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Transforming Process Industries

RAPID RACER AMPD: Back to the Future

Cheryl Teich
Teich Process Development LLC
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AIChE Process Development Division Webinar
7 June 2023

Process Development is What Brings Us Together

Successful PROCESS DEVELOPMENT*

Safe

Sustainable

Manufacturing USA®

RAPID RACER AMPD

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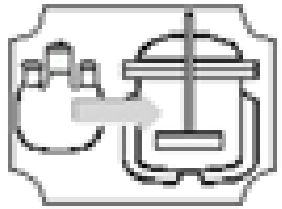
PROCESS DEVELOPMENT SYMPOSIUM



Process Development Division

AIChE The Global Home of Chemical Engineers

***Kamlesh Bhatia, DuPont (ret.)**
"The goal is commercial success."

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RAPID is part of Manufacturing USA®

Electronics	Materials	Energy/ Environment	Digital / Automation	Bio-Manufacturing
AIM photonics Integrated Photonics *Albany, NY* *Rochester, NY*	AFFOA Advanced Fibers and Textiles *Cambridge, MA*	RAPID Modular Chemical Process Intensification *New York, NY*	America Makes Additive Manufacturing *Youngstown, OH* *El Paso, TX*	biofabusa Regenerative Manufacturing *Manchester, NH*
NEXTFLEX Flexible Hybrid Electronics *San Jose, CA*	iacmi THE COMPOSITES INSTITUTE Advanced Composites *Knoxville, TN* *Detroit, MI*	REMADE INSTITUTE Sustainable Manufacturing *Rochester, NY*	ARM Advanced Robotics *Pittsburgh, PA*	NIMBL Biopharmaceutical Manufacturing *Newark, DE*
POWERAMERICA Wide Bandgap Semiconductors *Raleigh, NC*	lift Lightweight Materials *Detroit, MI*	CESMII Smart Sensors and Digital Process Control *Los Angeles, CA*	MxD Digital Manufacturing *Chicago, IL*	BioMADE Bioindustrial Manufacturing *St. Paul, MN*
			CYMANII Cybersecurity *San Antonio, TX*	

- Public-private partnership model to drive U.S. advanced manufacturing competitiveness
- Brings $1B (federal) and over $2B (private) to R&D, tech demonstration, and education
- Innovating new ways to manufacture in the U.S.
- Developing the next generation workforce

https://www.manufacturingusa.com/

Focusing on the Process Industries

- Manufacturing sector consumes ~25% of total US energy.
- Process industries are the largest consumers in the manufacturing sector.
- Process generally means integrated flow systems (solids, liquids, gases) not discrete products.
- Evolving process design and development to reduce the energy footprint of these industries.

Primary Metals
1608 TBTU

Petroleum Refining
6137 TBTU

Chemicals
4995 TBTU

Wood Pulp & Paper
2109 TBTU

Glass & Cement
716 TBTU

Food Processing
1162 TBTU

Adapted from Phil Westmoreland (2019)

RAPID's Mission

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Transforming Process Industries

RAPID's Institute Metrics...

- +20% Energy Efficiency
- 2X Energy Productivity
- 1000hr Pilot Demonstration
- 33 R&D Portfolio
- 50 Train-the-trainer
- 500 Educate Students
- $5M Self-Sustainment
- Industrial Roadmap
- −20% Module Cost
- −50% Cost of Deployment
- Diversity
- Annual Planning
- Supply Chain
- 31 Industrial Partnership

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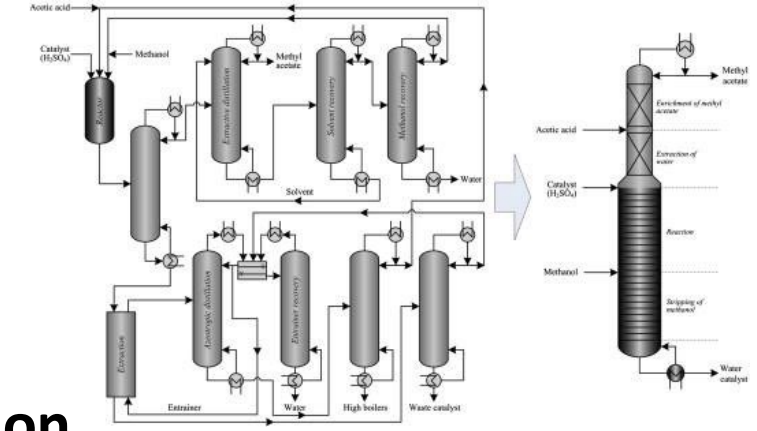
Modular Chemical Process Intensification (MCPI)

Modular Processing

- Rethinking systems to enable flexible, **distributed manufacturing**
- Shift from **bigger is better** paradigm to **small, modular** paradigm
- Transition from volume scaling to **numbering up**

Process Intensification

- Rethinking processes to dramatically **improve performance**
- Shift from **unit operations** paradigm to **integrative** paradigm
- Transition from **batch to continuous**
- Enable **decarbonization**



What is Process Intensification?

