Mass Transfer Rate Modeling Basics

Nathan A. Hatcher, P.E.

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Outline

- History of Process Simulation
- Briefly about the ProTreat® Simulator
- Characteristics of True Mass Transfer Rate Based Models
- The Ideal Stage
- Elements in a Rate Model

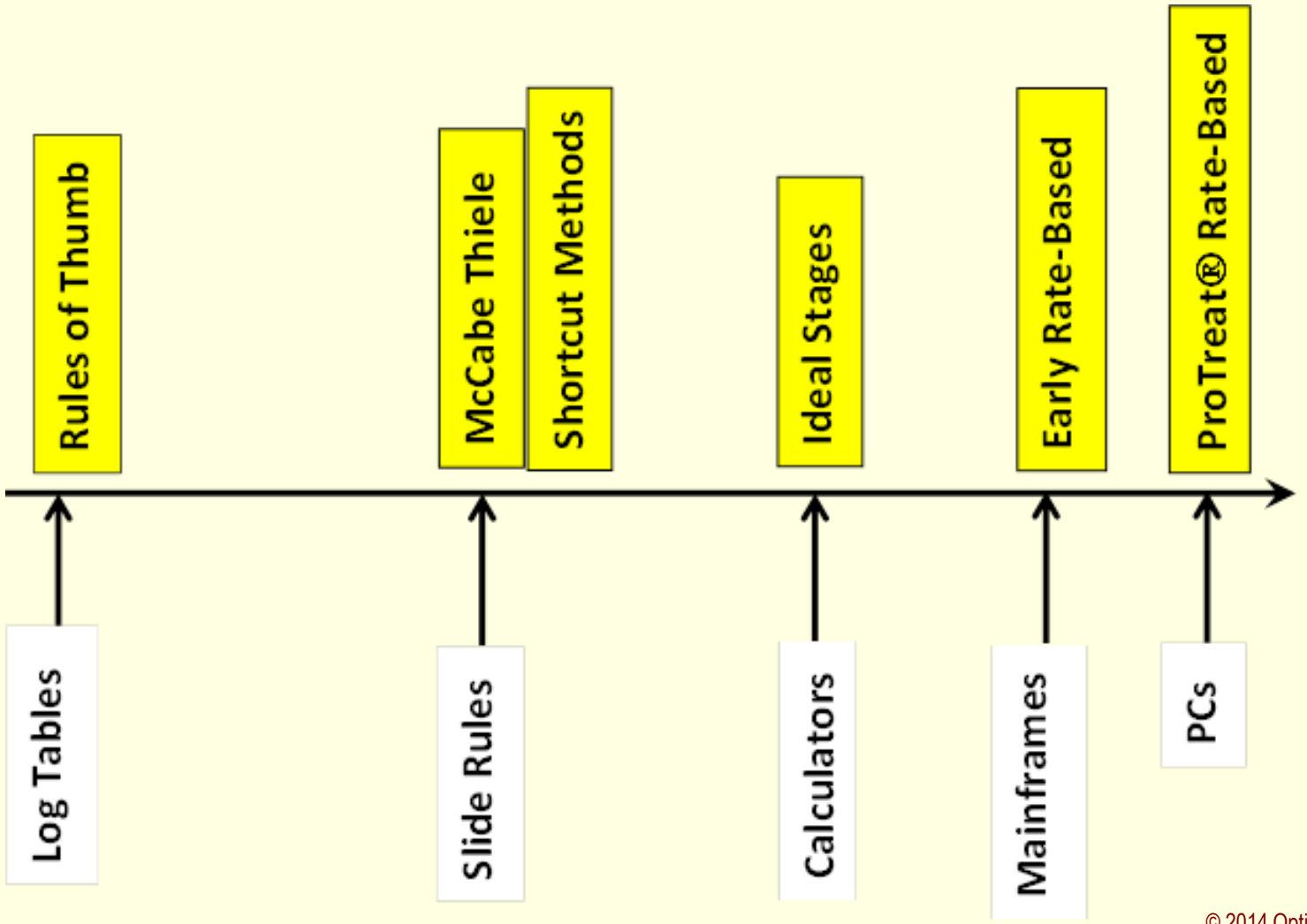
Background

- Survey……
- Process simulations are:
  - Physical and chemical mathematical models for processes taking place in process equipment
- Equations are either:
  - Empirical or Physically based

Brute force curve fits

Chemistry
Material & Energy balances
Vapor Liquid Equilibrium (VLE)
Mass & Heat Transport

Process Simulation Paleontology



Process Simulation

- Advantages over Hand Calculations
  - Speed of Computation
  - More Realistic Models
    - Better represent reality
    - Predictive and more confident extrapolation
- Match the Model to Needs

About ProTreat®

Mid 60s to Mid 80s	Dr. Ralph Weiland's university research on mass transfer rate modeling for mainframe computers (supported by Dow Chemical) led to the development of mass transfer rate models of AspenTech and SimSci
Late 80s	Engineering computations migrate from mainframes to PCs with Microsoft's launch of Windows®
1992	OGT, Inc. founded by Weiland & Dingman specifically to develop a rate-based simulator for Windows
2003	Commercial introduction of ProTreat®

