16th STS-AIChE Southwest Process Technology Conference

- Mass Transfer Rate Based Simulation of Liquid Treaters
- Prashanth Chandran & Ralph Weiland
- Affiliation- Prashanth Chandran is Technical Development Lead at & Ralph Weiland is Chairman at Optimized Gas Treating Inc.

Sept 22-23, 2025, University of Houston

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Speaker Bio

I work at Optimized Gas Treating (OGT) as a Senior Applications Engineer.

Education-E.I.T. Certification from the Texas Board of Professional Engineers and have a Bachelor`s Degree in Chemical Engineering. Also, hold an MBA from the University of Houston, Clear Lake, T X .

I have experience gained from employment in EPC Industry and in the manufacture of Mass Transfer & Heat Transfer products.

I love football and an avid fan of Houston Texans

Sept 22-23, 2025, University of Houston

Breakthrough in Modeling Technology - Mass Transfer Rate-Based Simulation of Liquid Treaters

Prashanth Chandran & Ralph Weiland

Optimized Gas Treating, Inc.

Outline

- Introduction
- Motivation (Why Rate-based?)
- Model Development
- Model Validation against plant data
- Case Study – Application to LPG treating
- Comparison of an ideal stage against real internals
- Ongoing and Future Directions

Liquid-Liquid Extraction

- Essential step in several chemical processes
- Applications
  - Refining
    - Aromatics removal from Lube Oil
    - Aromatics removal from Gasoline
  - Natural Gas Processing
    - LPG and Propane treating
    - Removal of CO_2, H_2S, COS and Mercaptans
  - Chemical
  - Pharmaceuticals & Biotechnology

Liquid-Liquid Extraction (Contd.)

- A slow mass transfer process
- Transfer between two dense phases
- Operated at low fluid velocities
  - Emulsification
  - Entrainment
- Factors affecting separation
  - Phase Equilibria
  - Fluid properties
  - Internals
  - Reactions in the system

Current Modeling Approaches

- Use of ideal stage models
- Rules of thumb for selecting number of stages
- Tray efficiency and HETP

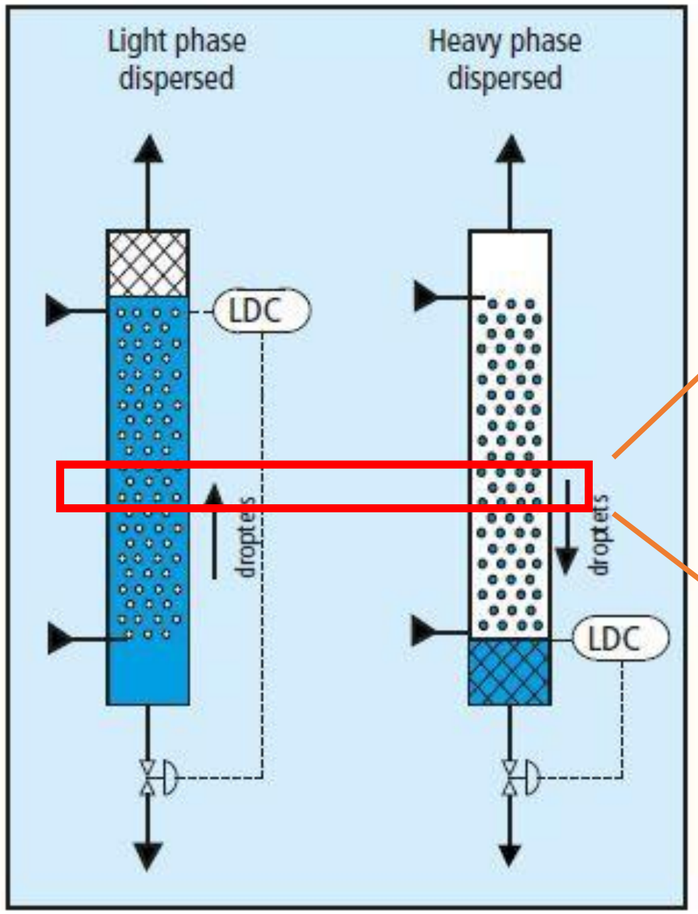
Why Rate-Based?

- Years of ProTreat® user feedback
- Rules of thumbs are often inaccurate
  - Doesn’t extend to all applications
  - Fails to predict behavior for different solutes
- Scarce literature on efficiency and HETP
- Rate models are well suited for slow mass transfer
  - Tray efficiency – 5 to 20 %
  - HETP – 10 to 20 feet
- Physically realistic
  - Accounts for true mass transfer internals and fluid properties

Why Rate-Based? (Contd.)