The RAPID Community: Academia, Industry, Federal Partners

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NIST Funded RAPID RACER AMPD under the American Rescue Act (Financial Assistance Award 70NANB22H006)

1. Develop and disseminate an accelerated process development framework that takes advantage of standardized modular process operations.

2. Setup and operate a modular process development Center of Excellence (COE) at AVN (formerly MATRIC) in South Charleston, WV, that will serve as a national asset testbed for future coronavirus response and a hub for job creation in the underserved Appalachian region.

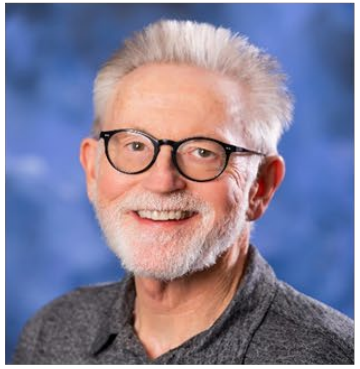
3. Demonstrate the accelerated process development framework for a currently offshored API precursor specialty chemical.

Never Let a Good Crisis Go to Waste: RAPID RACER AMPD and the Opportunity to Accelerate Modular Process Development

Patricia Gillenwater

Ignasi Palou-Rivera

Jack Dever



Mike Burgess

Rob Nunley

Teich Process Development LLC

Cheryl Teich

Nima Yazdanpanah

RAPID AMPD Tasks Overlap by Necessity

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Task 6 Report to NIST and Stakeholders Throughout Two Year Program

Teich Process Development LLC

Task 1 Benchmark Historical Process Development

Task 2 Construct Accelerated PD Framework

Task 3 Identify Precursor Candidates

Task 4 Construct Modular Testbed

Task 5 Validate Experimentally

PROCEGENCE ADVANCED MANUFACTURING AND EMERGING TECHNOLOGIES

AVN

RAPID AMPD Presentations (*Task 6*):

- **2022 AIChE Process Development Symposium (PDS)**
- **2022 AIChE Annual**
- **2023 PDS (June 13 – 15, 2023)**

March 2022 — March 2024

What We've Heard from Process Development Experts

- Chemical processing has not leveraged real advantages of modular designs
- Modular Technologies
  - Aren't "plug and play"
  - Still require significant process development
  - Follow same work process as non-modular equipment
- Why/how we "do" modular
  - Build at fabricator/designer's site: easier, cheaper, safer, minimizes downtime
  - Truck dimensions dictate skid and equipment sizes
  - Modules aren't "off the shelf"; each requires its own engineering
- In any case, it's all about the mass balance
  - "Know your Process" before using advanced modeling tools

June 22-25: 20th Anniversary of the

Frits Dautzenberg
ABB Lummus

Arthur Andrews
Merck

Kenneth Kem
Air Products

John Sofranko, Cawas Cooper (z"l)
AIChE Air Products

Dan Green DuPont | Christine Moore Pfizer | Ed Paul Merck | Paul Szabo Xerox | Kevin Joback Molecular Knowledge

Aaron Sarafinas
Rohm and Haas

Why are PDD T-shirts black?

Ed Paul (z"l)

Joe Cramer (AIChE), Terri Guitella (AIChE), George Liebermann (Xerox)