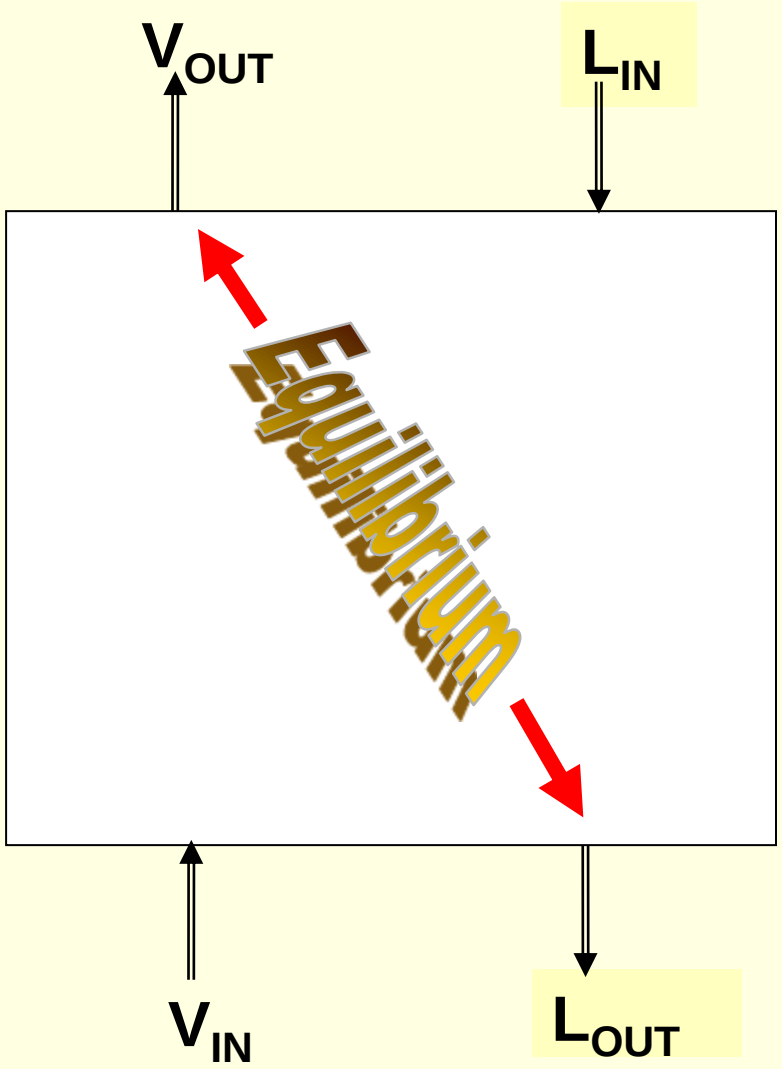
What can *ProTreat®* simulate?

- All amines plus 2- & 3-amine blends
- Physical solvents: DMPEG, MEG, DEG, TEG
- Specialty solvents
- Hydrocarbon, BTEX solubility
- Rate-based mercaptans, HCN, Phenol
- Heat Stable Salts (ionic contaminants)
- Ammonia & Sour Water Stripping
- Caustic treating with NaOH and KOH
- H_2S / CO_2 corrosion in amine and sour water

