Dynamic Modeling of Advanced Process Configurations for Post-Combustion Amine Scrubbing

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Challenges for CCS

Energy Penalty

~20-30% reduction in power plant output

Capital Cost

800 MW coal plant: > 3 billion ft^3/day flue gas

Tight Integration

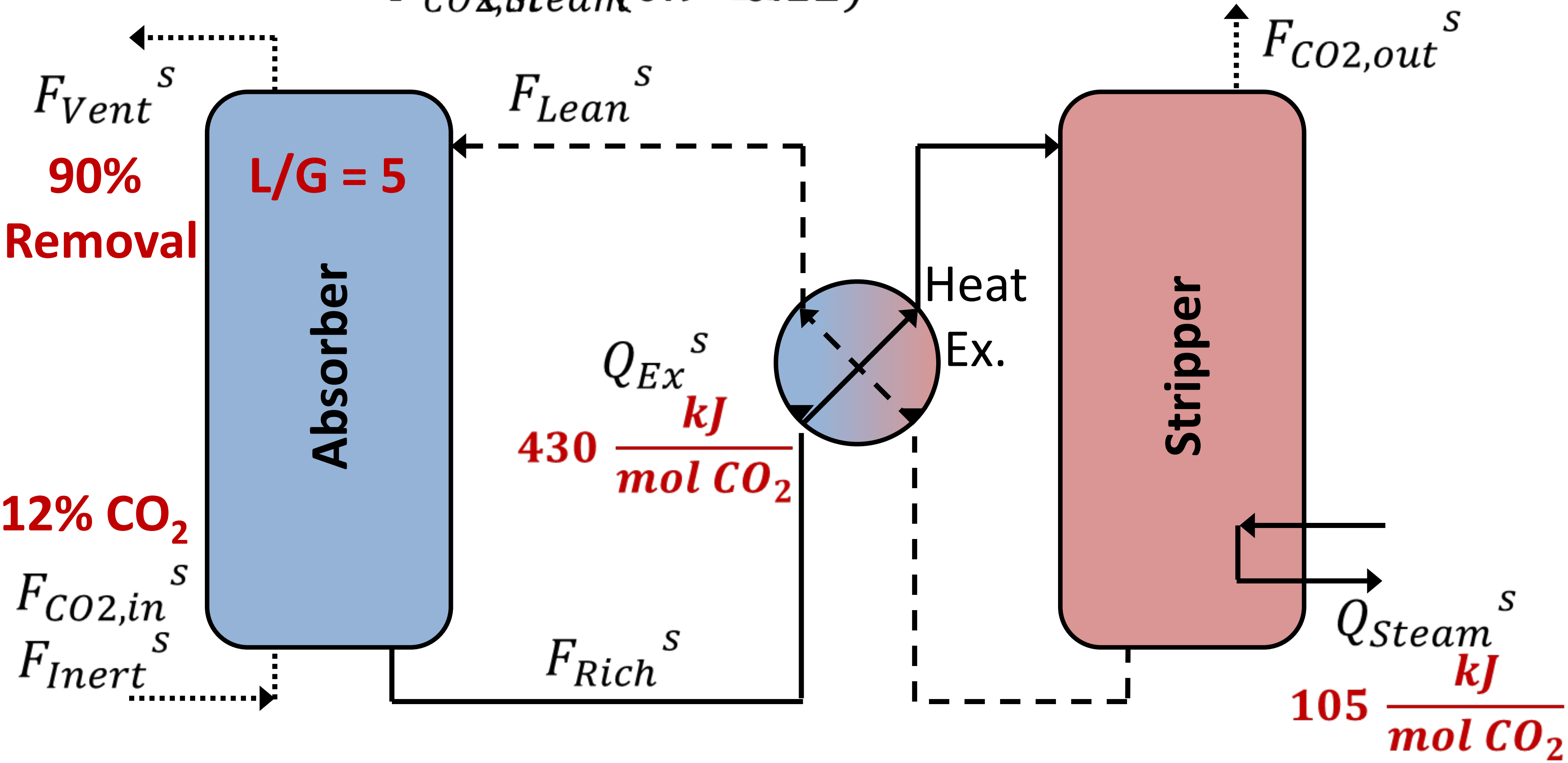
High material and energy recycle

Minimization of equipment size and solvent inventory

Heavy Material and Energy Recycle

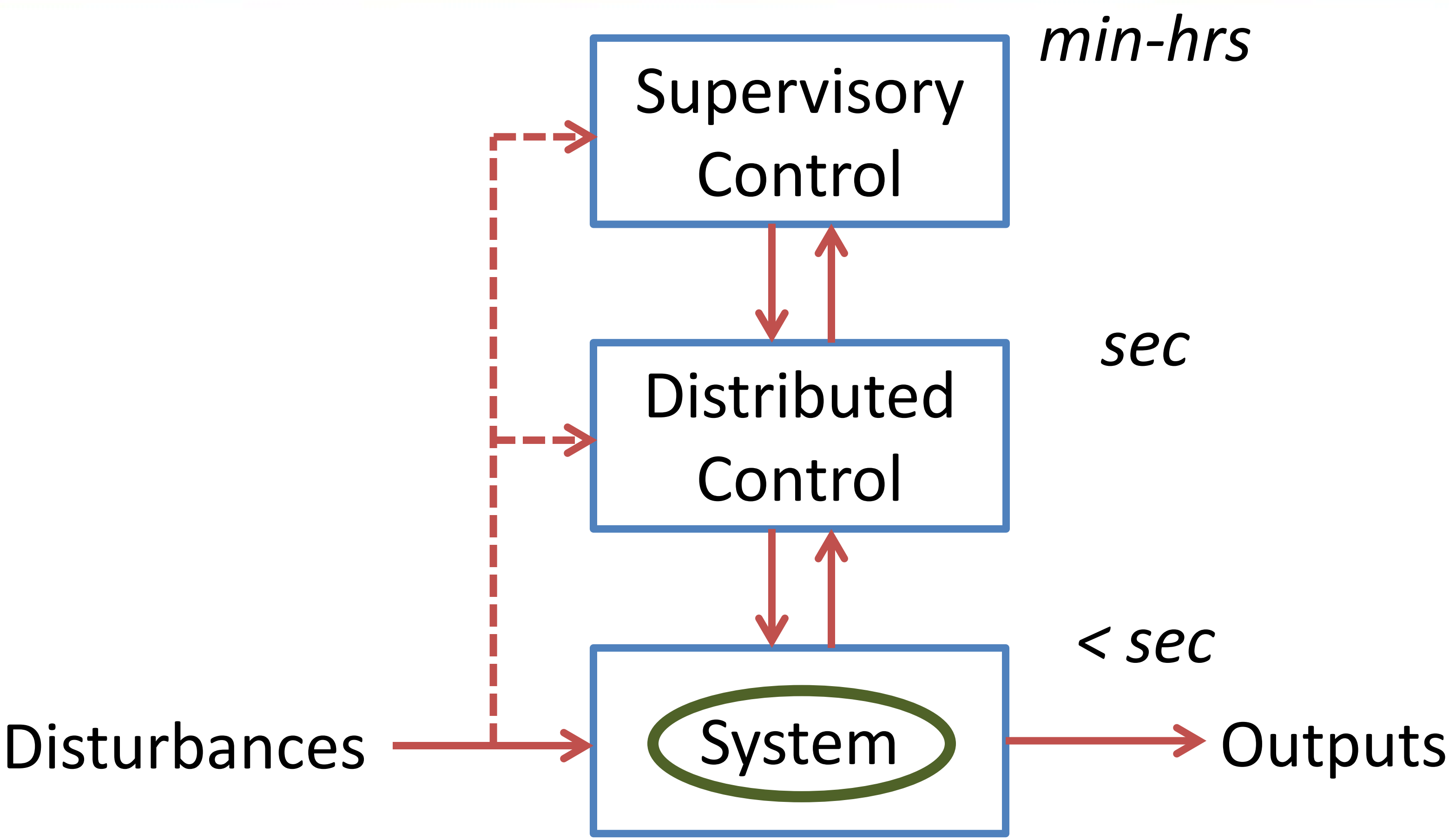
$$Rec = \frac{F_{Lean}^{s}}{F_{CO2,in}^{s}} = \frac{5}{(0.9 \cdot 0.12)} \gg 1$$