Chris Seymour
Pfizer

John Peragine
BMS

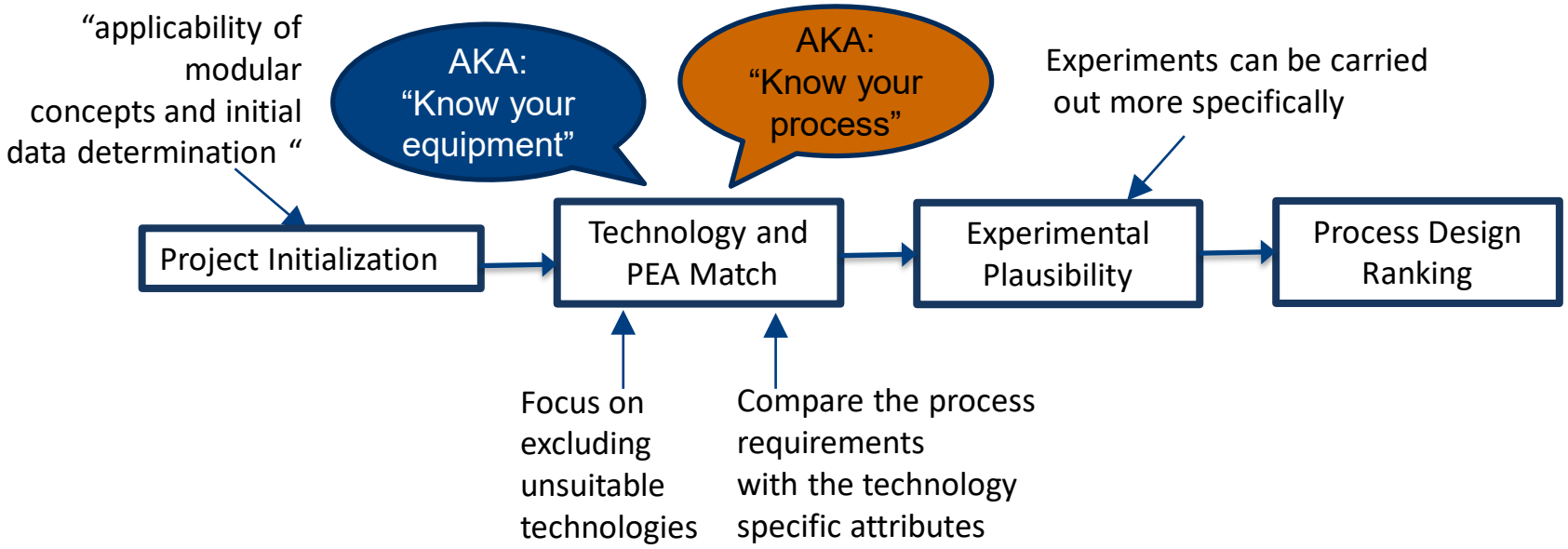
Christine Moore
Pfizer

https://web.archive.org/web/20050829025300/http://pd-aiche.com/archive/

Thanks to Ray Rooks

Benchmarking Process Development: "Everything Old is New Again"

"General approach for technology and Process Equipment Assembly (PEA) selection in process design", Schindel et al., Chem Eng & Proc: Process Intensification 159 (2021) 108223



Benchmarking Process Development: "Everything Old is New Again"

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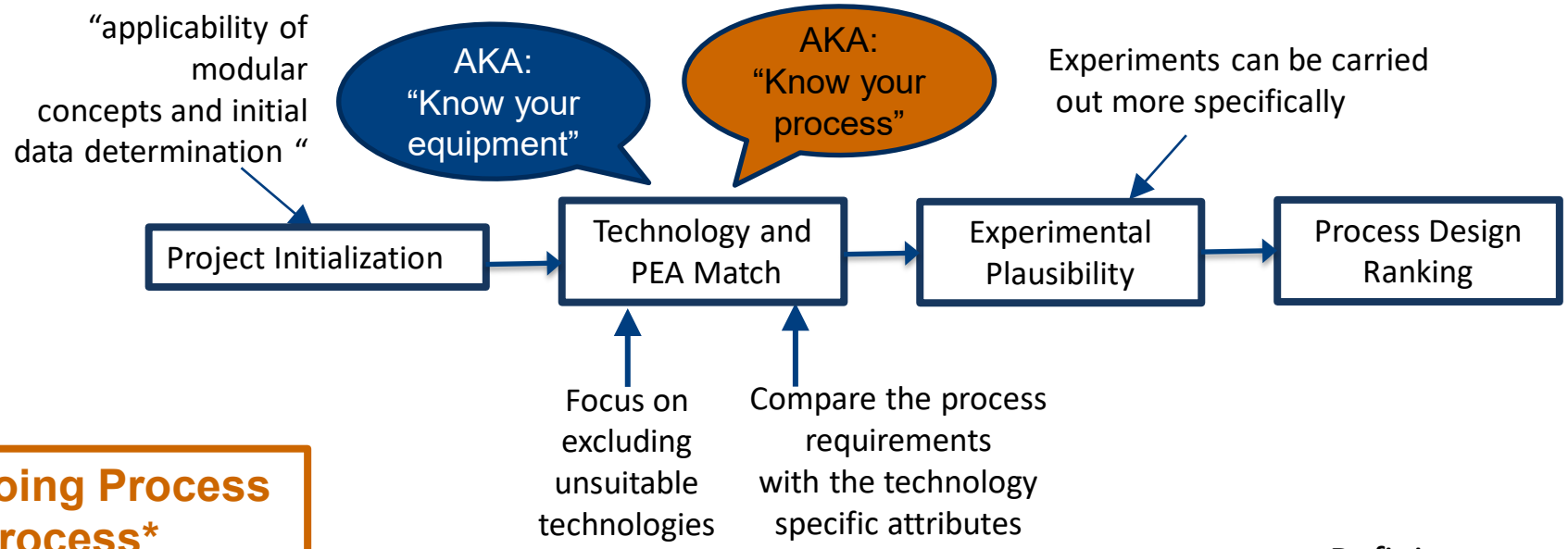
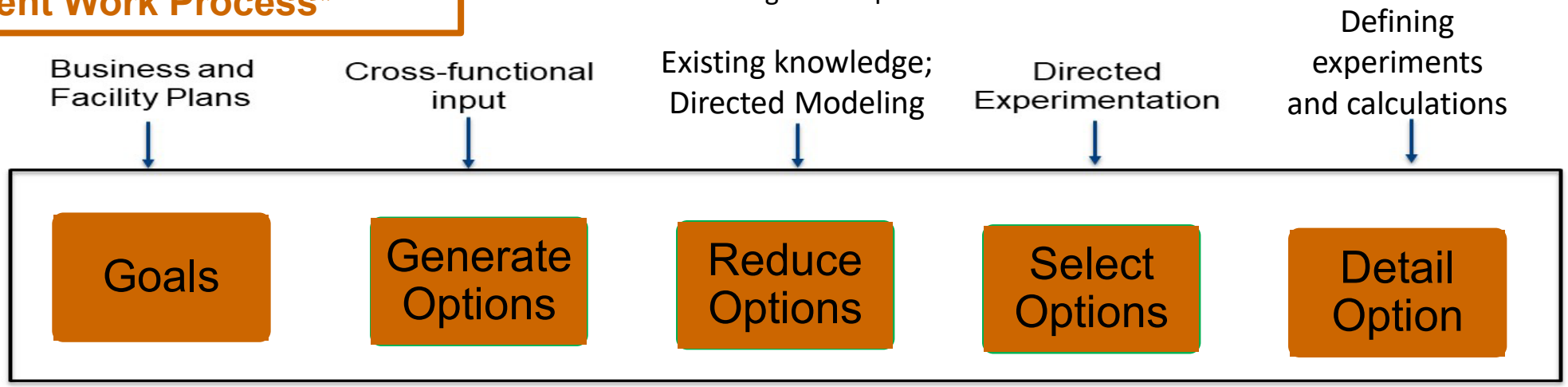