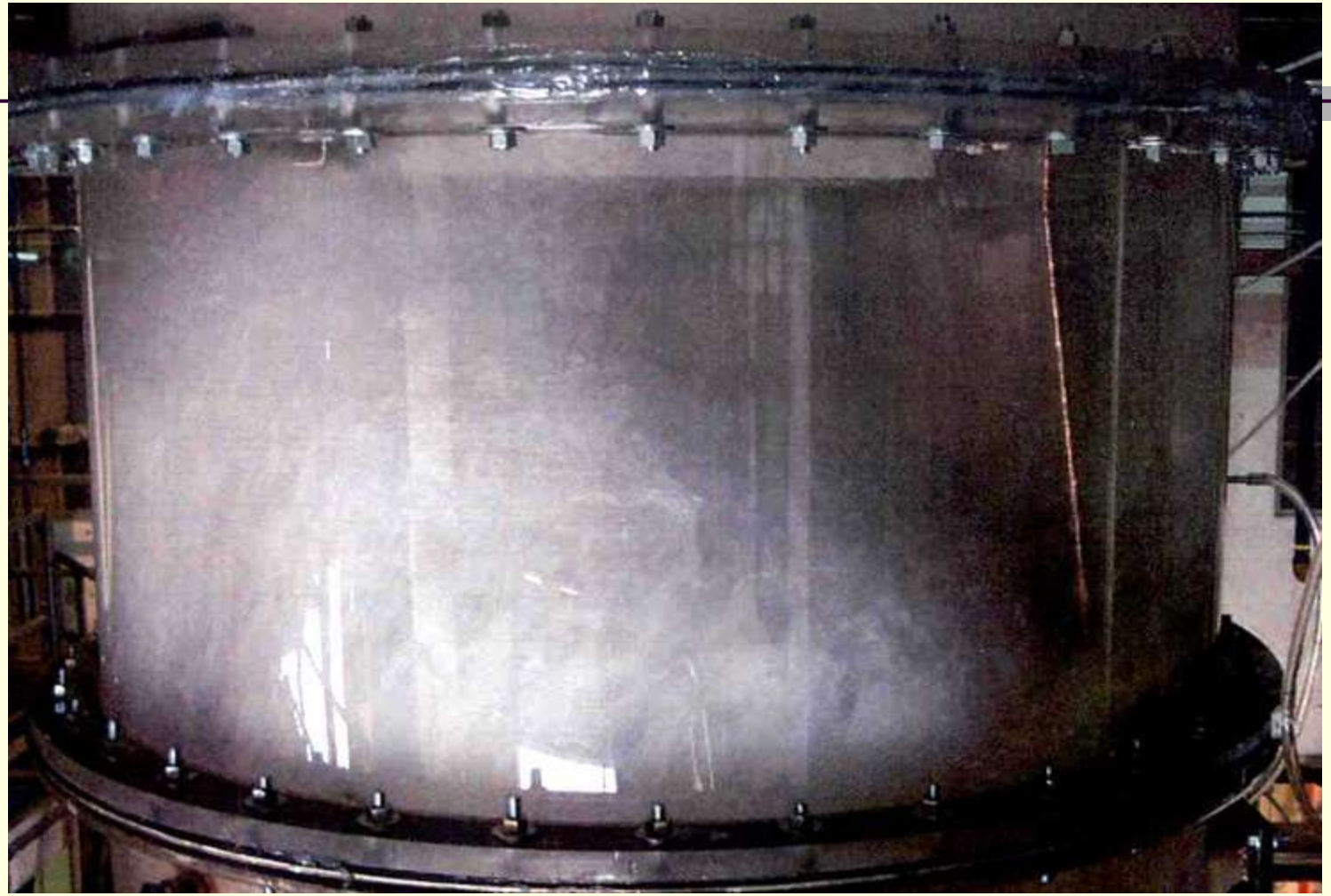
True MTR Distillation

- Directly calculates tray-by-tray & packed segment-by-segment performance
- No translation from ideal stages to real tower internals
- Real trays, random packing, structured packing — hydraulics & mass transfer
- Chemical reactions modeled and accounted for enhancement to mass transfer
- Flows/T/P/Composition impact separation through mass transfer as well as VLE