$$E = \frac{Q_{Ex}^{s}}{Q_{Steam}^{s}} = \frac{430}{105} \gg 1$$



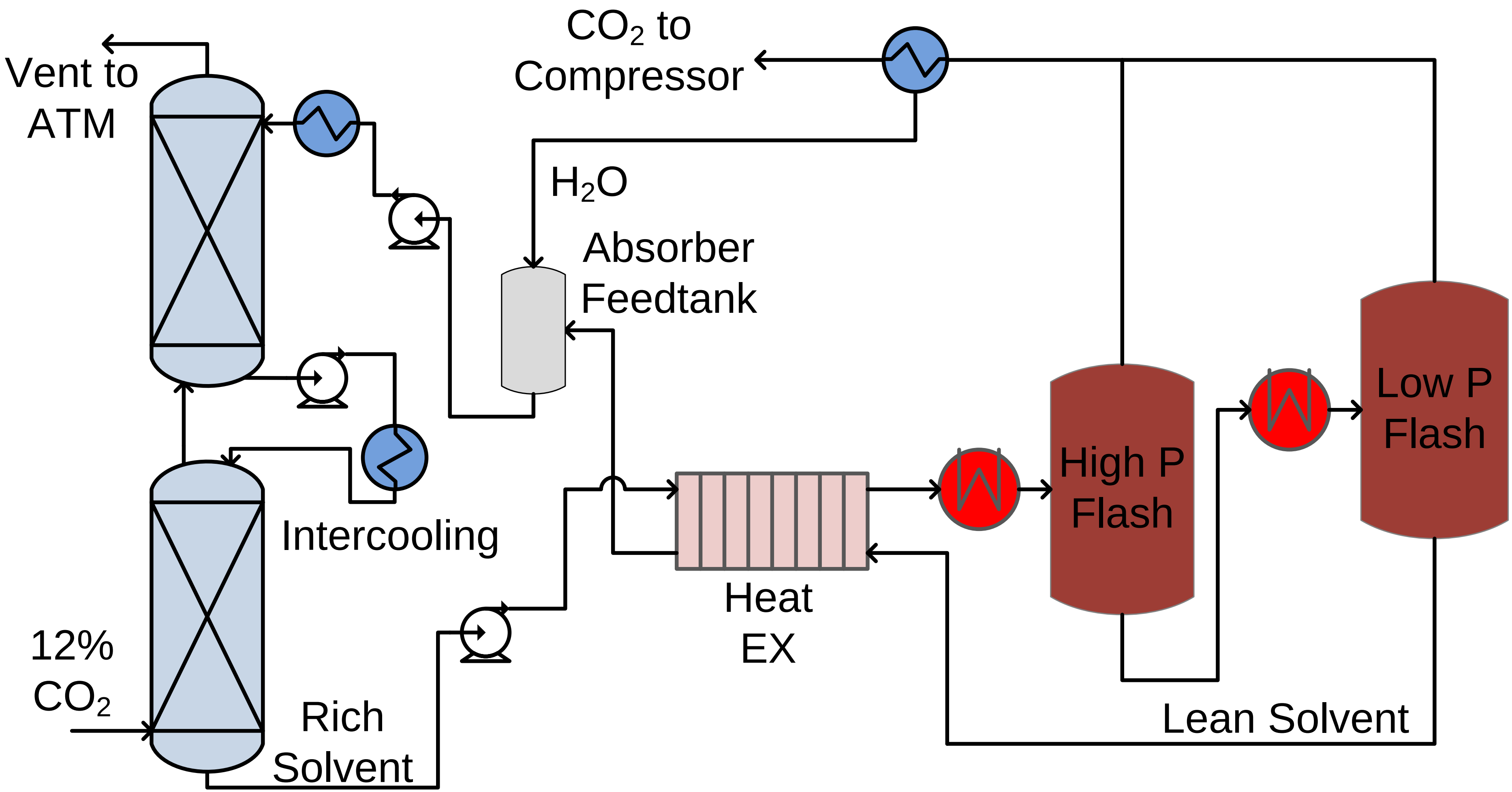
Baldea, M., Daoutidis, P. (2012). *Dynamics and Nonlinear Control of Integrated Process Systems*.

Hierarchical Controller Design



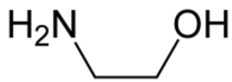
Goal: Develop dynamic model for control strategy design

Process Modeling: Advanced Configuration

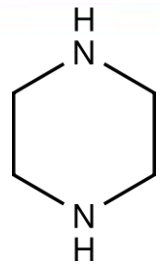


Process Modeling: Advanced Solvent

MEA:



PZ:



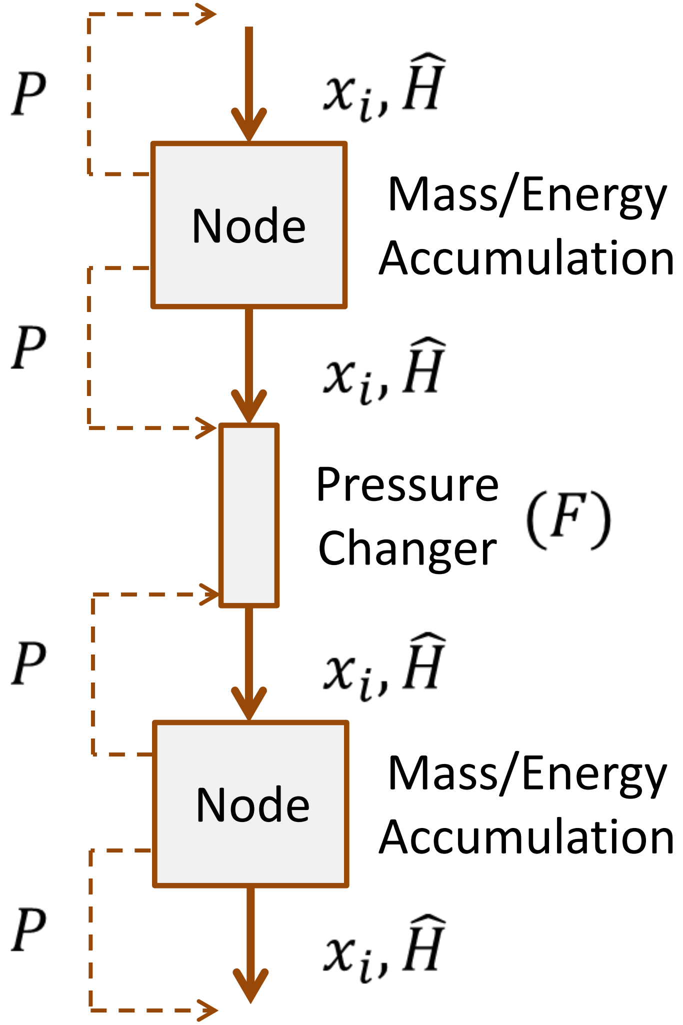
Previous Works ↓ **This Research** ↓

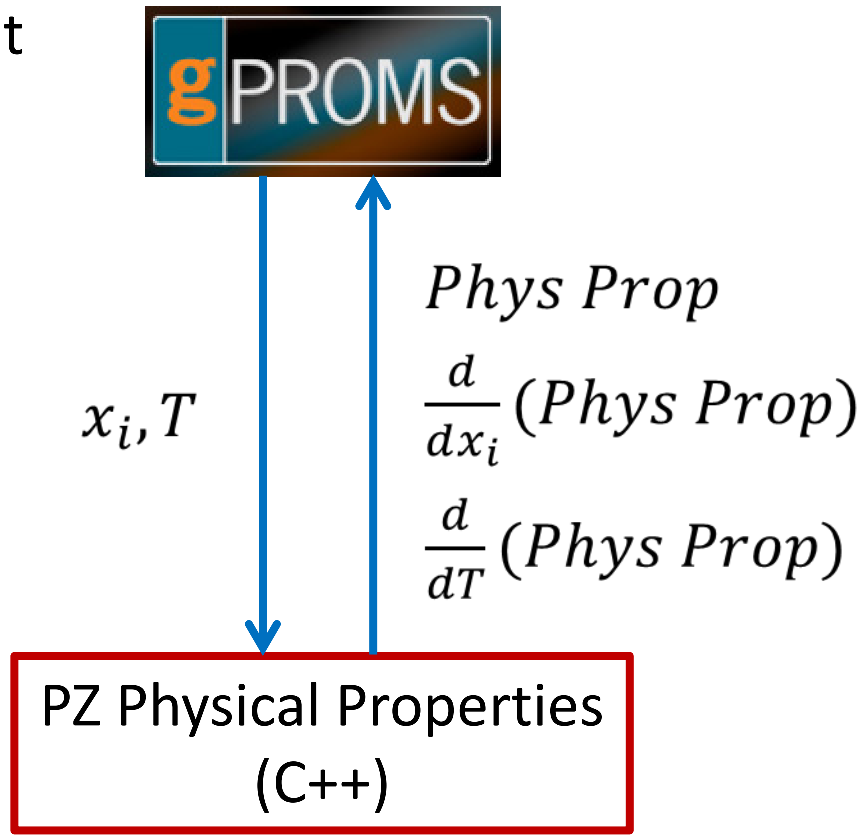
Property	7 m MEA	8 m PZ
$k_g' \times 10^7$ (mol/Pa·s·m^2)	4.3	**8.5**
Capacity (mol CO_2/mol PZ + H_2O)	0.67	**0.88**
Degradation T (°C)	121	**163**
Max stripper P (bar)	4	**16**
Degradation rate at 120°C (1/week)	8.1%	**0.07%**
C_{amine} in gas at 40°C (ppm)	13	**8**
ΔH_{abs} at lean ldg (kJ/mol CO_2)	**-76**	-71

Rochelle et al. (2011). *Chem Eng*, *171*(3), 725-733.

Modeling Software: gPROMS©

Equation-oriented process flowsheet





ΔH_{abs}, C_p, P^*_{CO2}, ρ, μ

Model Validation: SRP Pilot Plant

Stripper

Absorber

Two-Stage Flash

Validation Data:

Fall 2011

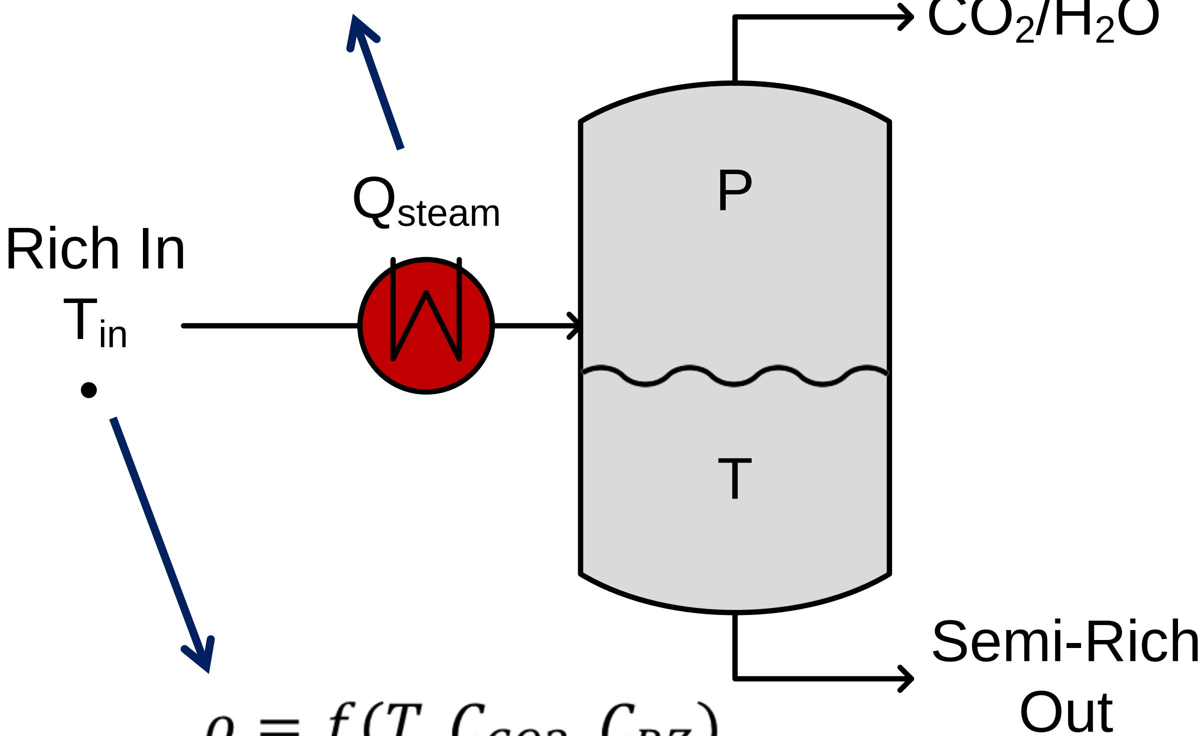
PZ Solvent

Two-Stage Flash Stripper

Intercooled Absorber

Flash Tank Model

$$Q_{eff} = Q_{steam} - Q_{loss}$$
$$Q_{loss} = UA(T - T_{amb})$$



$$\rho = f(T, C_{CO2}, C_{PZ})$$
$$\frac{\rho}{\rho_{H2O}} = \left(\frac{\rho}{\rho_{H2O}}\right)_{meas} + \left(\frac{\rho}{\rho_{H2O}}\right)_{bias}$$

