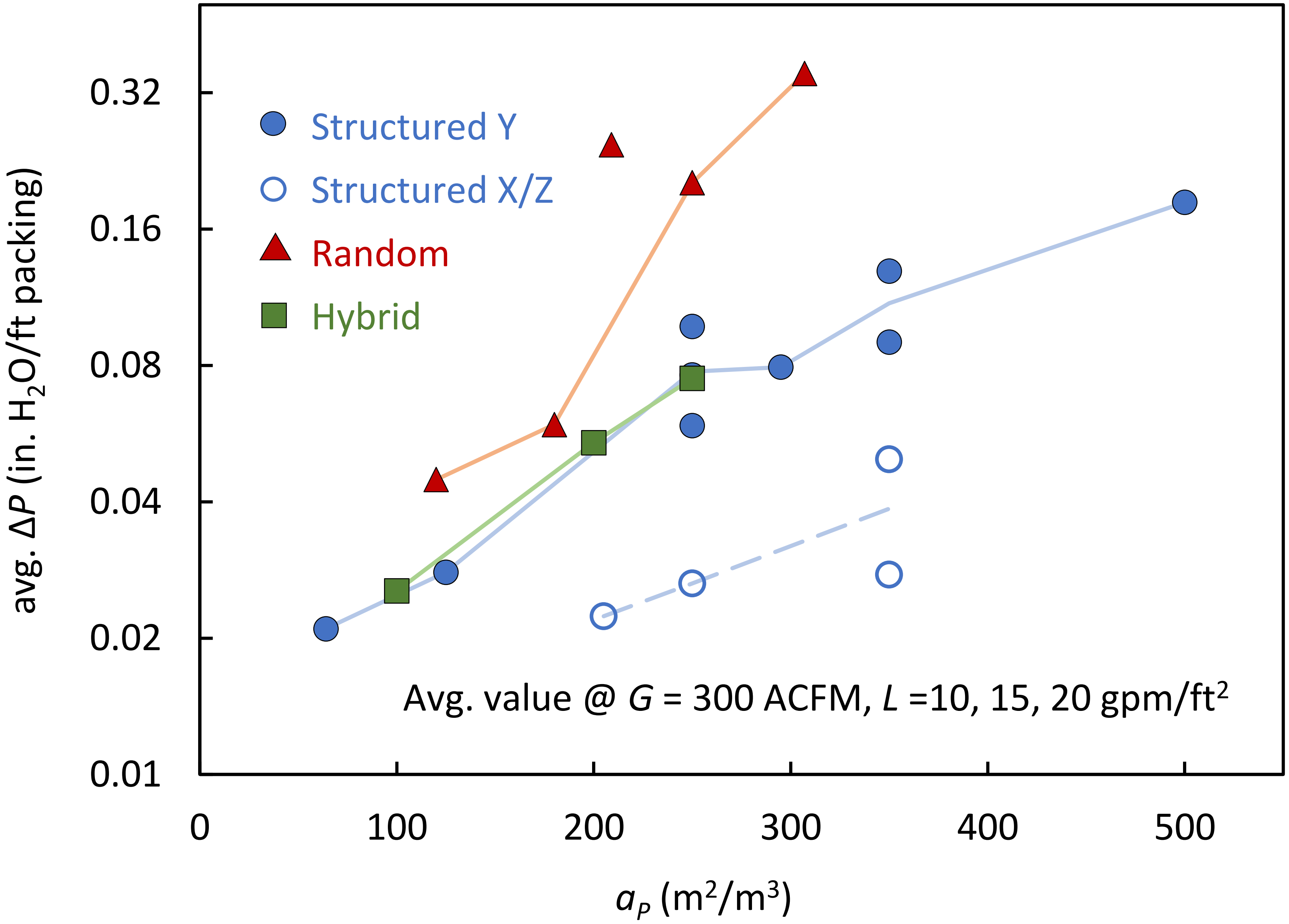
Measured and calculated k_{Alk}



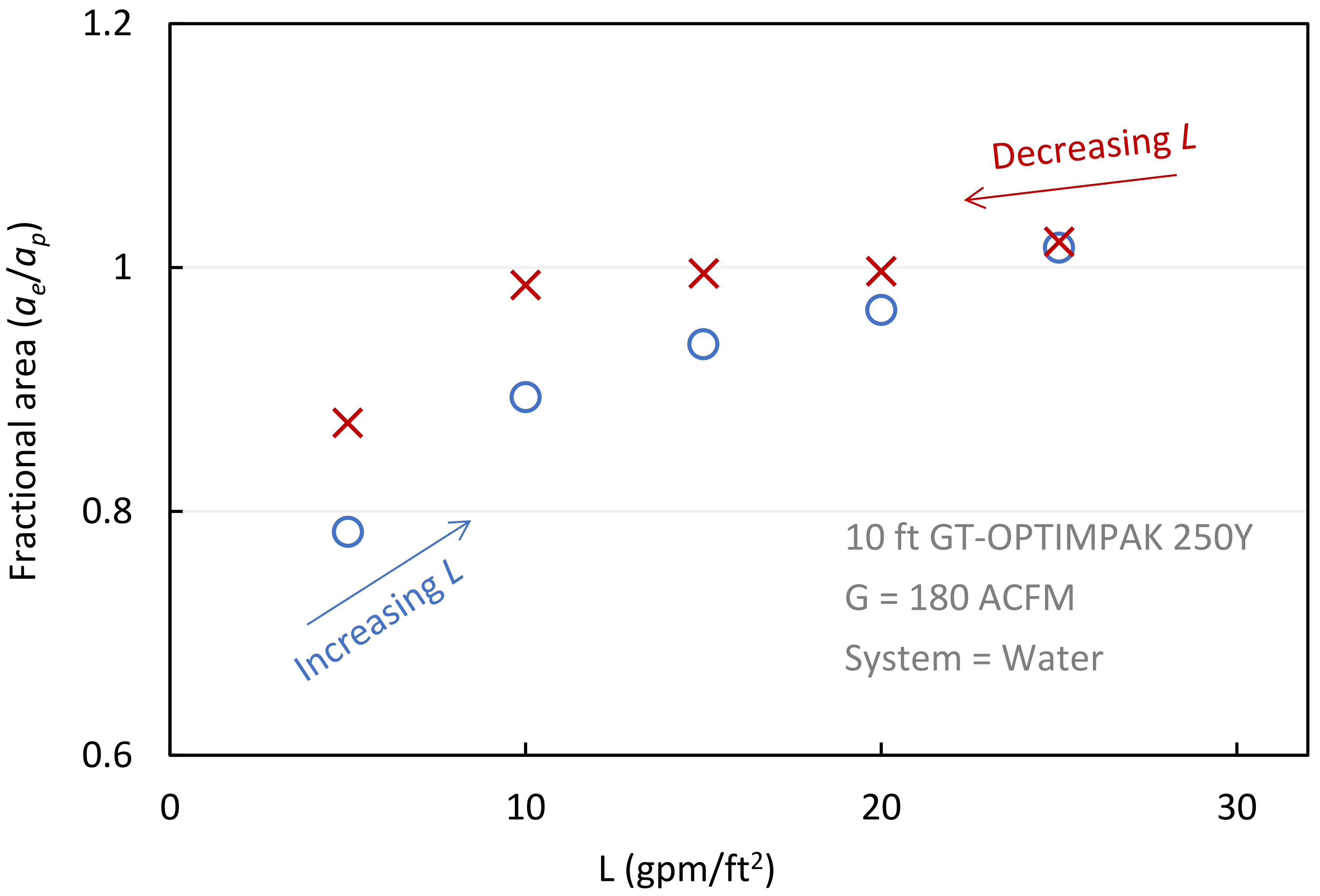
Surface depletion of alkalinity for WWC runs