The Ideal Stage



Low Gas Flow

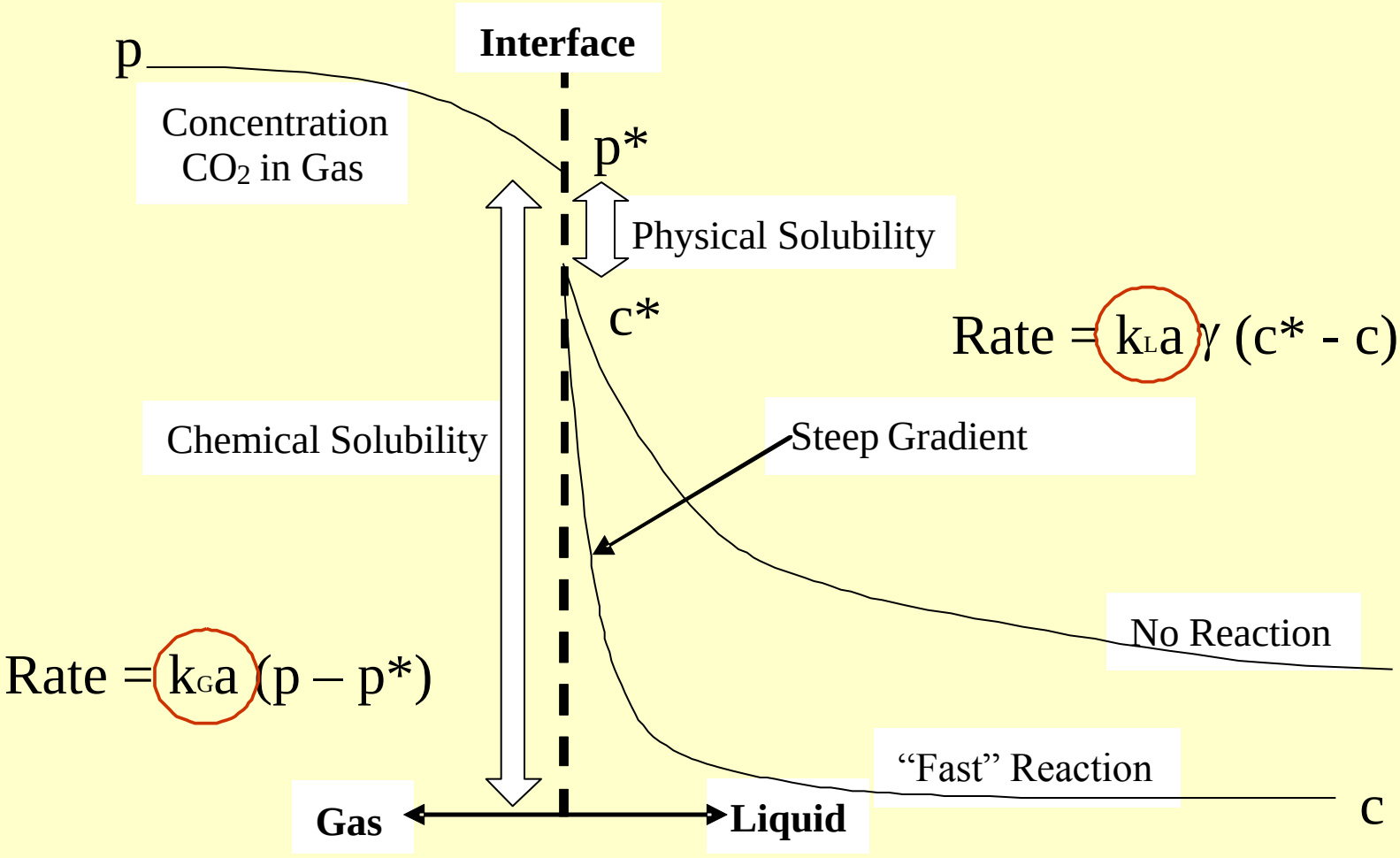


Medium Gas Flow

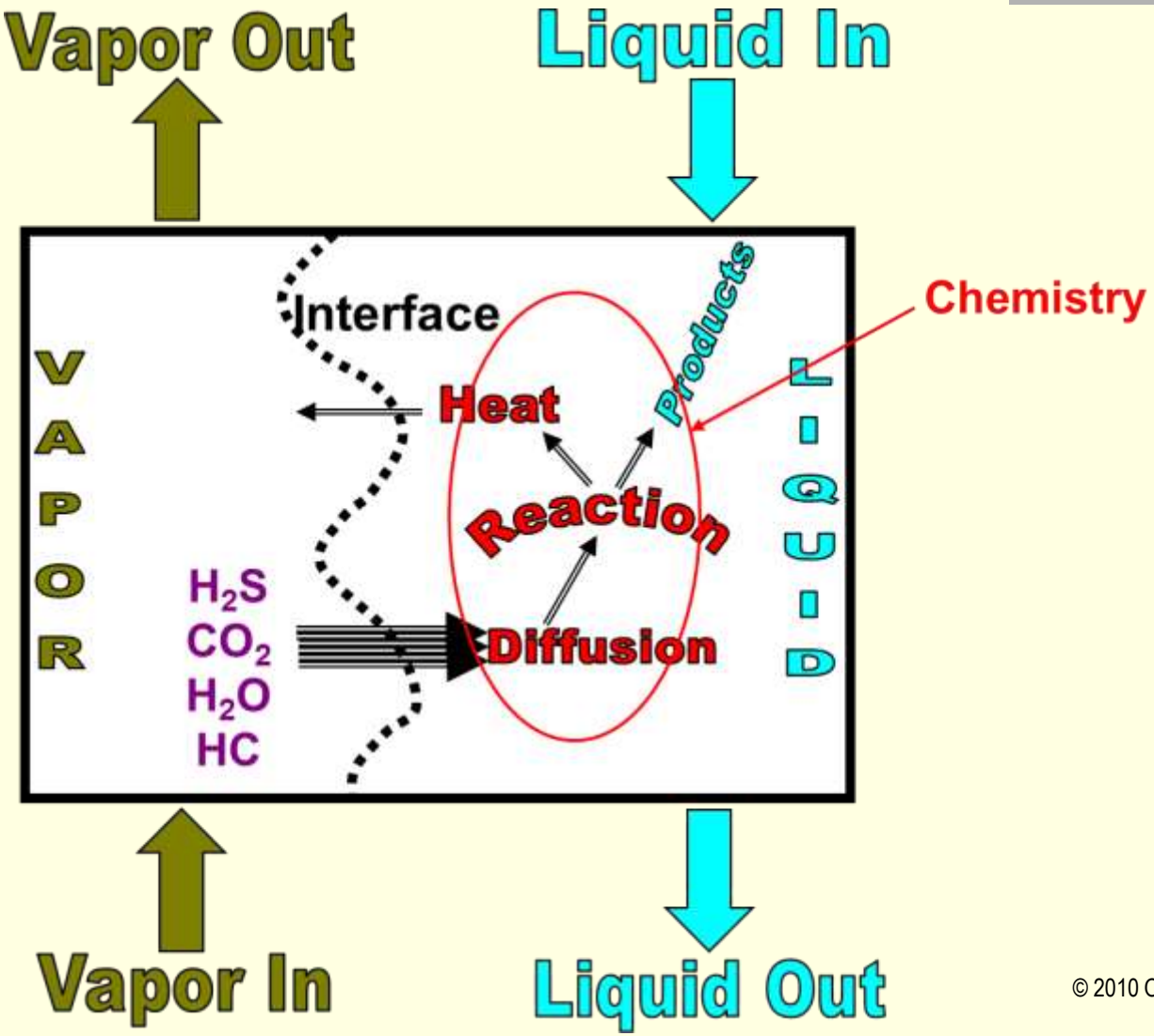
High Gas Flow

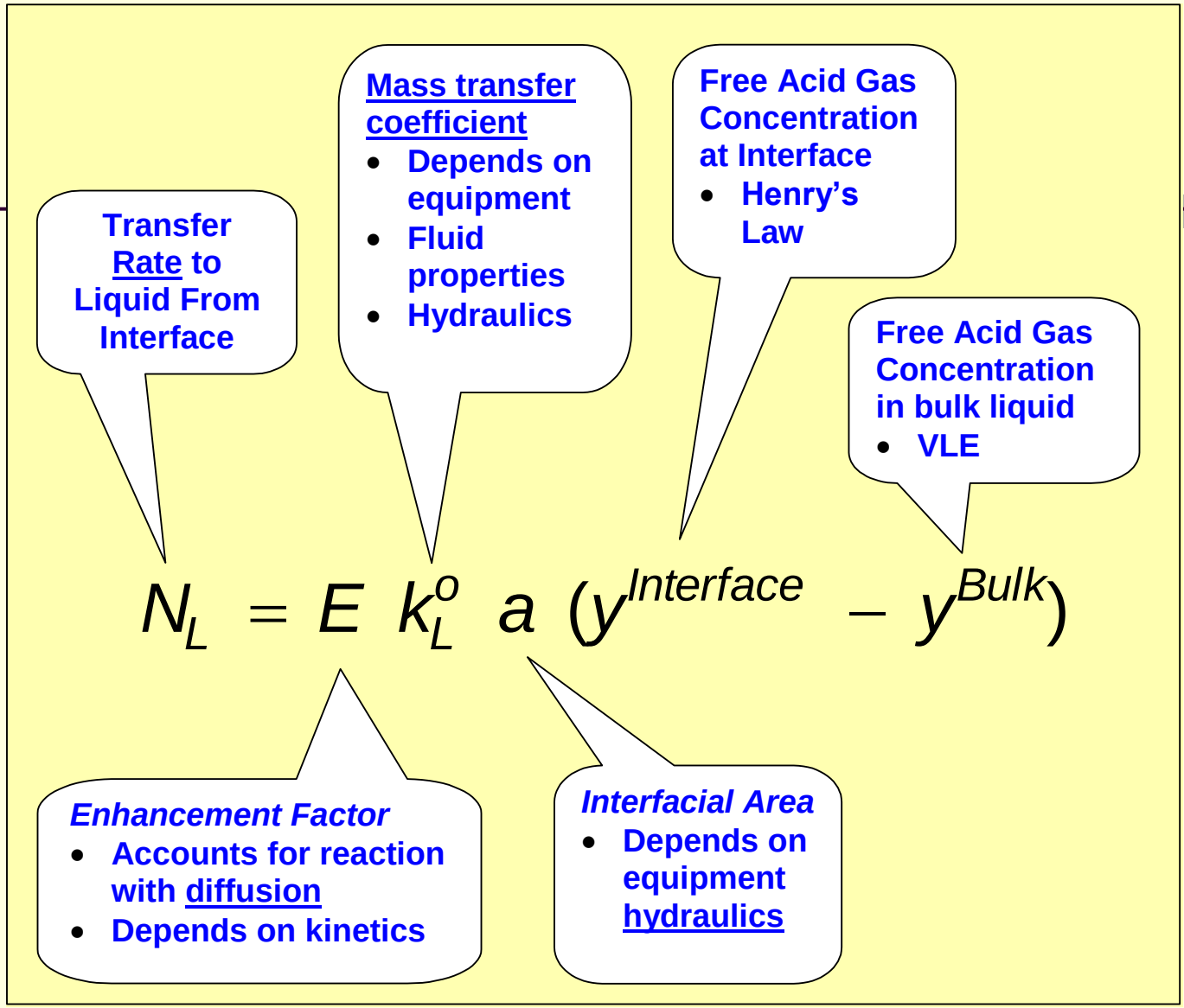
Onset of Flood in Structured Packing

Mass Transfer – Gas Absorption



MTR Segment





Mass Transfer Rate

Depends on...

- Area available for mass/heat transfer
- Phase resistances
  - Gas & liquid loads
  - Hydraulics (specific tower internals)
  - Physical properties (density, viscosity, diffusion)
- Driving force (extent that phases are not in equilibrium)