- Lack of commercial models
- Leverage ProTreat’s Gas Treating Model
  - Rigorous and accurate electrolytic thermodynamics for amine treating
  - Well established, accurate and time-tested rate model for gas treating, carbon capture and sulfur recovery
  - Flexible flowsheeting software

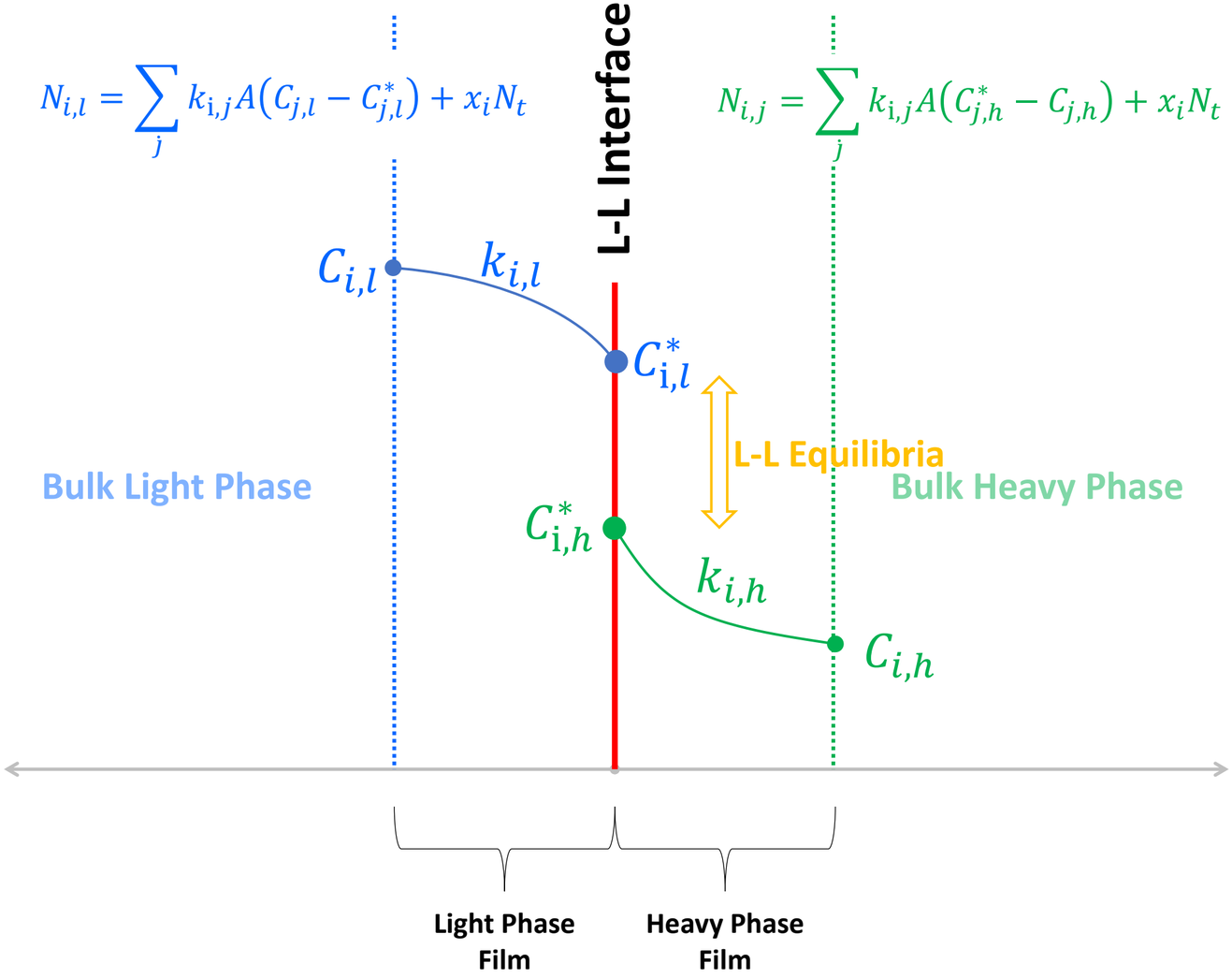
Rate Model



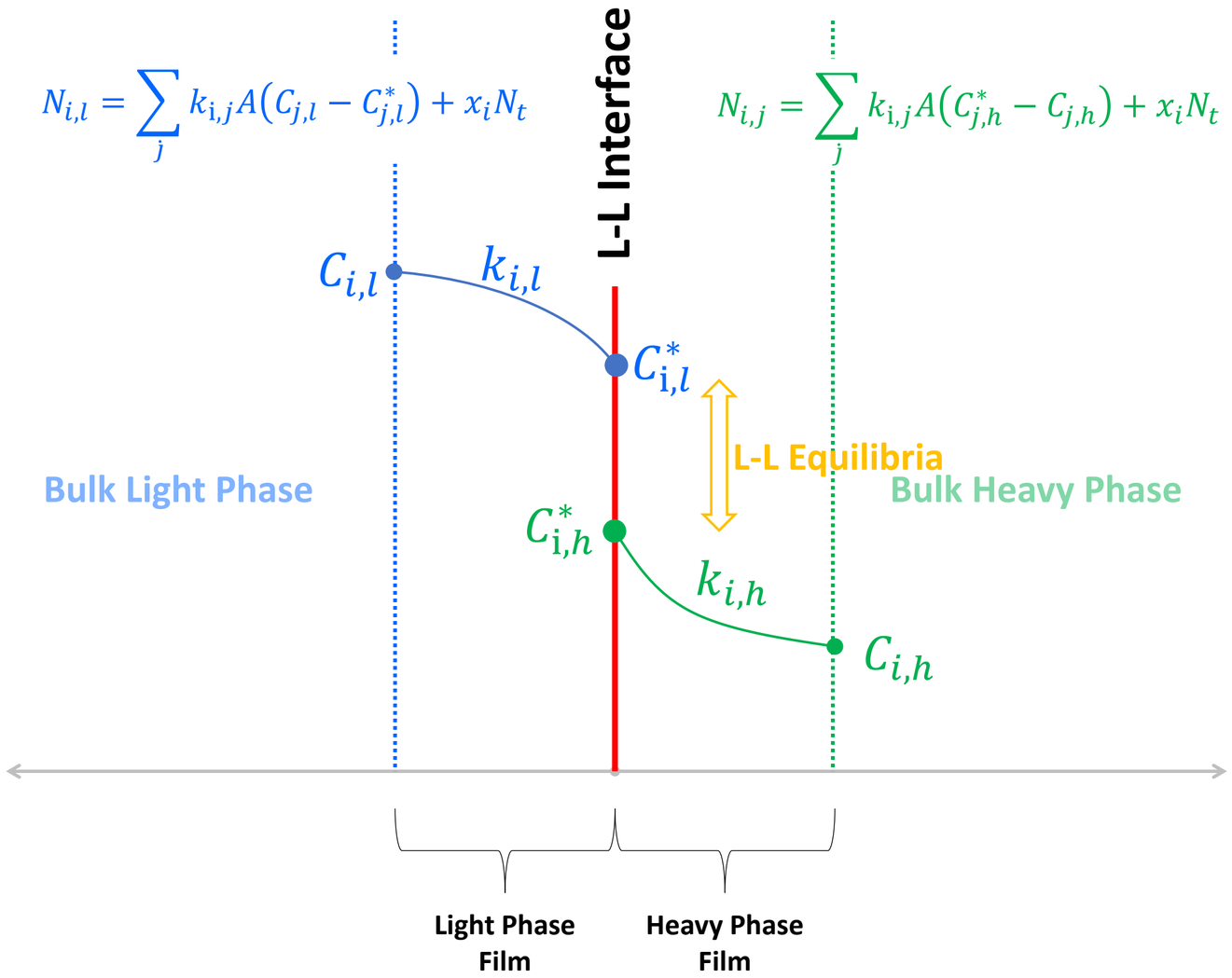
Reference: https://www.schulzpartner.com/products/thermal-processes/liquid-liquid-extraction