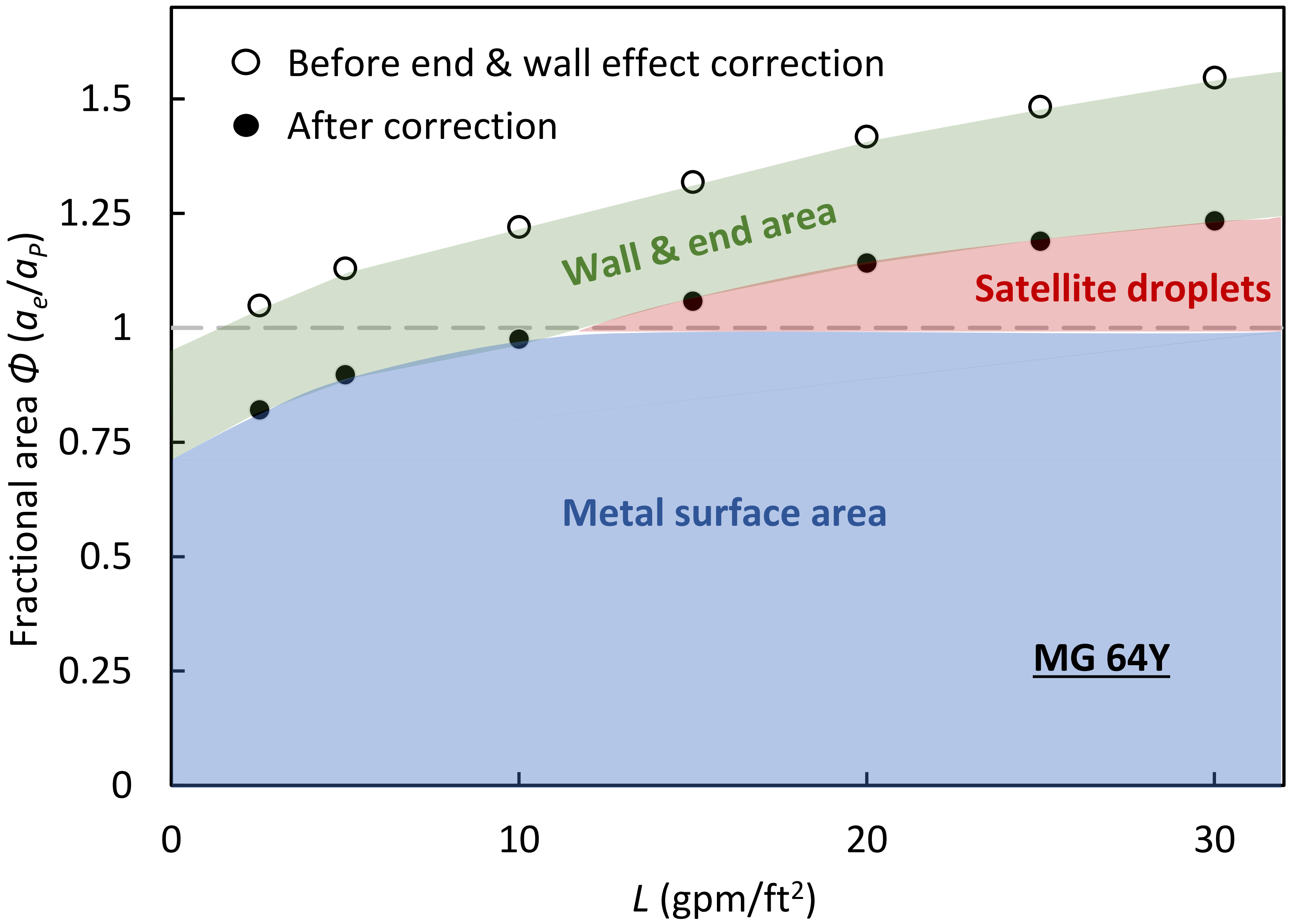
Pressure drop



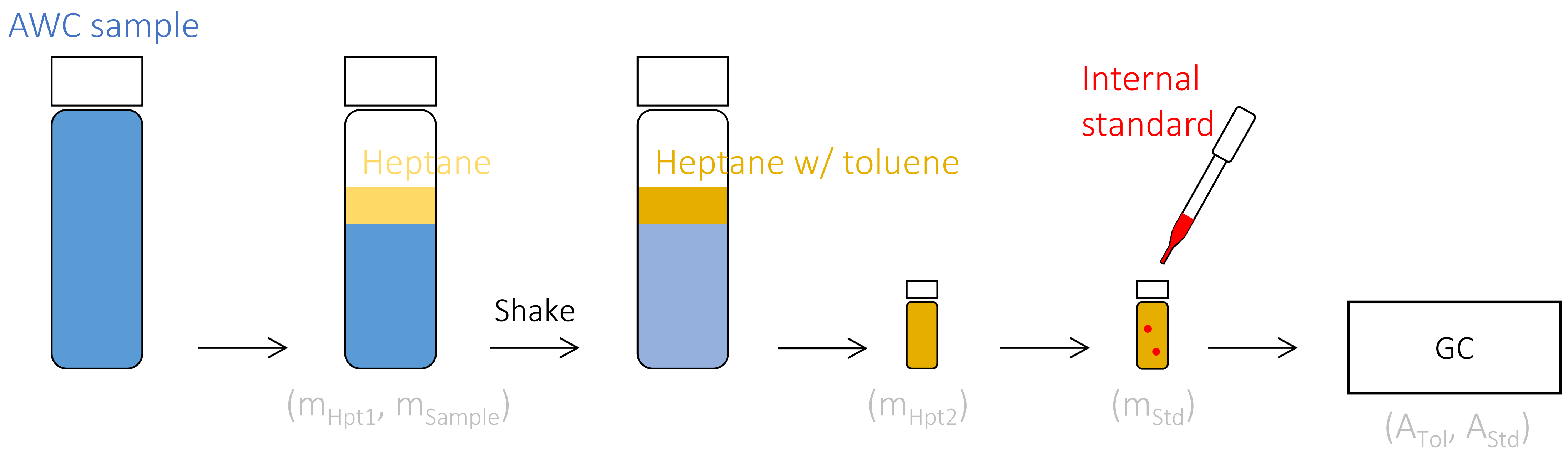
Effect of flow rate sequence on a_e