Mass Transfer Rate

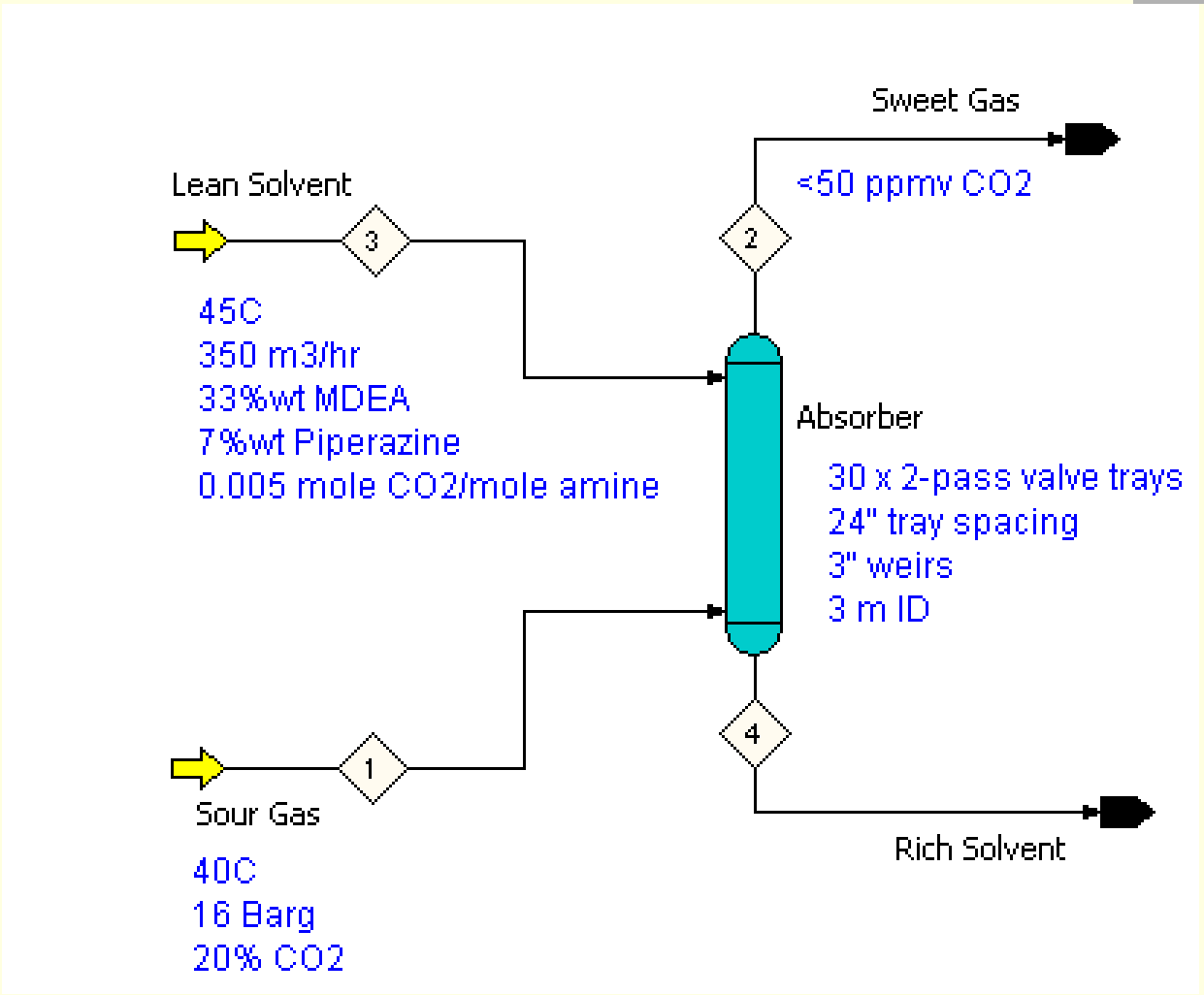
Results…

- Learn how much CO_2 and H_2S are actually removed on each individual REAL tray and in each segment of REAL packing
- You are *not* asked for
  - Number of theoretical stages
  - Liquid holdup per theoretical stage
  - Tray efficiency or packing HETP
- You *are* asked for
  - Tray details (as per tray drawings)
  - Column details (as per PFDs)
  - Packing type & size by Vendor designations (as per PFDs)

Phase Equilibrium

- Just as important as in ideal stage models
- But not the whole story
- If the VLE is wrong, the rate model will follow suit

Case Study



Ideal Stage "Tuning"

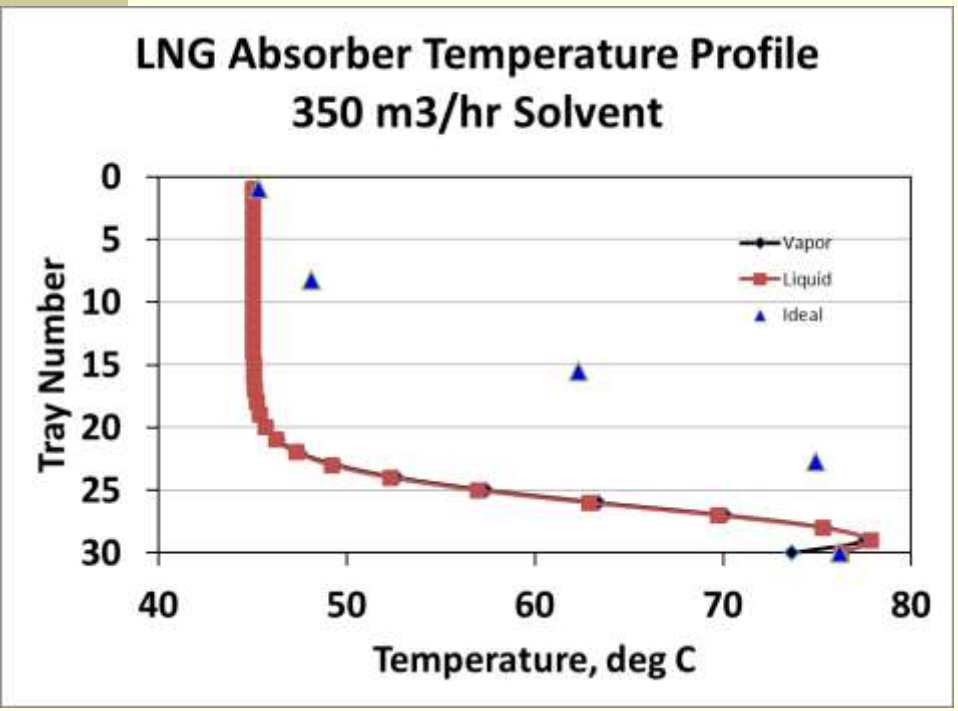
Match CO_2 performance at 350 m3/hr solvent

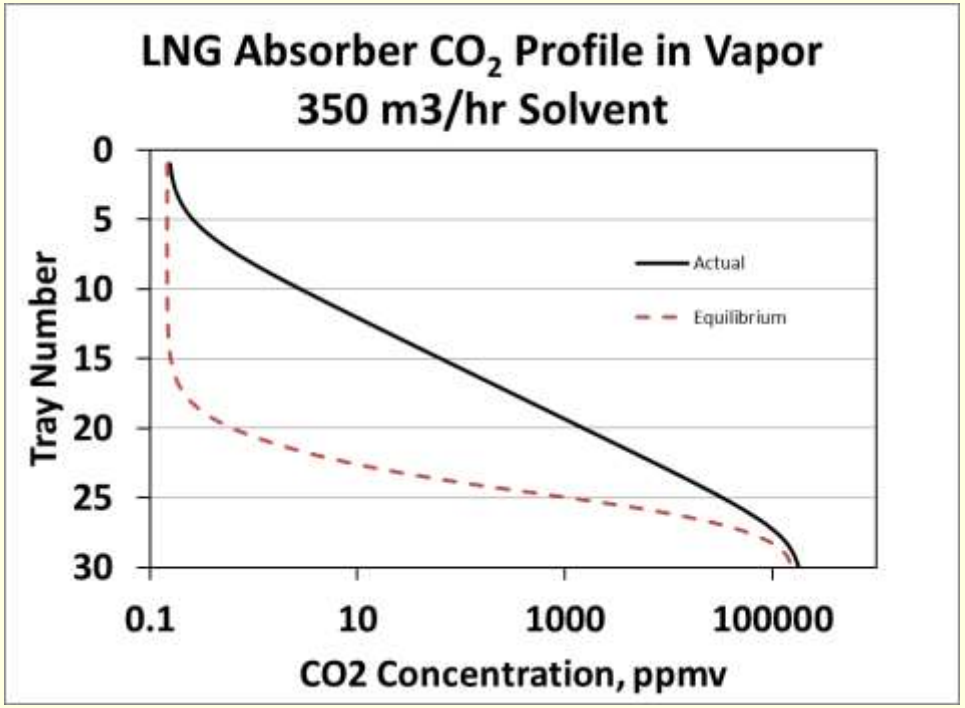
Ideal Stages	CO2 Out, ppmv
3	745
4	1.14
5	0.150
6	0.146