$$N_{i,l} = \sum_j k_{i,j} A\left(C_{j,l} - C^*_{j,l}\right) + x_i N_t$$

$$N_{i,j} = \sum_j k_{i,j} A\left(C^*_{j,h} - C_{j,h}\right) + x_i N_t$$



Rate Model - Segment Equations



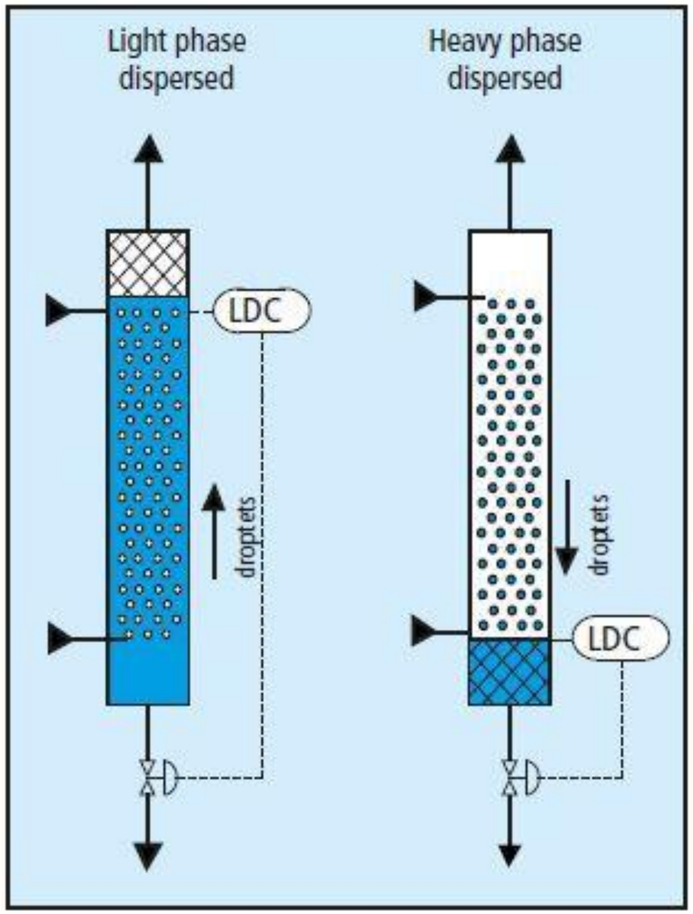
System of Non-Linear Equations

- Material Balance
- Liquid-Liquid Equilibria
- Mass Flux Equations
- Interface Energy Balance
- Bulk Phase Energy Balance

Solution:

- Phase Flows, Composition, Temperature
- Interface Composition and Temperature
- Component Fluxes