Rohm and Haas Ongoing Process Development Work Process*



**Aaron Sarafinas, Rohm and Haas Company, "Successful Process Development: Profitable Specialty Chemical Products Using Winning Work Processes, AIChE Process Development Symposium, June 2003*

"New" Process Equipment Assembly Workflow Aligns with Established Workflows in Other Organizations

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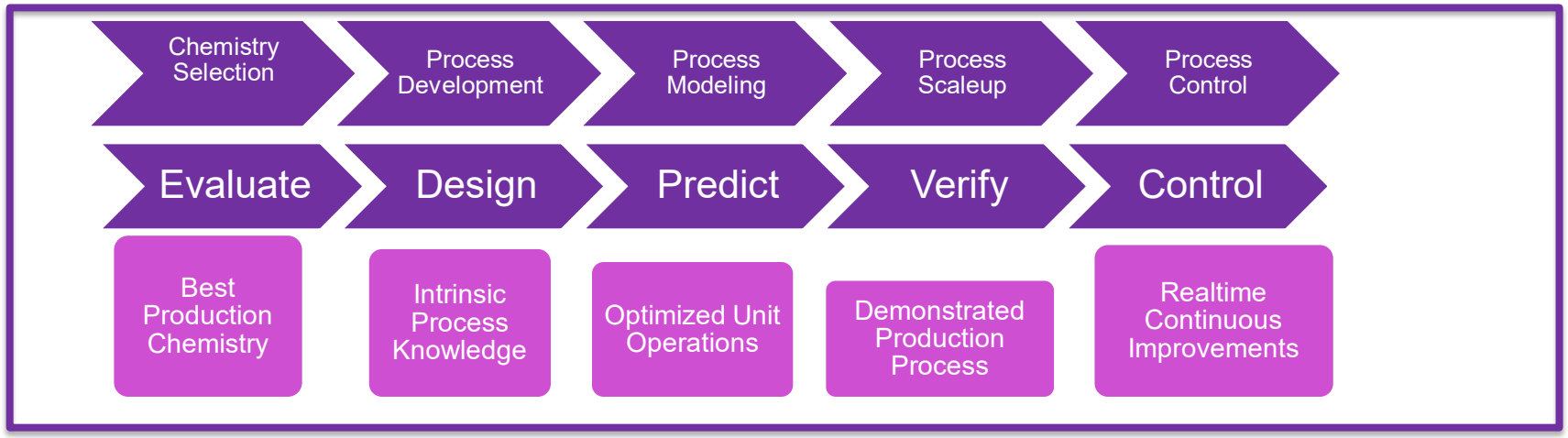
San Kiang, BMS, 2003 PDS

BIG Pharma



Paul Szabo, Xerox, 2003 PDS Specialty Chem

Molecular Design | Synthetic Chemistry | Process Optimization | Benchscale Engineering | Scale-Up | Process Design | Plant Design and Operation