← Closest representation

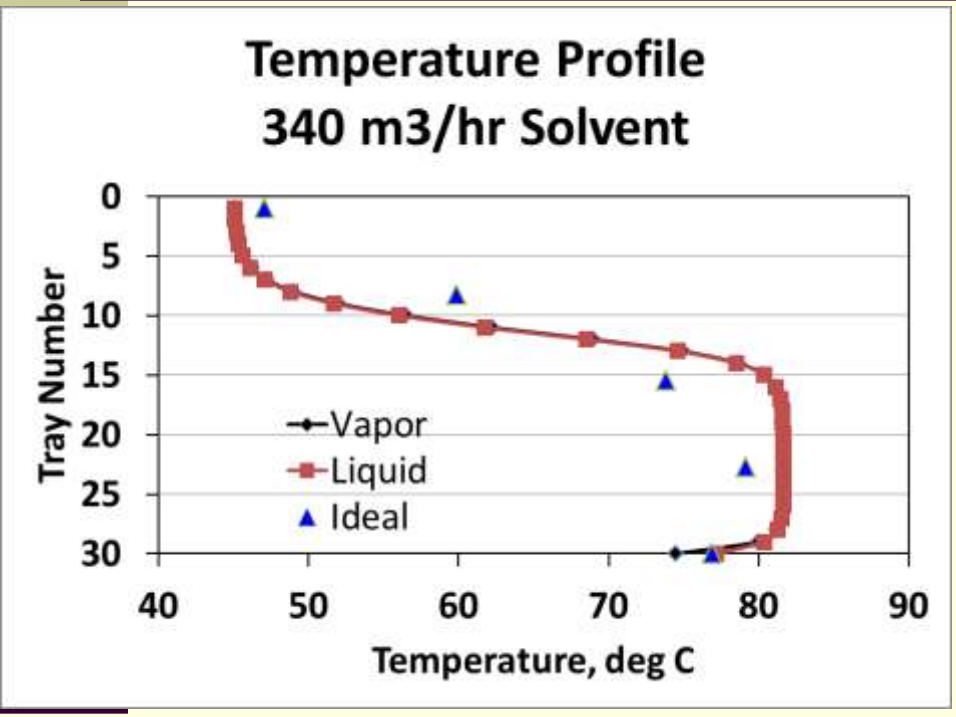
ProTreat Rate Model Outlet CO2: 0.156 ppmv