Rate Model



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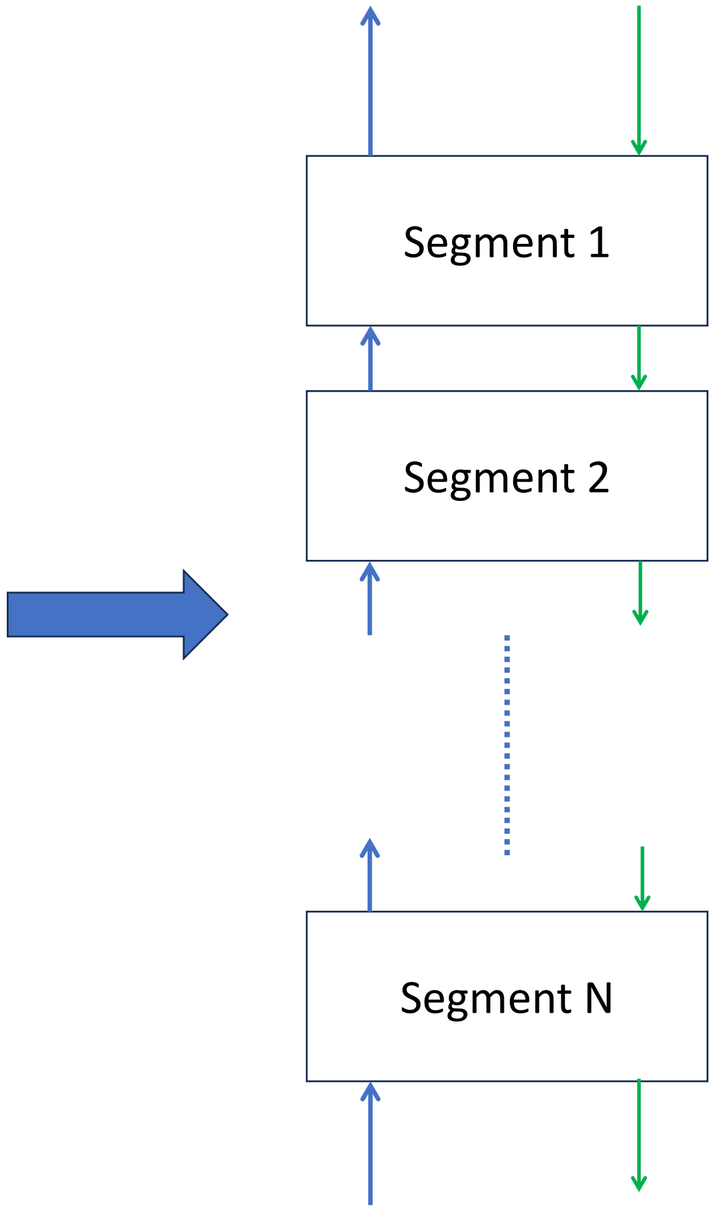
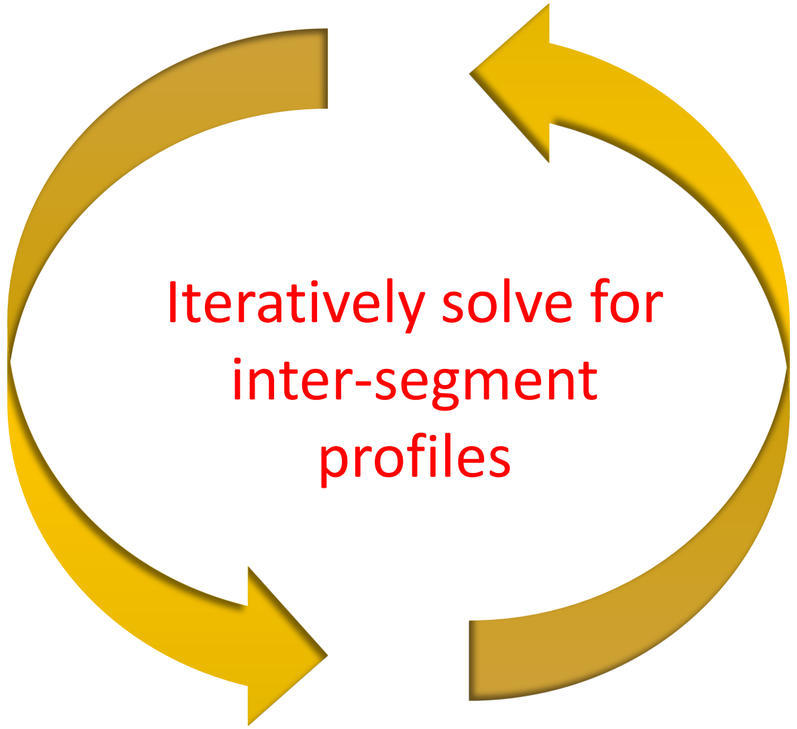




Features implemented

Sieve Trays

- Hole Size
- % Open Area
- Tray spacing
- Downcomer clearance

Packings

- Packed Depth
- User Defined Packing
  - Surface Area
  - Void Fraction
- Existing Packing Database

Spray Column

- Mass Transfer Zone Depth
- Distributor hole size
- Distributor total hole area

- Select heavy or light phase as dispersed
- Hydraulics - Rate or size columns
- Physical and Reactive solvents

Diagnostic Benefits

- Sauter Mean Diameter of dispersed phase
- Interface compositions and fluxes
  - Understand operating regimes
  - Phase equilibria limited
  - Mass transfer limited – On which phase?
- Interfacial Area
- Liquid-Liquid Interfacial Tension
- Hydraulic outputs and warnings