Need Identification

Product Design

Basic Chemistry Detailed Chemistry

Task Identification

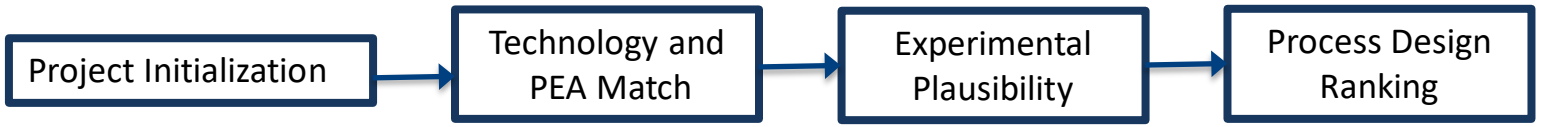
Equipment Design

Vendor Equipment Tests

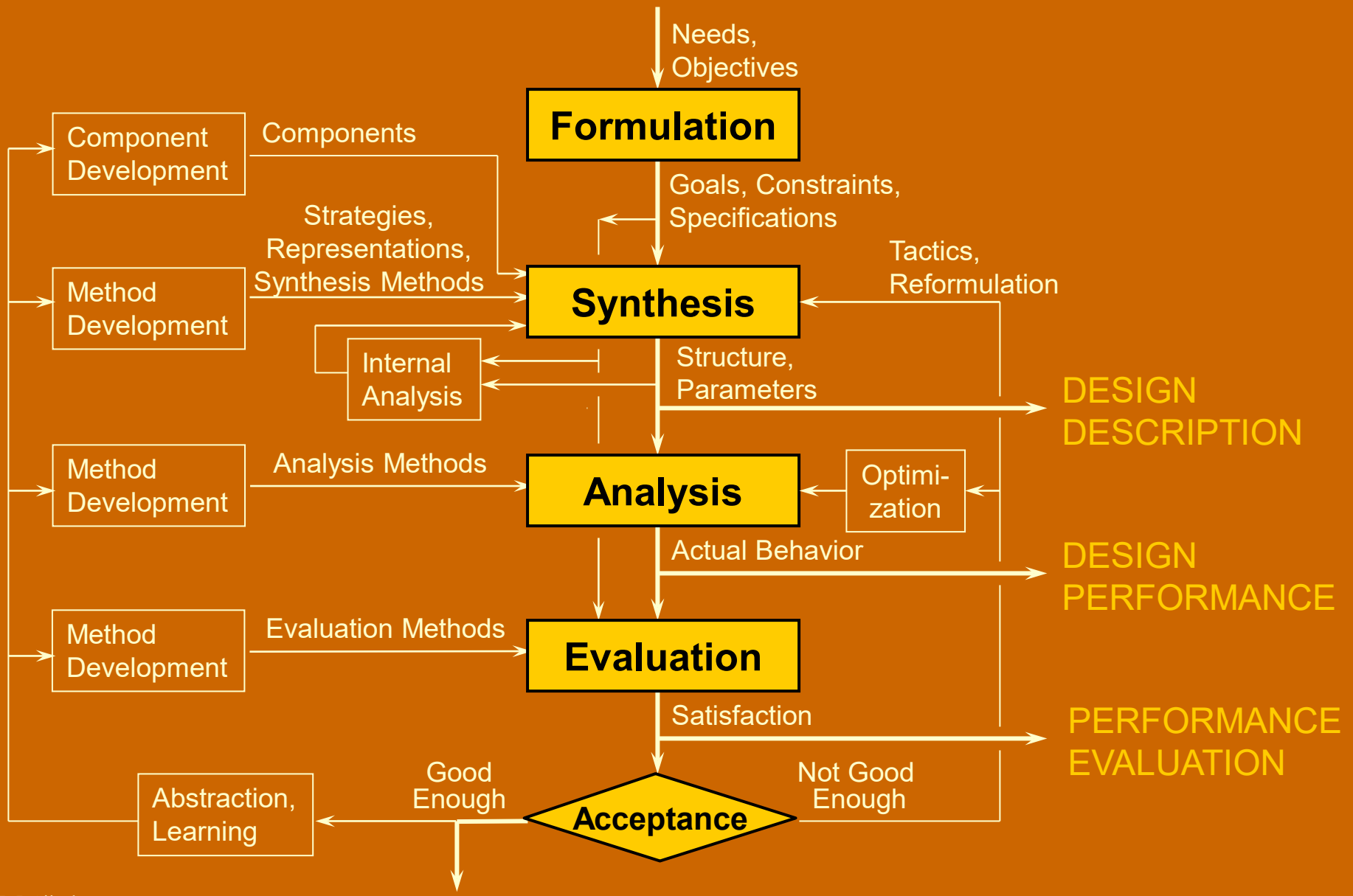
Equipment Design
Plant Engineering
Detailed Engineering
Vendor Specifications
Component Acquisition
Construction Plan, Schedule
Plant Construction
Operating Procedures
Commissioning/Startup
Production Plan/Schedule
Operation