Different a_e regimes



GC sampling technique

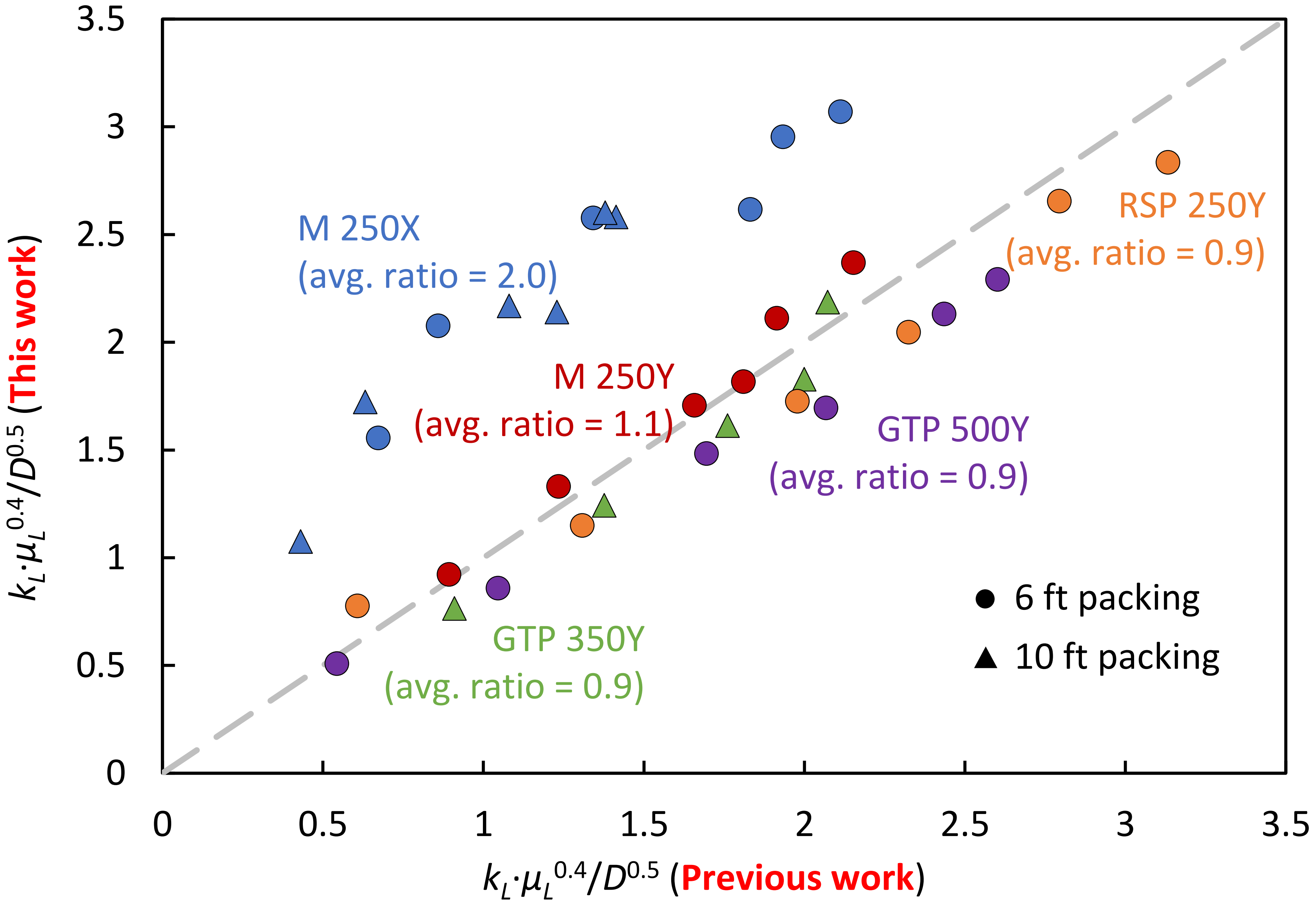


$$\frac{w_{Tol,GC}}{w_{Std,GC}} = \frac{R_{Tol} \times