Model Validation – Plant Data Used

- Total of 15 LPG treaters
  - 7 Sieve Tray Columns
  - 8 Packed Columns
- Solvent used - MEA (1), DEA (10), MDEA(4)
- Up to 2.5 mol% H_2S
- Up to 4000 ppm Total Mercaptans and COS

Plant Data – Trays

- Tray diameter was known in all cases
- 10 to 25 Sieve Trays in each
- Tray diagrams were not available in any of the cases
- Assumptions for trays
  - 2 feet spacing
  - ¼ inch holes
  - 70% Active Area
  - 8% Hole Open Area

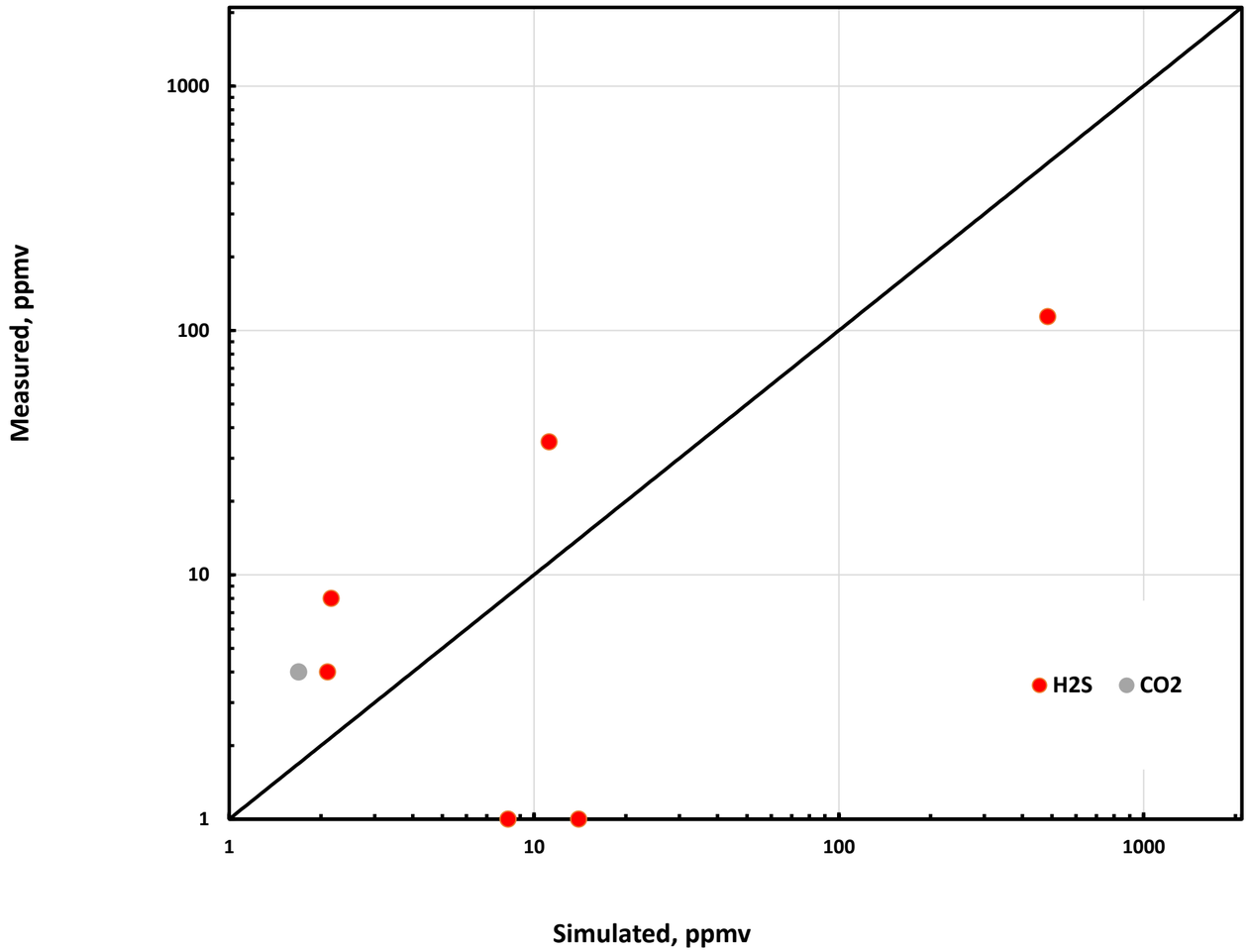
Plant Data – Packings

- 20 to 40 feet of packing
- 3 cases using 2” Raschig Rings
- 2 cases of 1” Raschig Rings
- 3 Unknowns – Assumed to be 2” Raschig Rings