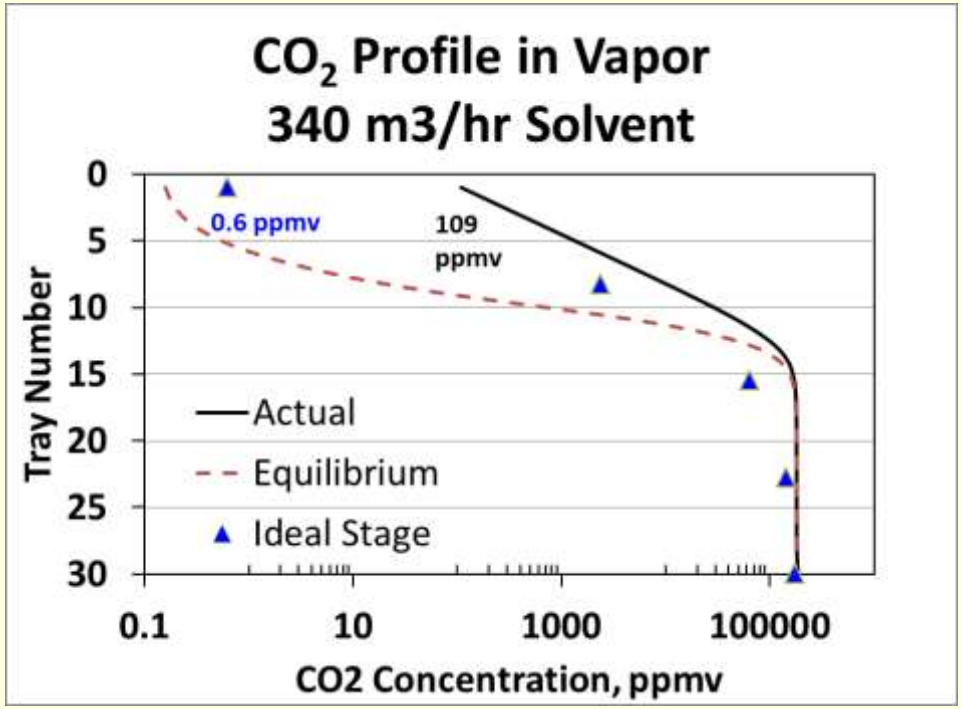
Column Profiles
350 m3/hr Solvent Rate





Column Profiles
340 m3/hr Solvent Rate



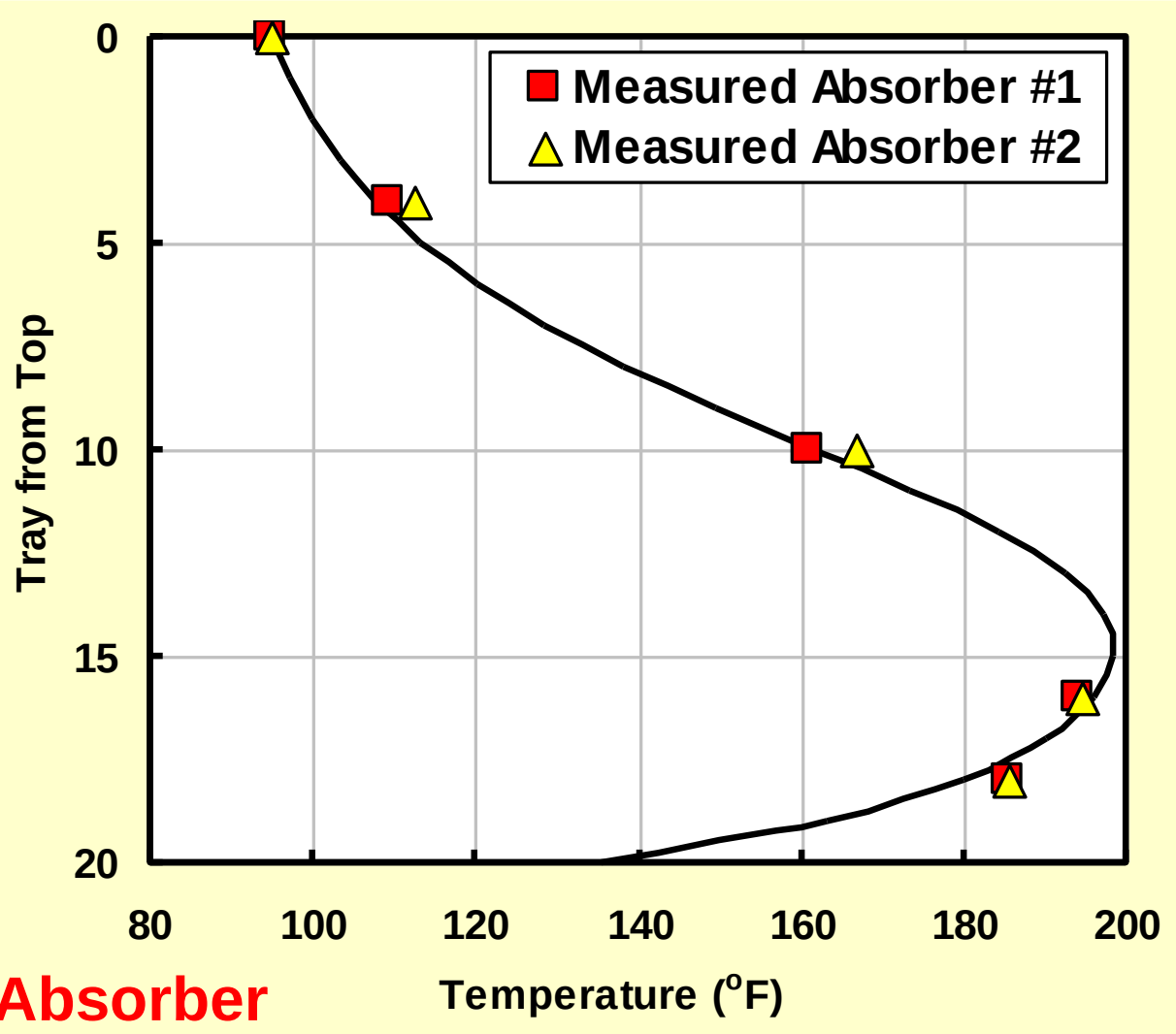


Mass Transfer Rate Models

- Answers don't depend on how well you can play the "guess the efficiencies" and "guess a residence time" game. They depend on what the tower internals can really do!
- A mass transfer rate model sets up a virtual plant based on REAL WORLD REALITY and sound engineering science
- You don't pick parameter values to match the data — the simulation matches good data or you go looking for what's wrong with the plant

Why a Rate Model?

- Predictive
  - Tower internals do matter, packing characteristics (type, size, structured, random, etc.) enter directly into calculations
- Highly reliable for selective gas treating
  - Selectivity is a competition between CO_2 and H_2S absorption rates.
- Works correctly with mixed amines
  - Mixed amine performance depends on altering mass transfer rates, and mass transfer rates are the very basis of a rate model



Gas Treating Absorber Temperature Profile

Summary

- Directly tied to internals type, detail, & operating conditions via hydraulics & quality of contact
- Separation depends on physical & transport properties (c_P, μ, σ, ρ) — so does the rate model
- A truly predictive tool—needs no operating experience to get answers
- Relates to actual hardware
- Tells you what a plant *should* be doing

ProTreat®

Taking the Guesswork

Out of Process Simulation