Fitted:

$$\left(\frac{\rho}{\rho_{H2O}}\right)_{bias} = 0.0082$$

~4% Increase in experimental loading

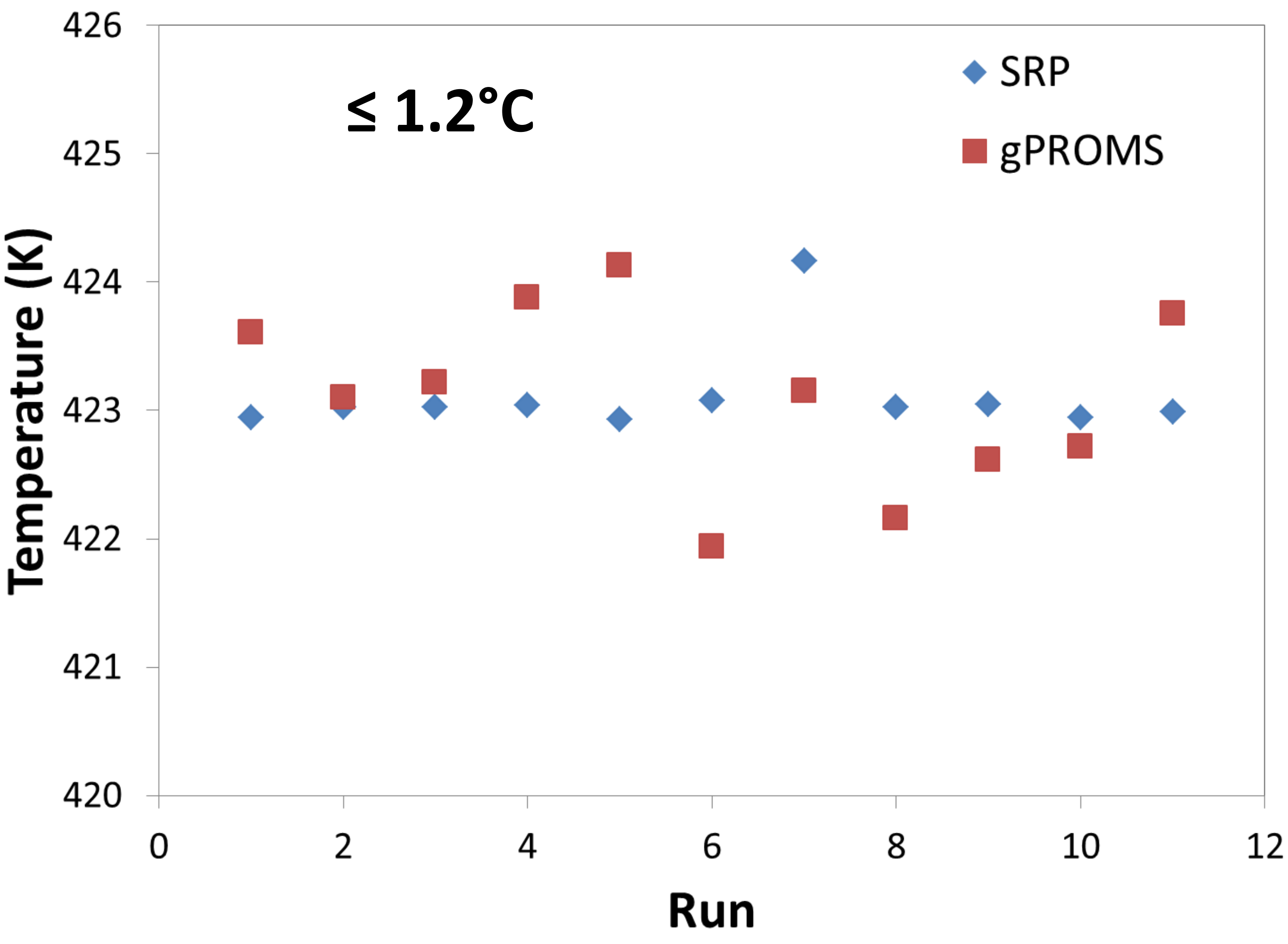
Fitted:

$UA = 0.075$ kW/K

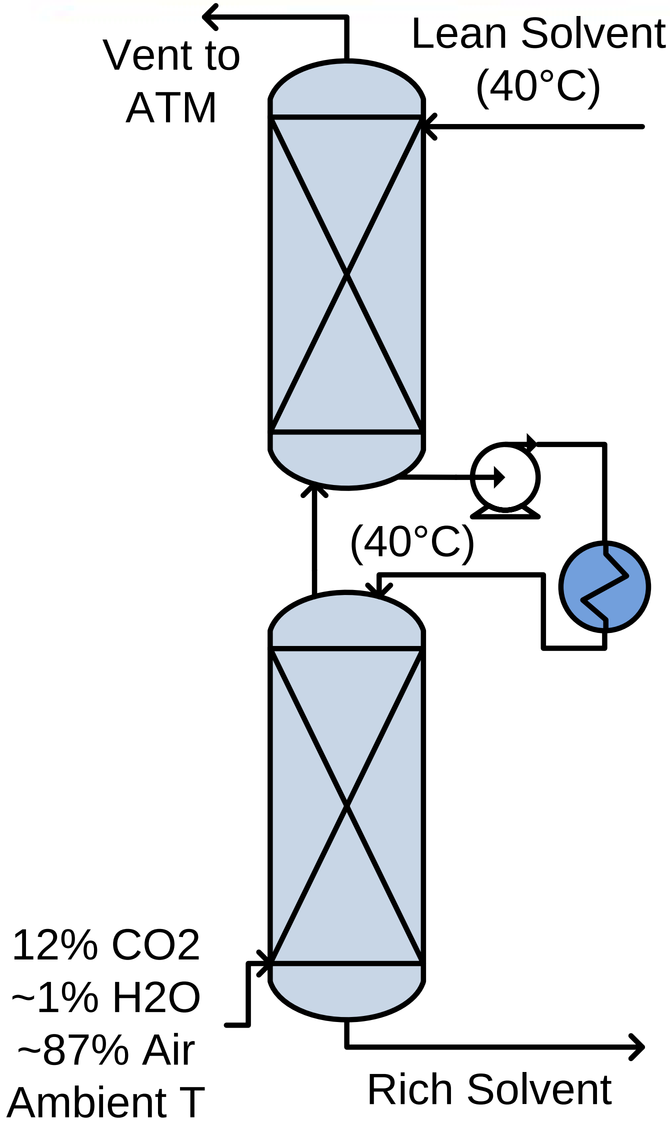
Experimental (both tanks):