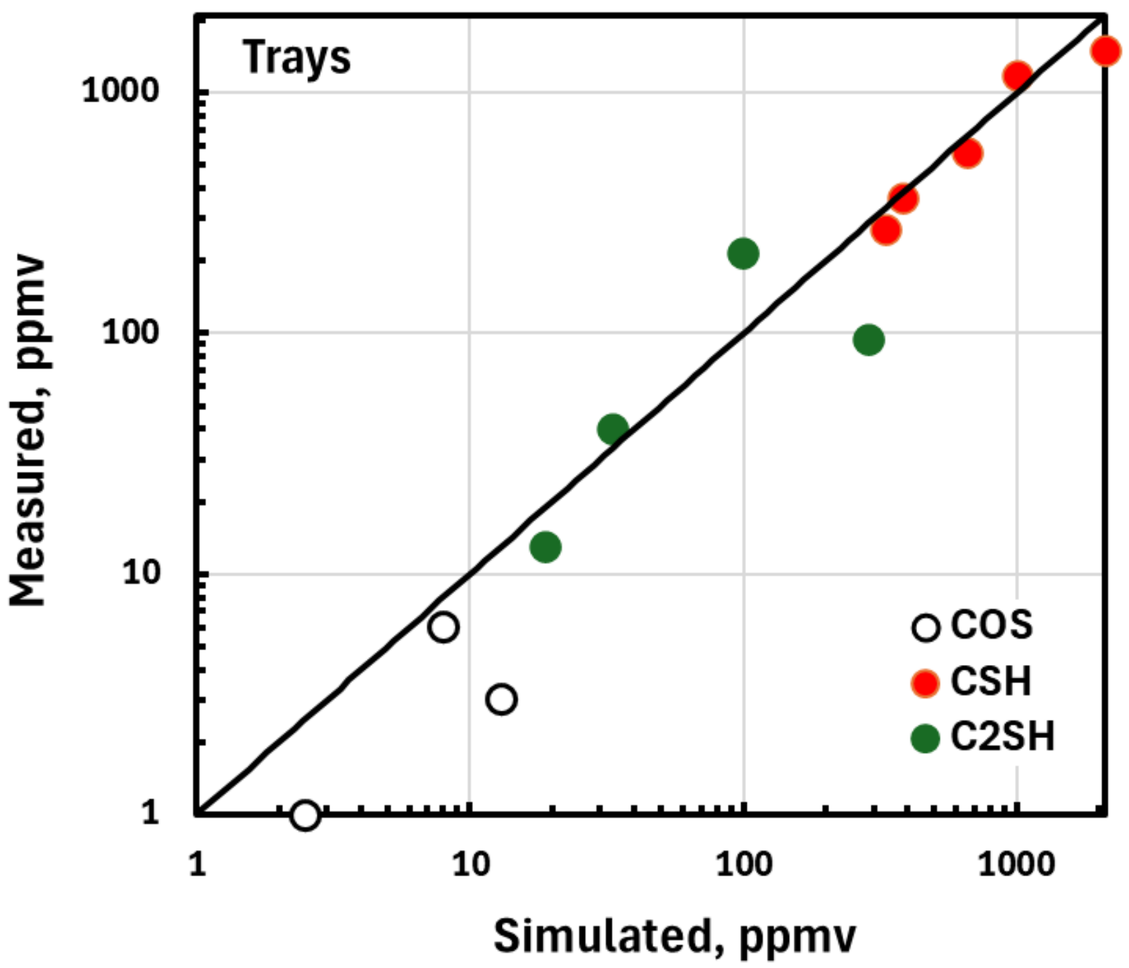
Model vs Data – H_2S

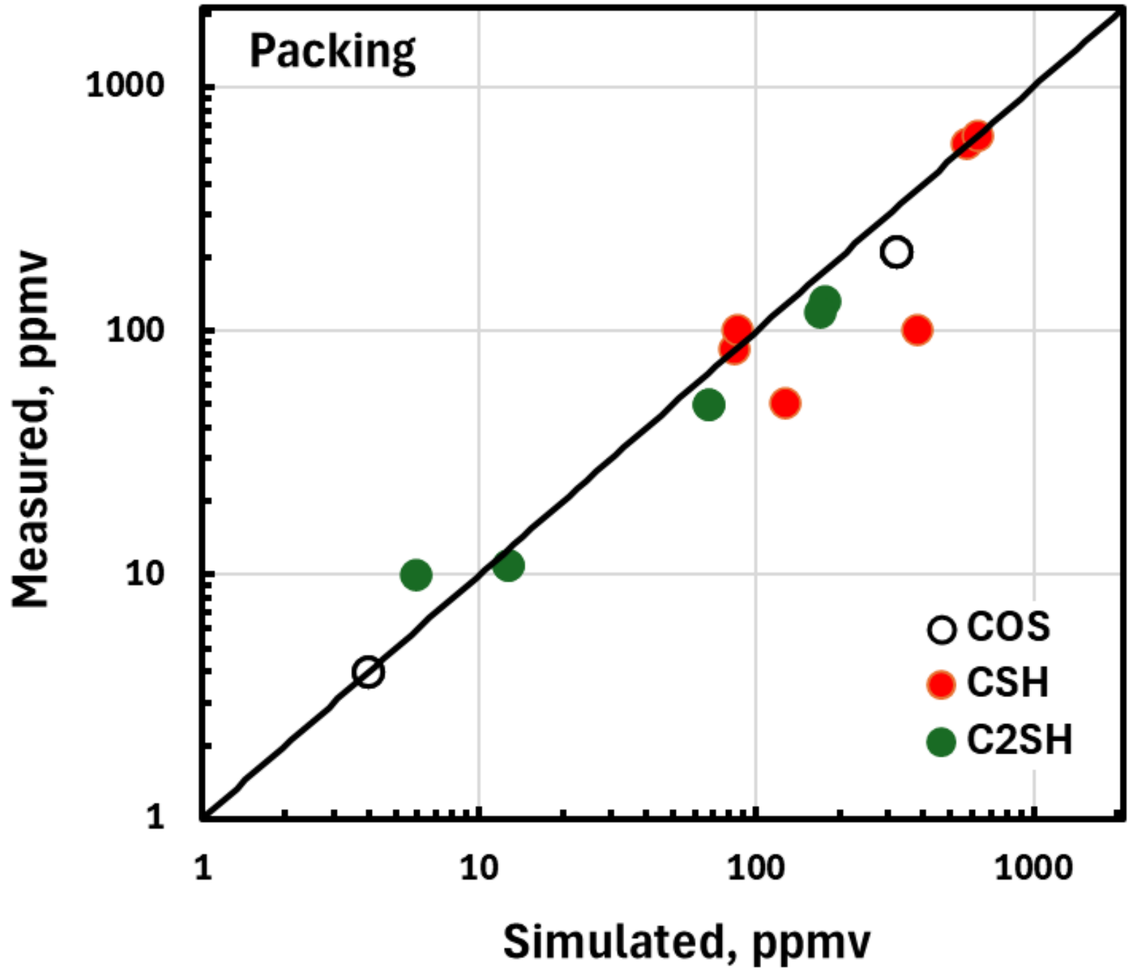
- H_2S in almost all cases were reported to be < 1 ppm
- Simulated predictions were in the range of 0.3 – 2 ppm