A_{Tol}}{R_{Std} \times A_{Std}}$$

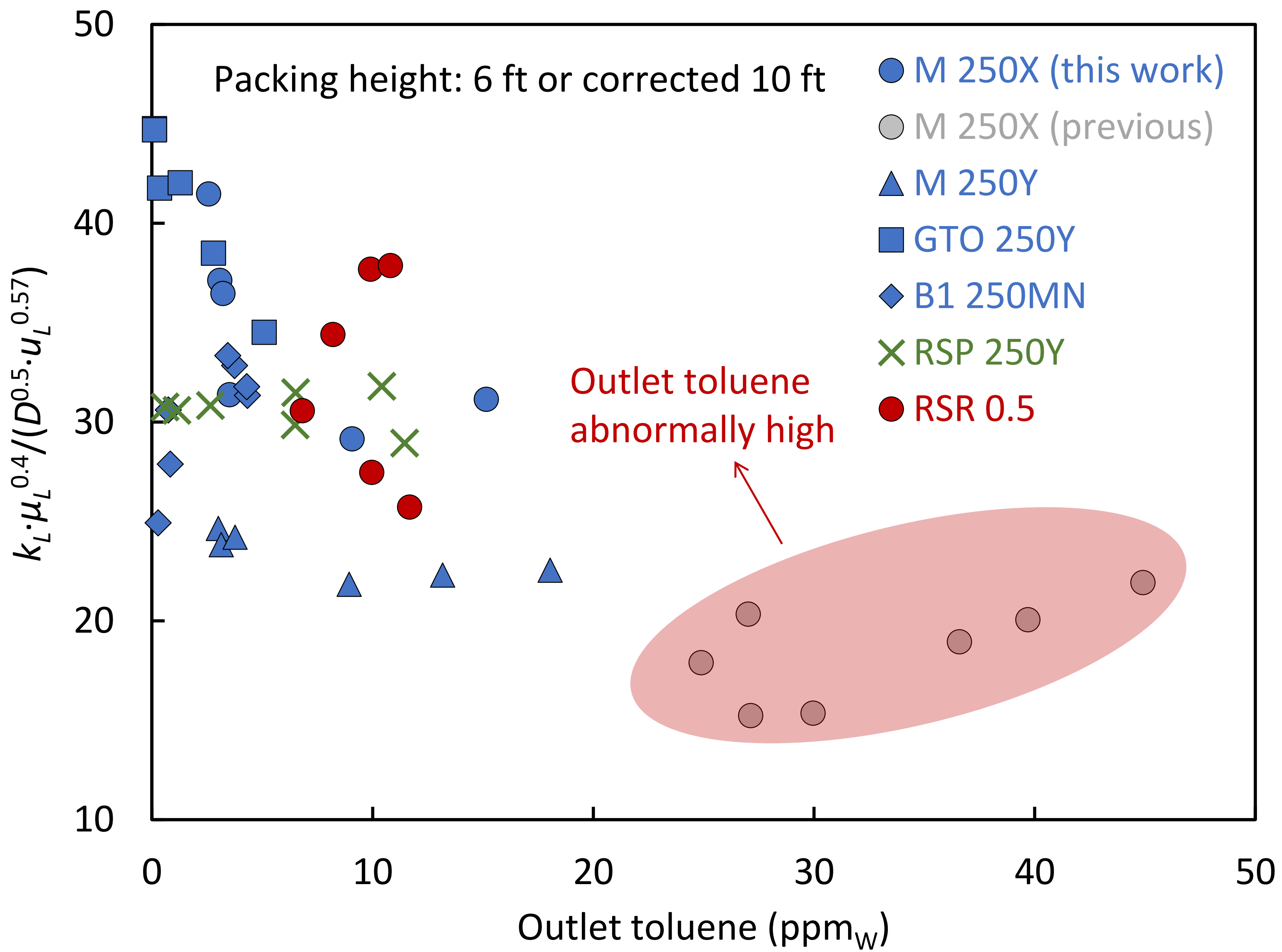
$$w_{Std,GC} = \frac{m_{Std}}{m_{Hpt2} + m_{Std}}$$