Large-scale, Commodity Chem

Schindel et al., Chem Eng & Proc: Process Intensification 159 (2021) 108223



Siirola Design Paradigm



Jeff Siirola

Technology Fellow (ret.), Eastman Chemical Company

Professor of Engineering Practice, Purdue University

Adjunct Professor of Chemical Engineering, Carnegie Mellon University

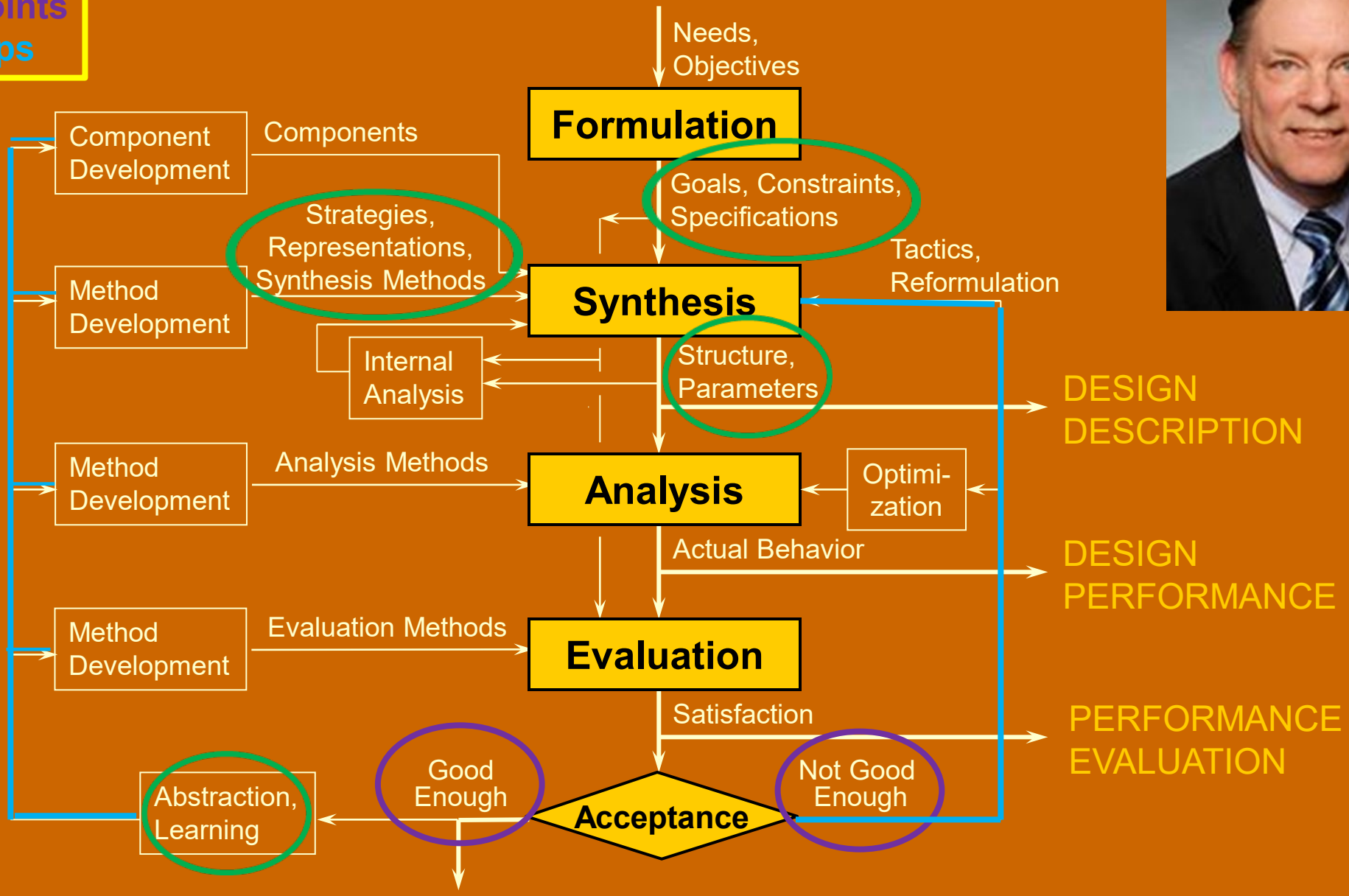
Member, National Academy of Engineering

AIChE Fellow

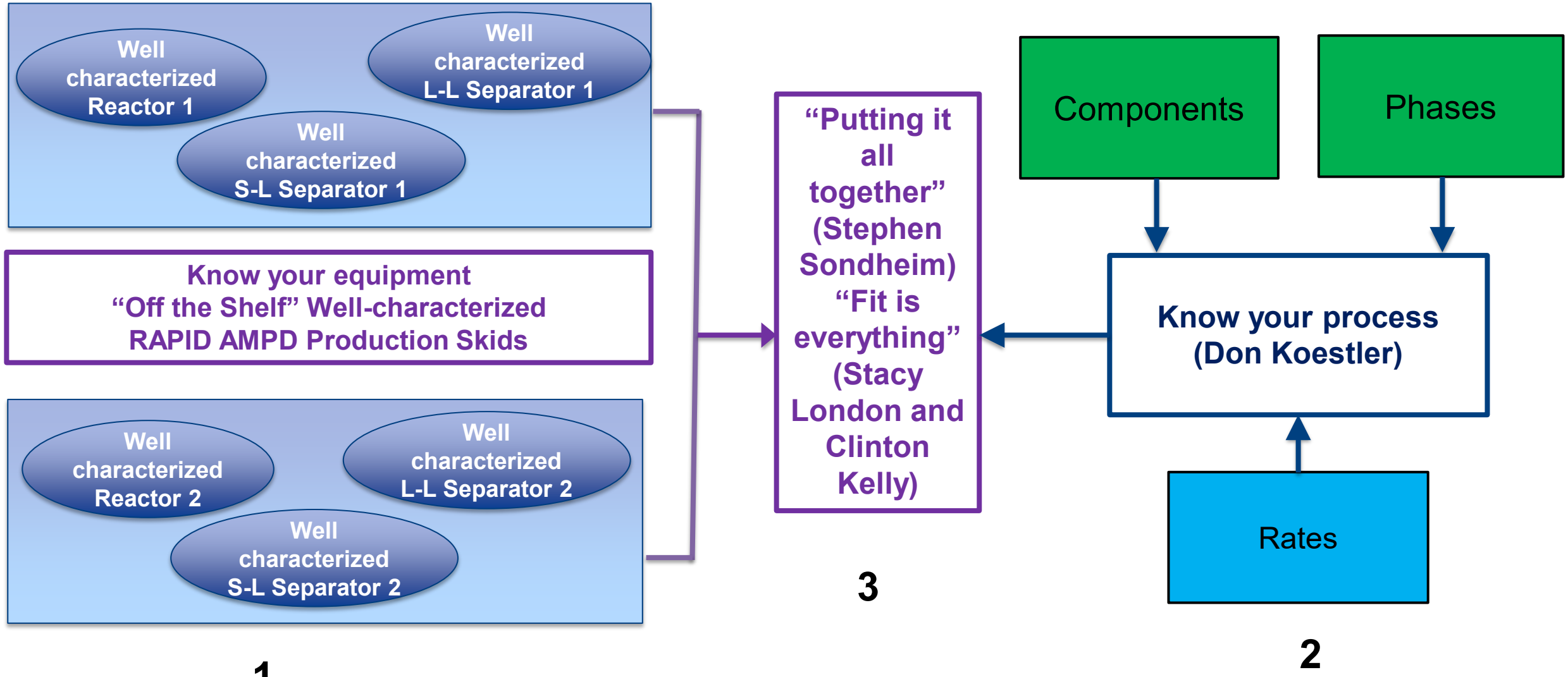
2005 AIChE President

Siirola Design Paradigm

Note
- deliverables
- decision points
- recycle loops



RAPID RACER AMPD Accelerated Process Development: 3 Steps



Step 1: Know Your Equipment!

Know Your Equipment!!!

Fully Characterized, Modular, "off the shelf" RAPID AMPD Skid

Reactor Residence time/distribution, k_La, disengagement, heat transfer, P/V

Liquid-Liquid Separator Residence time/distribution; Mass transfer, Loading, P/V

Solid-Liquid Separator Residence time/distribution, Mass transfer, Loading, P/V

Vision

"We've got Elegance"*

Douglas on Conceptual Cost Estimates

Roberge and Lonza co-workers on Continuous Reactors/Microreactors

Doherty and Malone on Reactive Distillation

*Songwriter: Jerry Herman
Elegance lyrics © Edwin H. Morris & Co. Inc.