Model vs Data – H_2S



Model vs Data – Mercaptans and COS





Case Study - LPG Treating

- Removal of H2S, CO2 and other trace Sulphur species (COS and mercaptans)
- Solvent - DEA
- Compare performance of a single ideal stage against actual internals

Reactions – Mass Transfer Enhancement

$$H_2O \rightleftharpoons H^+ + OH^-$$

$$Am + H^+ \rightleftharpoons AmH^+$$

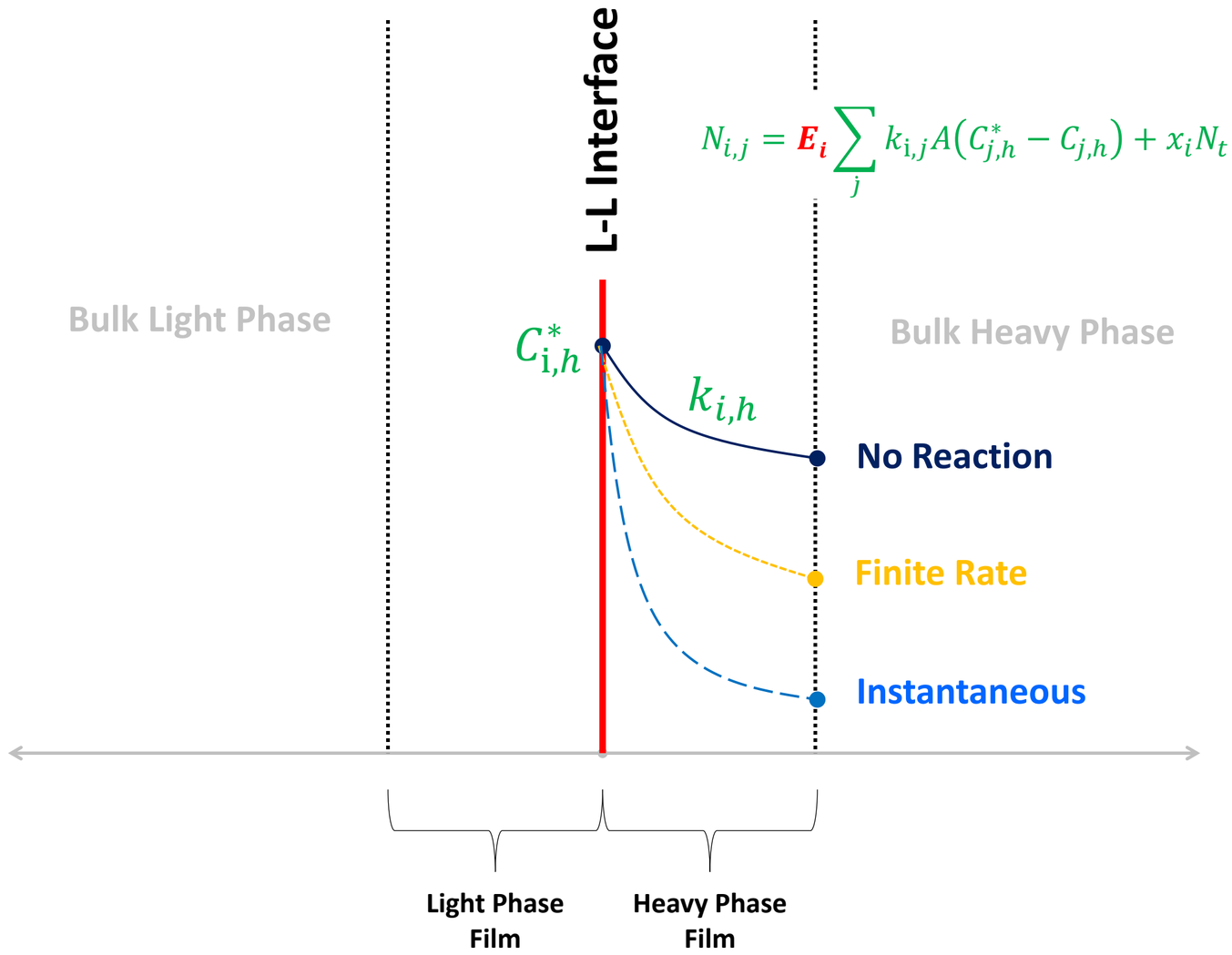
$$CO_2 + H_2O \rightleftharpoons H^+ + HCO_3^-$$