$$w_{Tol,Sample} = \frac{w_{Tol,GC} \times m_{Hpt1}}{m_{Sample}}$$

k_L reproducibility is good



Outlier: M 250X



"Big rivulet" assumption

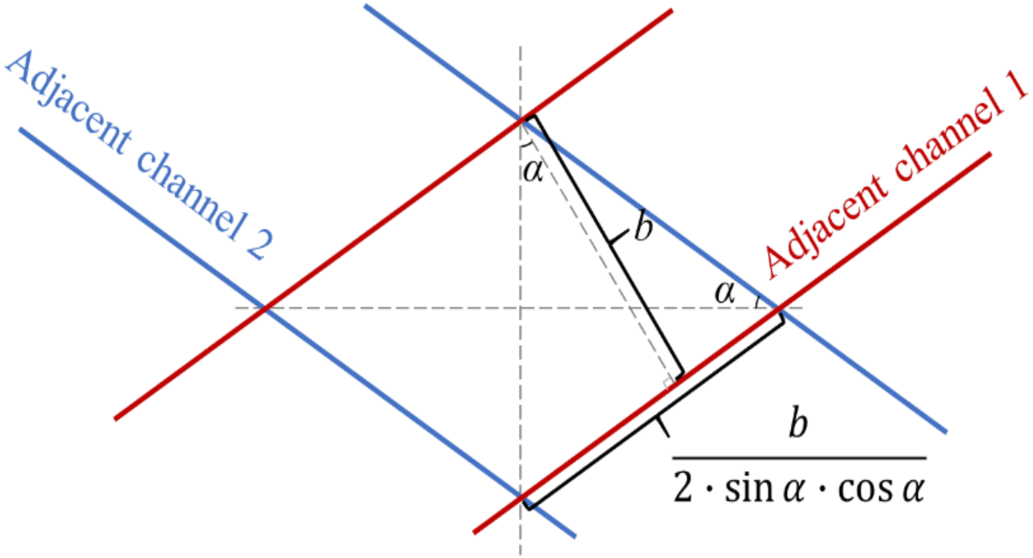
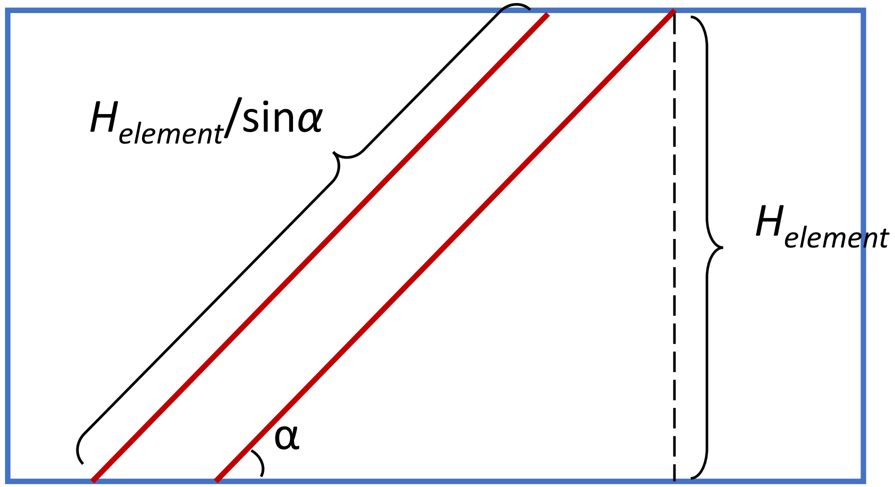
Flow regimes	Thin, spread film	Thick, big rivulets
Contribute to a_e ?	Yes	Yes
Contribute to k_L ?	**No**	Yes
f (a_P)	Increase w/ a_P	Decrease w/ a_P