$UA = 0.054$ kW/K

Steady State Flash Tank Validation

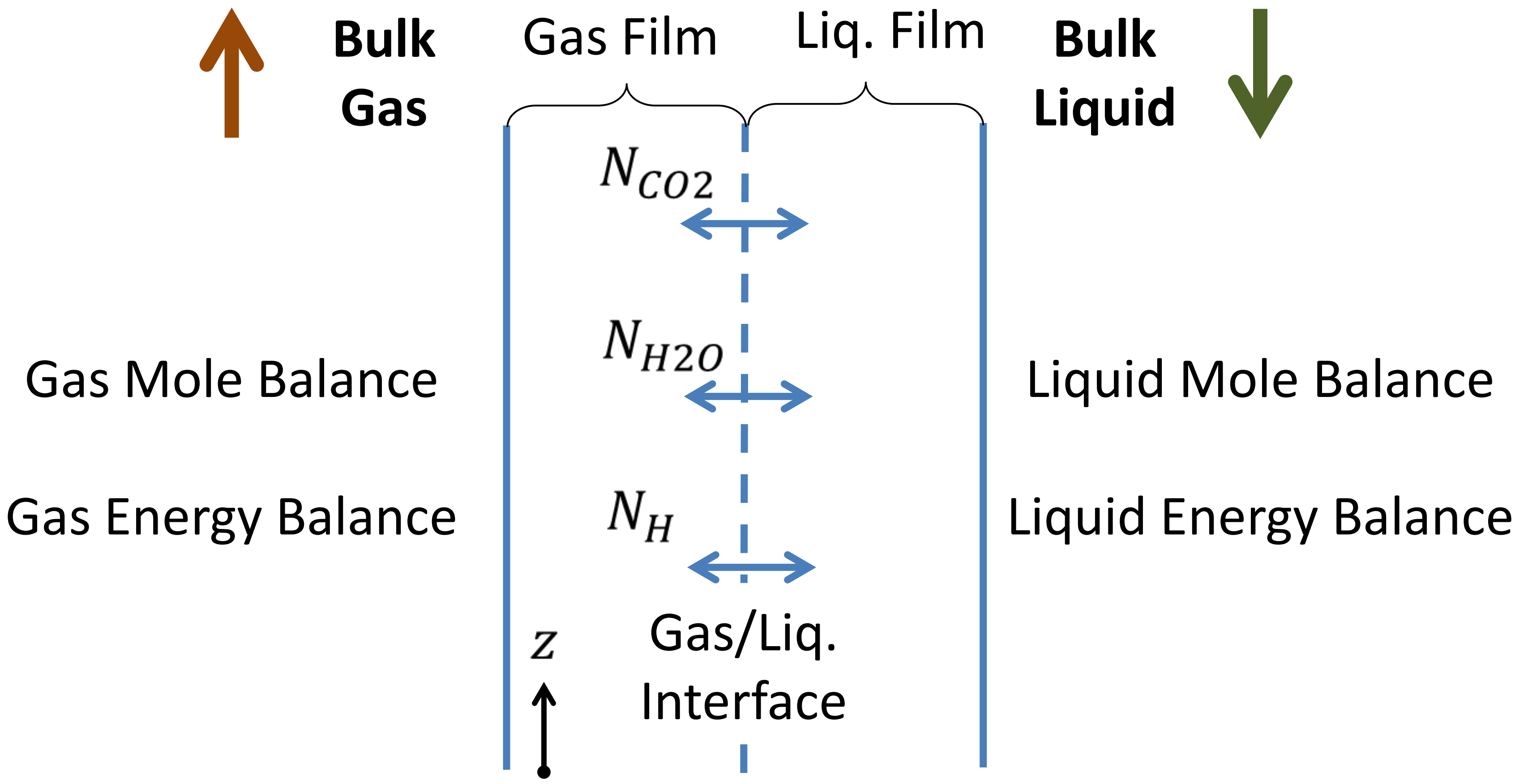


Intercooled Absorber Model



- Ideal gas law is valid
- PZ is nonvolatile
- Mass transfer of H_2O is gas film controlled
- Heat transfer is gas film controlled
- Equilibrium at the gas/liquid interface
- No accumulation at the gas/liquid interface
- Constant pressure drop
- Plug flow regime

Absorber Model Development



Absorber Mass Transfer

Liquid film:

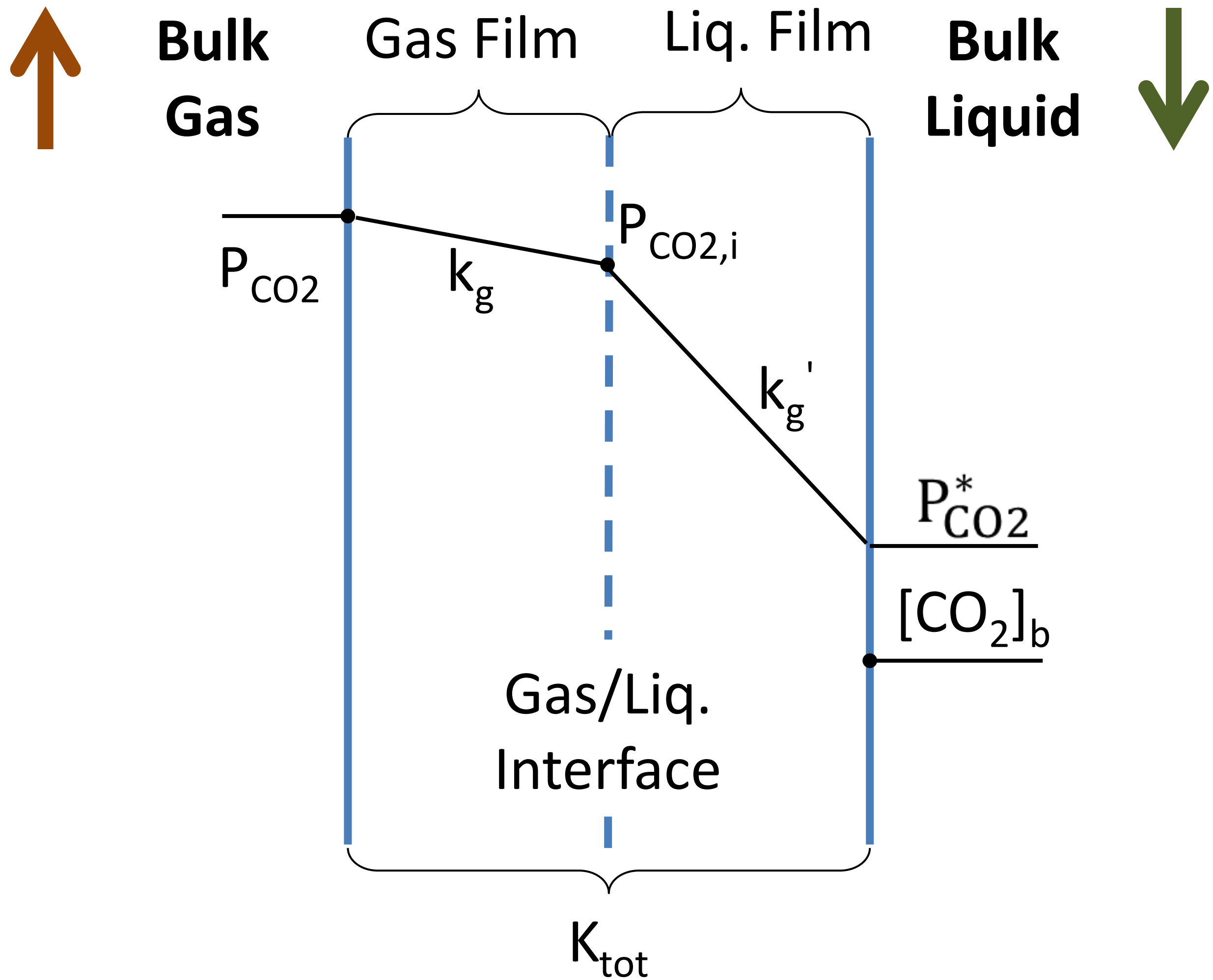
$$k_g' = f(\propto)$$

Overall Mass Transfer Coefficient:

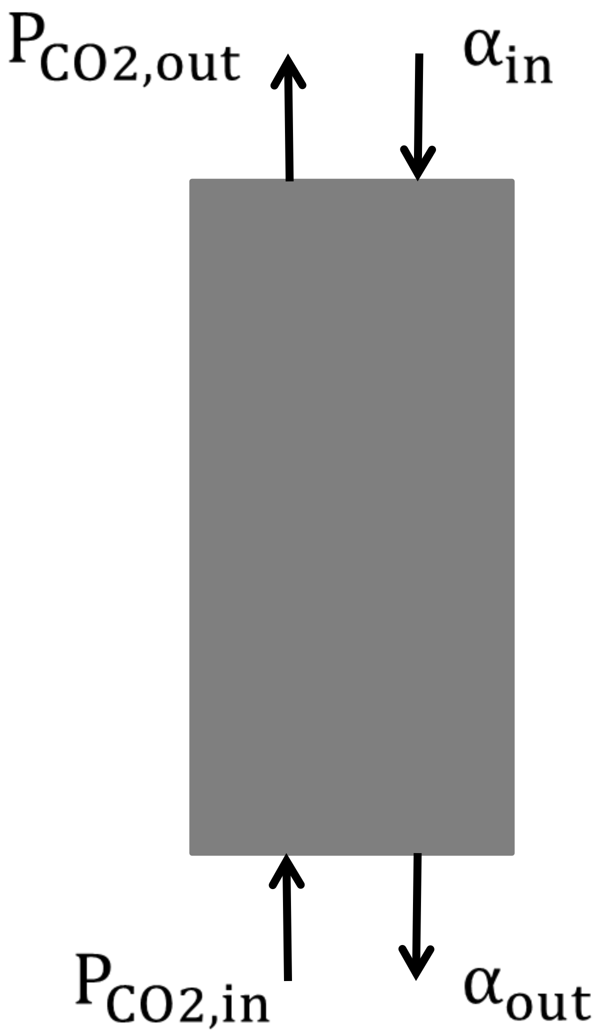
$$\frac{1}{K_{tot}} = \frac{1}{k_g} + \frac{1}{k_g'}$$

Rate-Based Flux:

$$N_{CO2} = K_{tot}(P_{CO2} - P^*_{CO2})$$



Wetted Wall Column Validation



Cooling Oil

T = constant

$$\frac{\partial E}{\partial t} = 0$$

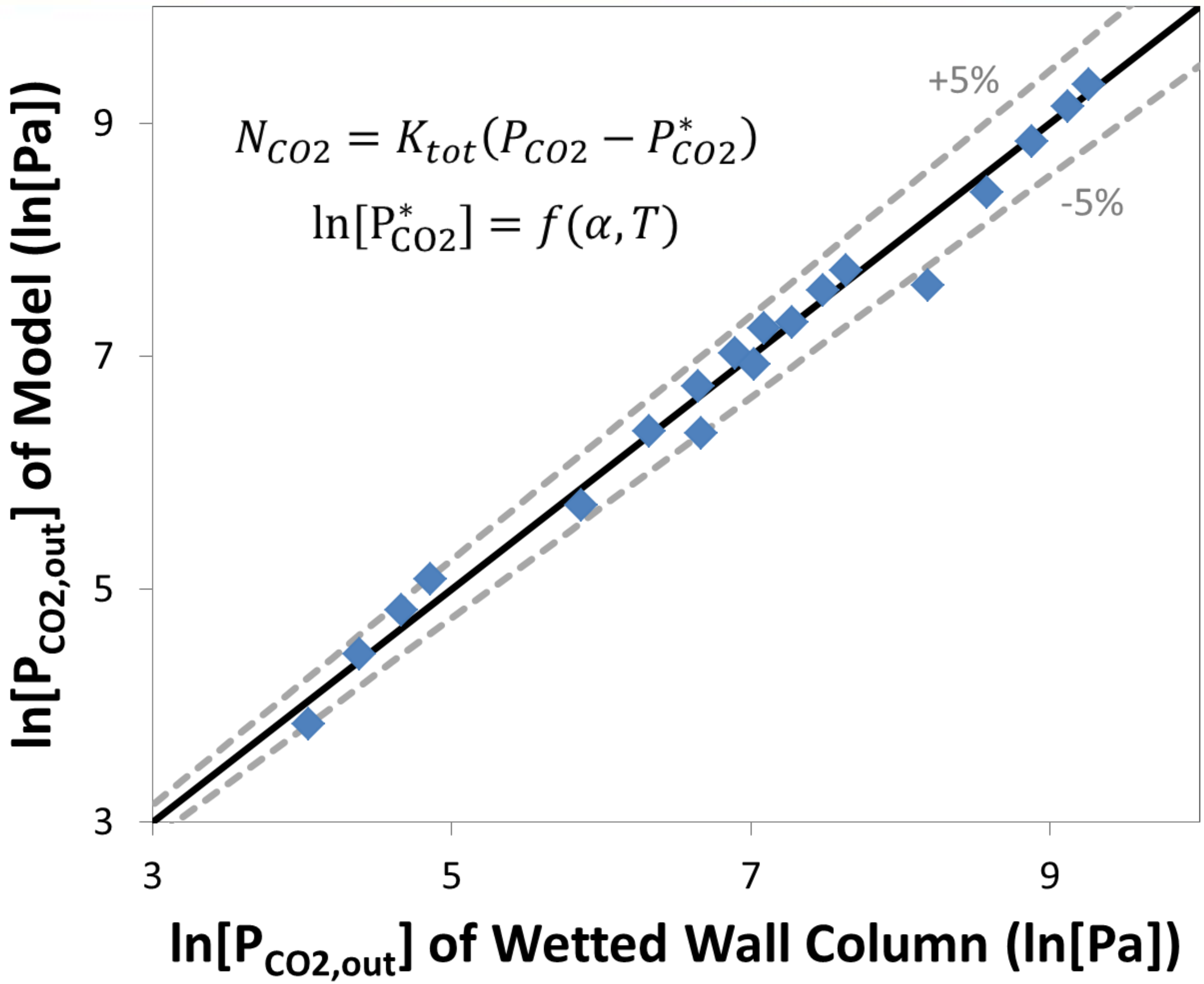
$$\alpha_{in} \approx \alpha_{out}$$

$$\ln[P^*_{CO2}] = f(\alpha, T)$$

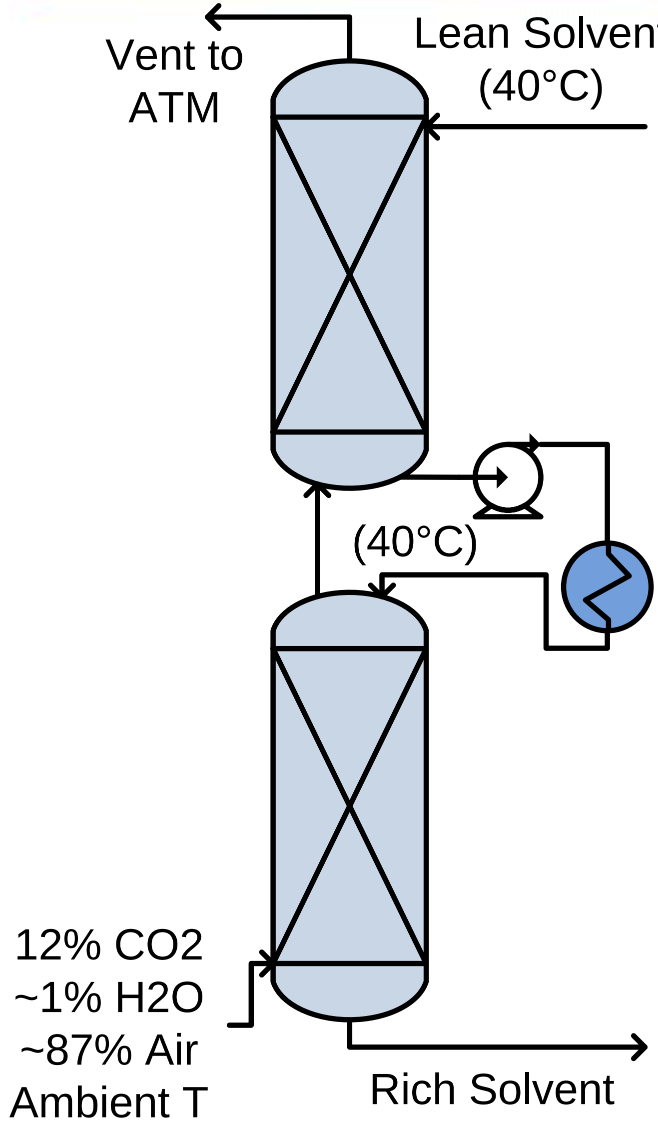
Given loading

Predict Flux

Wetted Wall Column Validation Results



Steady State Absorber Validation



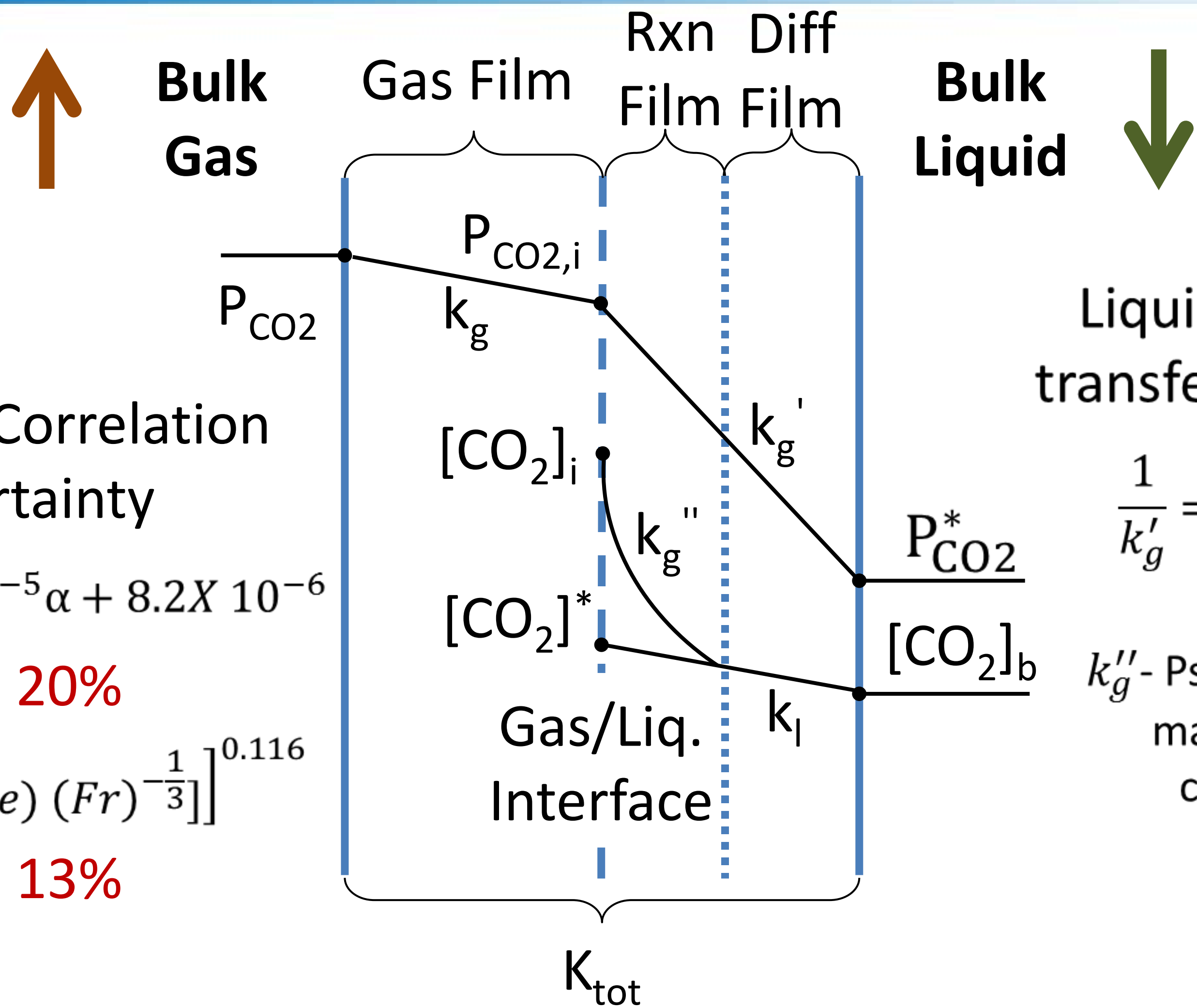
$\alpha_{lean} = 0.26$ **Input**

$k_g' a_e$ Factor
0.74

Consistent with Schade (2012)