$$HCO_3^- \rightleftharpoons H^+ + CO_3^{2-}$$

$$2\,Am + CO_2 \rightleftharpoons AmH^+ + AmCOO^-$$

$$H_2S \rightleftharpoons H^+ + HS^-$$

$$HS^- \rightleftharpoons H^+ + S^{2-}$$



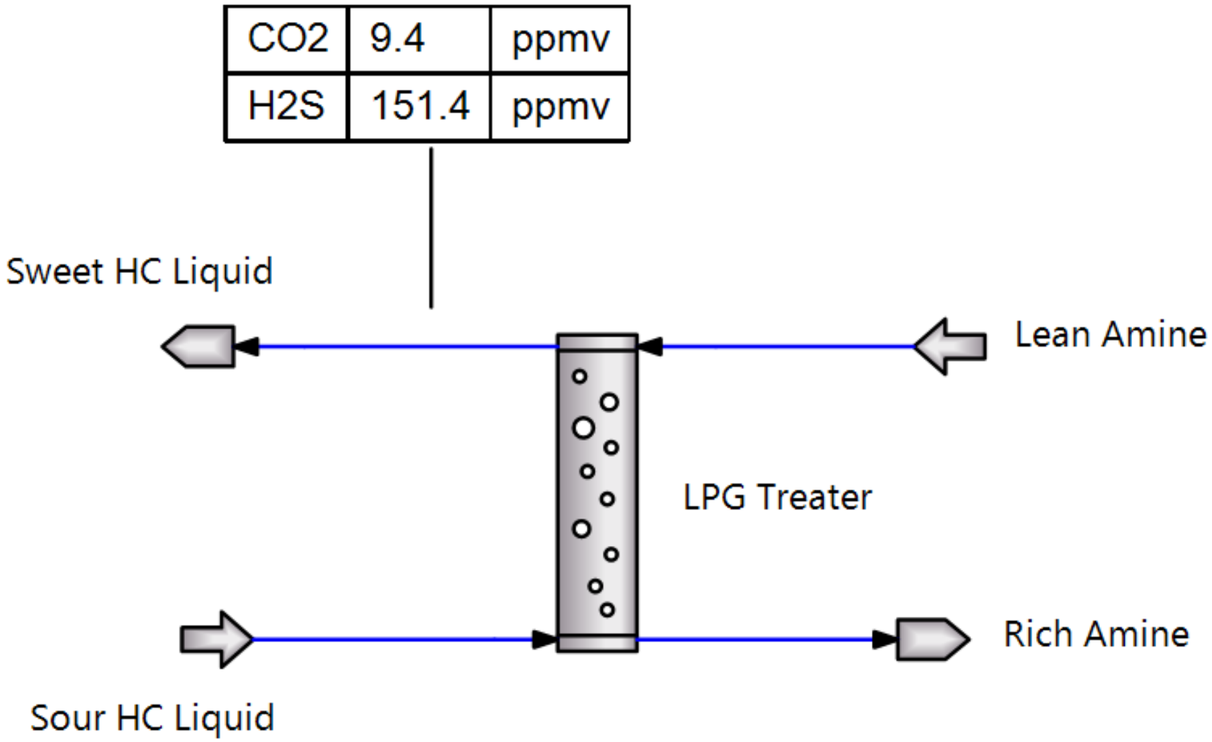
LPG Treater

LPG Feed

- 400 US Gal/min
- 5000 ppm CO_2
- 5000 ppm H_2S
- 500 psig
- Dispersed phase

Solvent

- 30 wt% DEA
- 100 US Gal/min
- Continuous Phase



Single Ideal Stage

Internals Comparisons

Internals	Specs	Performance	
		CO_2	H_2S
		ppmv	
Ideal Stage	**1 Equilibrium Stage**	9	151
Sieve Tray	2-ft Spacing 10-mm Hole, 10 % Open Area **5 Trays**	197	207
Packing	2” Raschig Rings **5.8 Feet**	213	157
Spray Column	10-mm Distributor Holes 15 % Open Area **44 Feet**	136	154

Internals Comparisons

Internals		Performance	
		CO_2	H_2S
Sieve Tray	Overall Efficiency	11 %	20 %
Packing	HETP (feet)	11	5.8
Spray Column		63	44

Ongoing & Future Directions

- Beta testing with customers
- Validation against operating plant data
- To be included in the upcoming OGT ProTreat® 9.0 release
- Implement agitated internals (RDC and Pulsed)
- Implement additional Mass Transfer and Hydraulic correlations
- Explore other applications apart from Propane and LPG treating

Thank you

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