Measured area > a_e for k_L

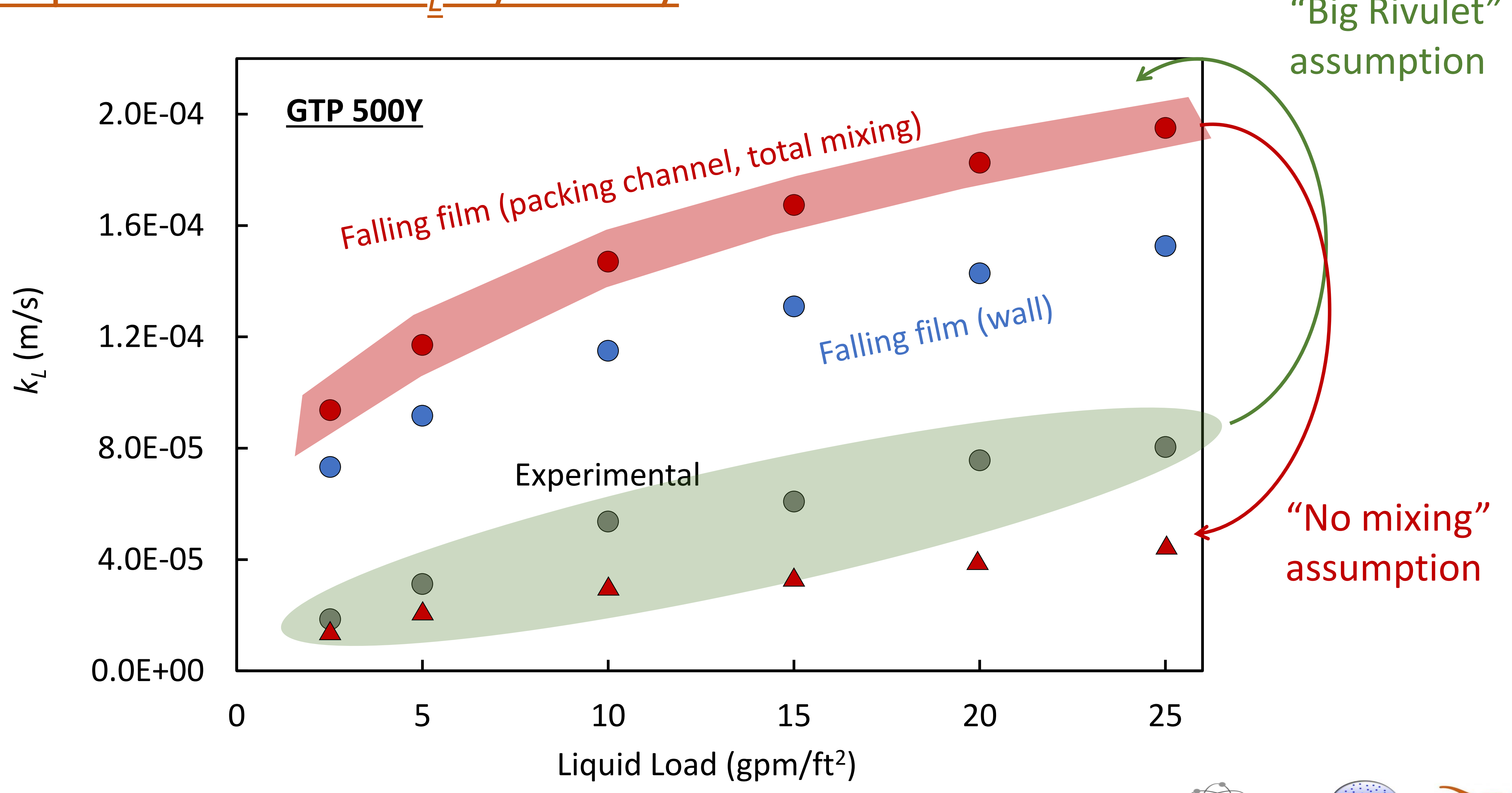
(underestimate k_L)