$\alpha_{rich} = 0.36$ **Match within 7%**

Mass Transfer Coefficient Uncertainty



Empirical Correlation Uncertainty

$$k_g' = -2.0\,X\,10^{-5}\alpha + 8.2X\,10^{-6}$$

± 20%

$$\frac{a_e}{a_p} = 1.34\left[(We)\,(Fr)^{-\frac{1}{3}}\right]^{0.116}$$

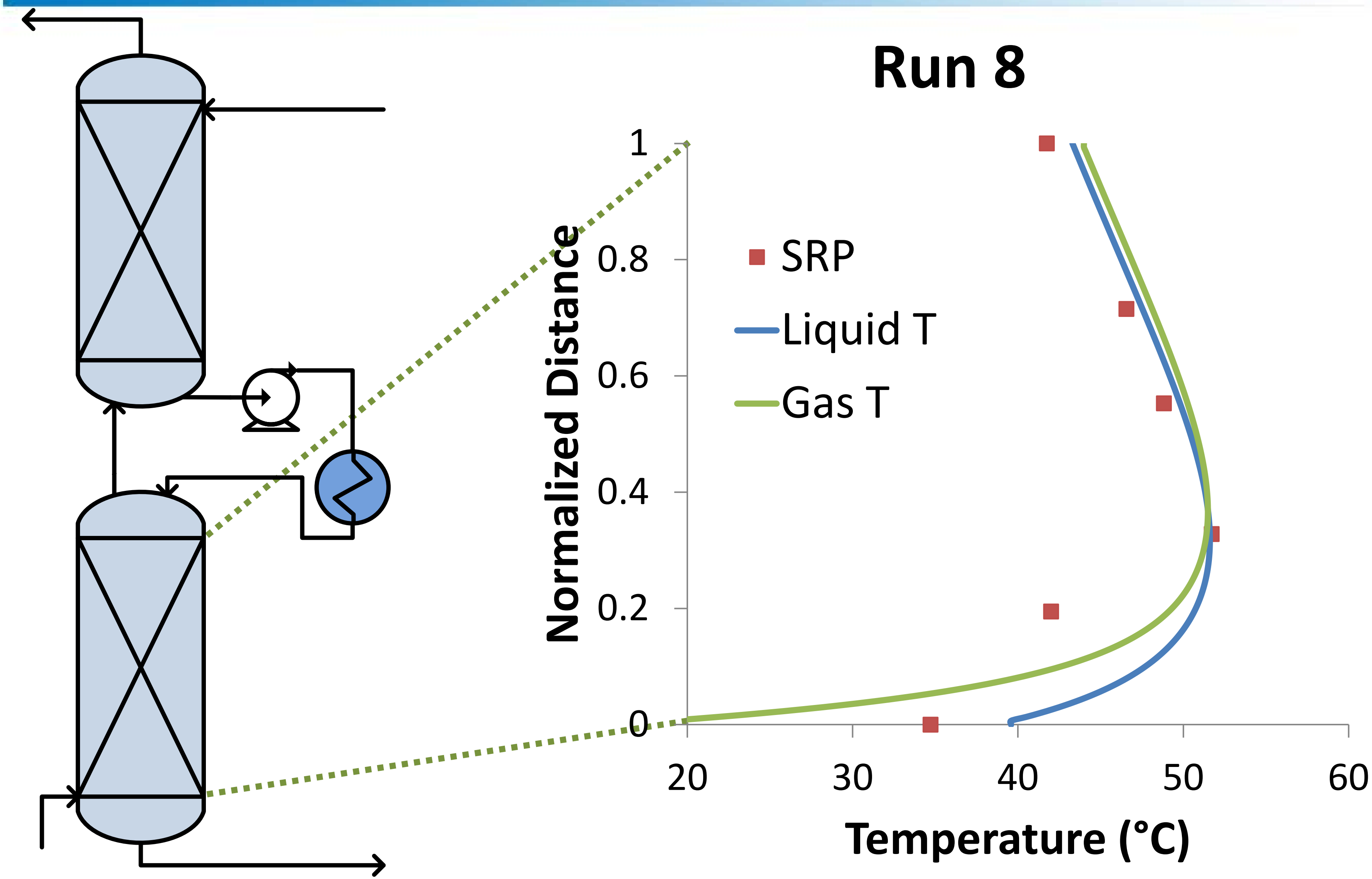
± 13%

Liquid film mass transfer coefficient:

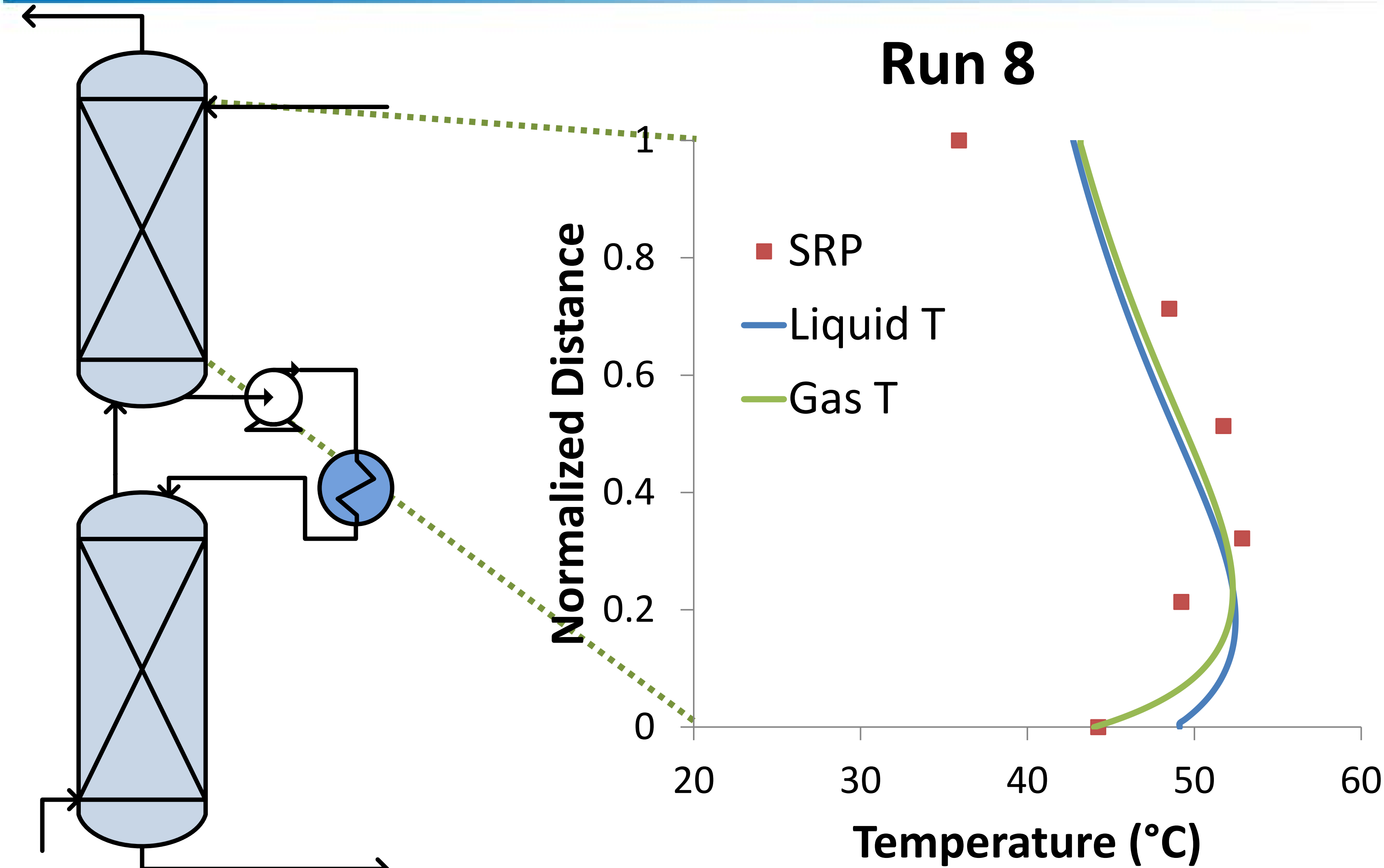
$$\frac{1}{k_g'} = \frac{m_{CO2}}{k_l} + \frac{1}{k_g''}$$

k_g''- Pseudo 1st order mass transfer coefficient

Steady State Absorber Validation



Steady State Absorber Validation



Conclusions

- Heavy energy and material recycle lead to multiple time scale behavior in the amine scrubbing system
- Flash tank temperature predicted within 1.2°C after adjusting loading by 4% heat loss by 40%
- Absorber with $k_g' = f(\alpha)$ predicts experimental $\ln[P_{CO2}]$ for wetted wall column with average error of 2.2%
- Absorber loading matched within 7% with 26% decrease in $a_e k_g'$
- Behavior of absorber temperature profile consistent with pilot plant measurements

Questions?

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