Δa ↑ for finer packings

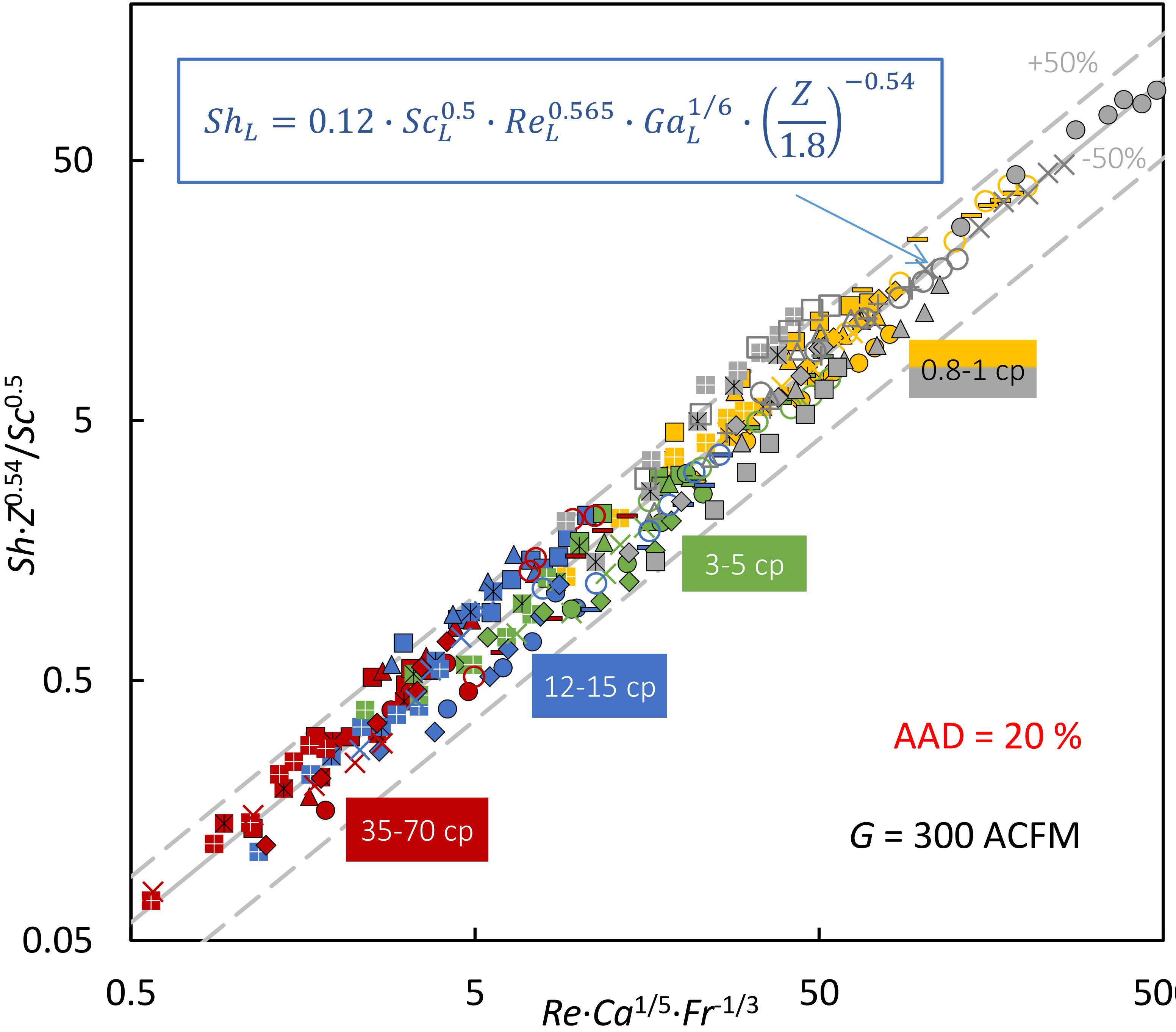
“No mixing” assumption

	“Mixing point”	“No mixing”
Sketch		
L	$\frac{b}{2 \cdot \sin\alpha \cdot \cos\alpha}$	$H_{element}/\sin\alpha$
$f(a_P)$	a_P ↑ L ↓ Q/W ↓ k_L ↑	a_P ↑ L — Q/W ↓ k_L ↓

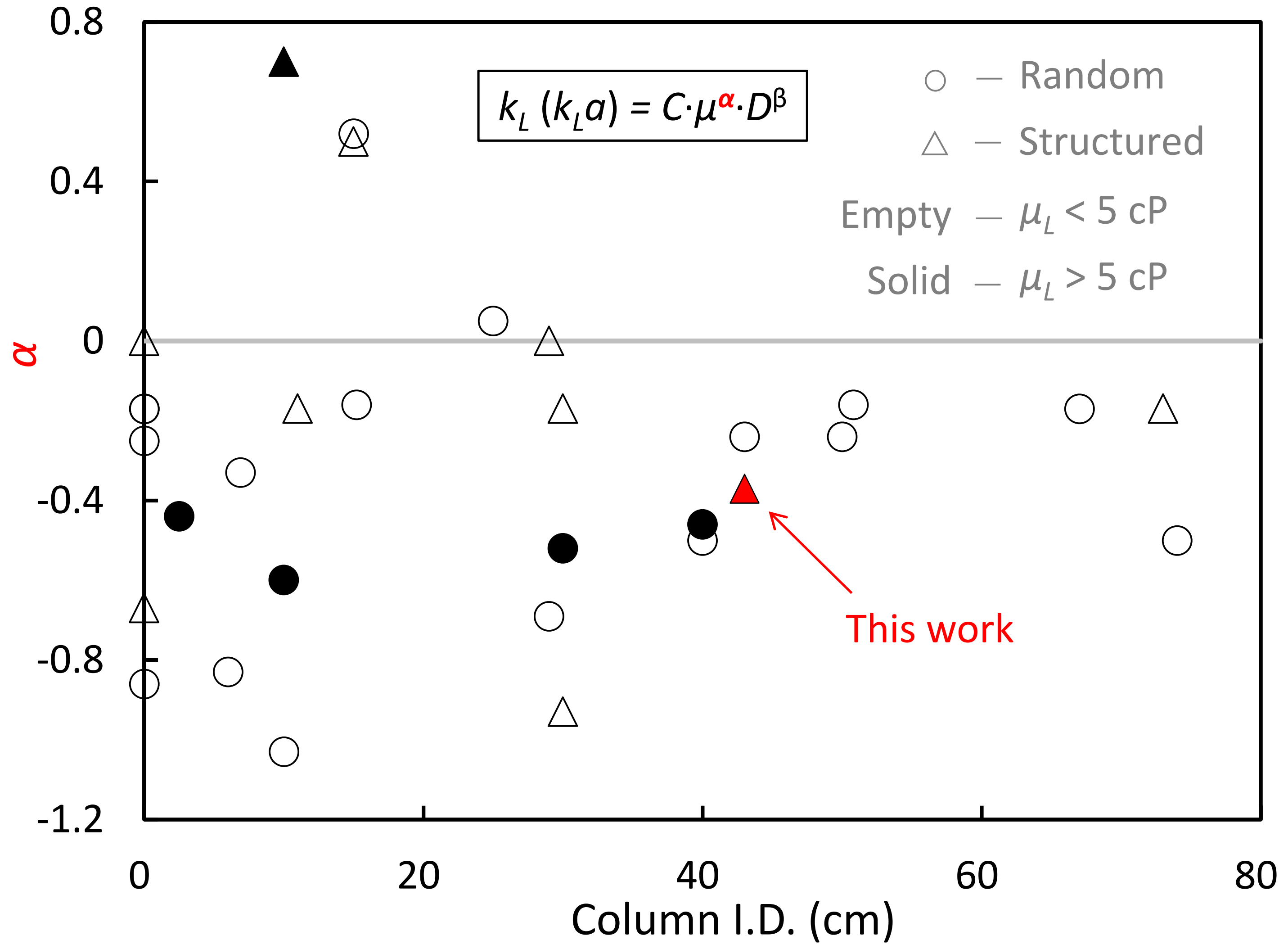
Compare measured k_L w/ theory



Liquid film mass transfer coefficient: k_L



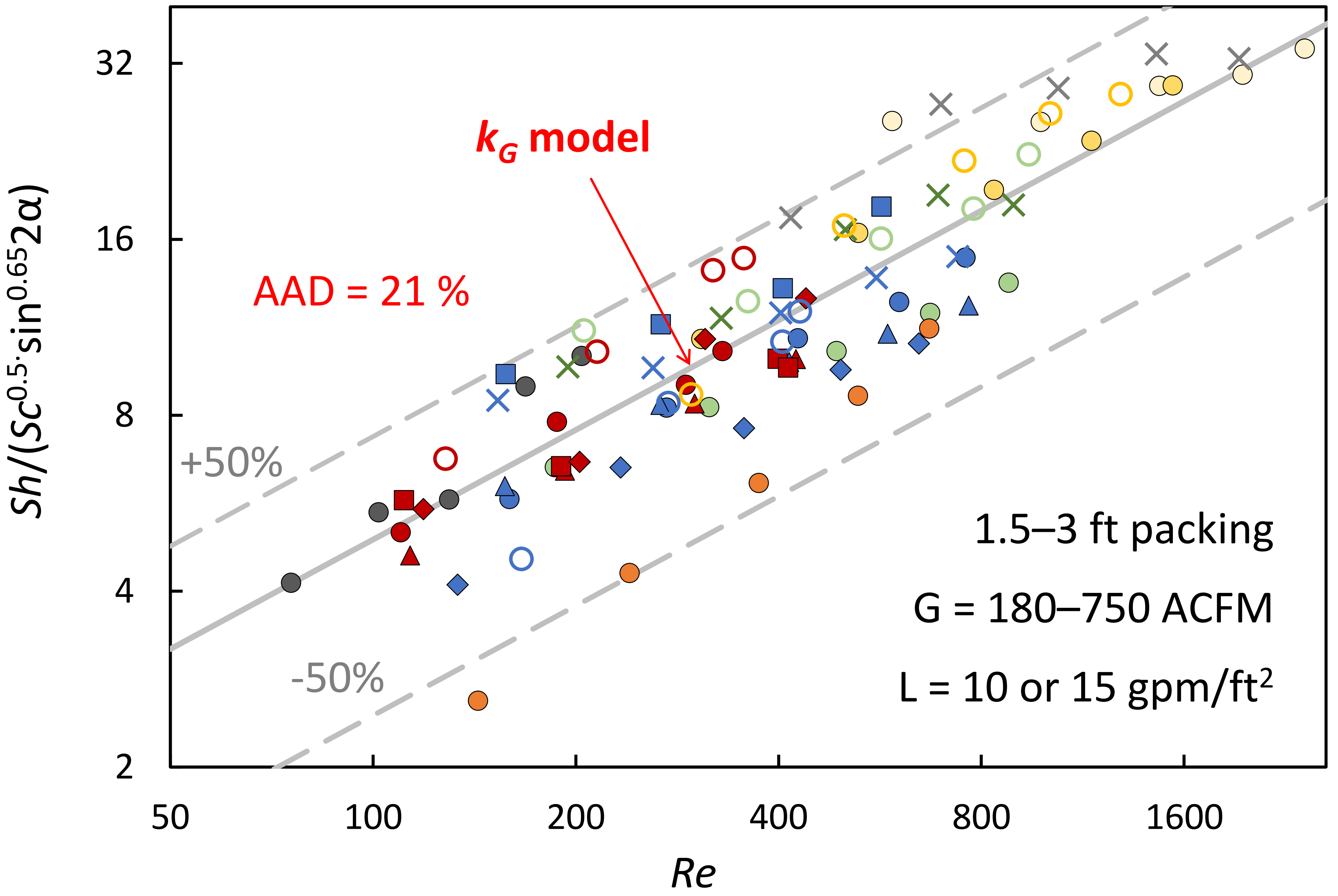
This work compared to literature



❑ This work

- Greatly expand packing database
- Greatly expand μ_L variance
- Reliable a_e (kinetic) data
- Relatively large column size

k_G Model



k_G model
AAD = 21 %
+50%
-50%
1.5–3 ft packing
G = 180–750 ACFM
L = 10 or 15 gpm/ft^2
32
16
8
4
2
50
100
200
400
800
1600
$Sh/(Sc^{0.5} \cdot \sin^{0.65} 2\alpha)$
Re