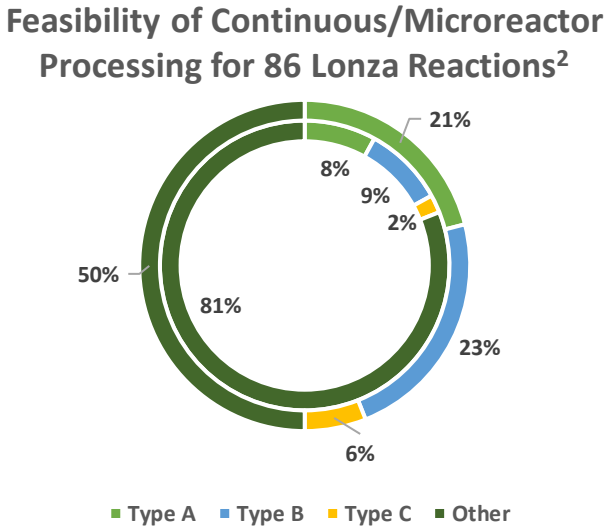
Roberge: Focus on Data-Rich Experiments to Characterize Reactions and Rank Reactor Options

Ideal process development[1]

- Early phase RC-1 to establish: Enthalpy, Kinetics, Mass balance, Type of phases
- Screening DOE
- Optimization DOE } DAC
- RC-1
- Pilot or large-scale production

Classify Reactions to Assess Reactor Options[2]

- Type A: Fast, $t_{1/2} < 1$ s
- Type B: Rapid, 1 s < $t_{1/2}$ < 10 min
- Type C: Slow, $t_{1/2} > 10$ min, but continuous brings safety and/or quality improvement
- Other: Go batch or semi-batch



Solids limit use of microreactors

Lonza

[1]Roberge, **"An Integrated Approach Combining Reaction Engineering and Design of Experiments for Optimizing Reactions,** Org Proc Res & Dev **2004**, 8, 1049-105

[2]Roberge et al, **"Microreactor Technology: A Revolution for the Fine Chemical and Pharmaceutical Industries?",** Chem. Eng. Technol. **2005**, 28, No. 3

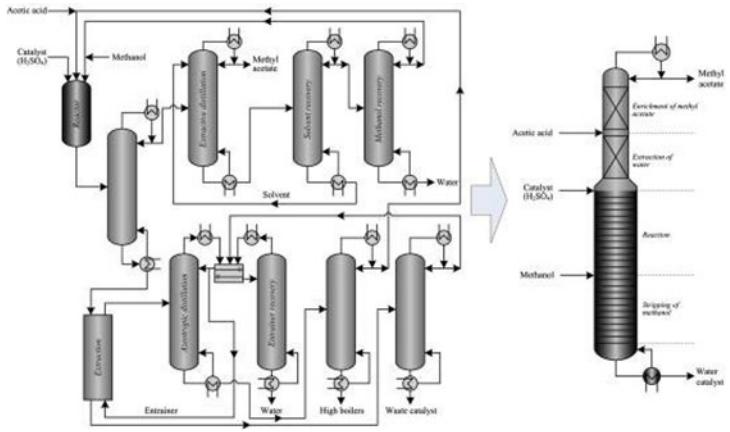
Doherty and Malone Established Feasibility Regions for Reactive Distillation

- It's all about the
  - Phases (Thermo)
  - Components (Thermo)
  - Rates (Kinetics)
- Chemical reaction will affect the vapor – liquid equilibrium
  - Things can become more complex
- But . . .fast reactions reaching chemical equilibrium quickly can simplify the separation
  - Azeotropes may disappear

EASTMAN

Eastman Chemical Methyl Acetate Process

OLD NEW



M.F. Doherty and M.F. Malone, "Conceptual Designs of Distillation Systems, McGraw-Hill, 2001.
V.H. Agreda et al, "High-Purity Methyl Acetate via Reactive Distillation", CEP 86(2), 40 – 46, 1990.
R.S. Huss et al, "Reactive distillation for methyl acetate production", Comp. Chem Eng., 27 (2003), 1855 – 1866.

Applying the Approach to RAPID RACER AMPD: Modular Skid Equipment Designed to Accommodate Multi-phase Processes at AVN

- Reactors
  - 20 L Hastelloy CSTR with Pitched Blade Turbine Impeller
  - 20 gal Glass-lined CSTR with Retreat Curve Impeller (RCI)
  - Multiple 10 ft x 2 in tubular
  - Multiple 10 ft x 1 in tubular
- Multiple Distillation columns and peripherals
- Crystallizer
- Filter/dryer

Per Jeff Siirola, what is “good enough”?

“Good enough”: Calculate Transfer Rates with Well-established Correlations

Agitated Vessels/Reactors

Miscible Liquid-liquid Blend time

Tackling Difficult Mixing Problems

DAVID S. DICKEY
MIXTECH, INC.

www.aiche.org/cep August 2015 CEP

Minimize Blending Time

https://www.chemicalprocessing.com/print/content/11373993

Gas-liquid Mass Transfer
Middleton and Smith, “Gas-Liquid Mixing in Turbulent Systems”, Chapter 11

S-L Mass Transfer
Atiemo-Obeng et al., “Solid-Liquid Mixing”, Chapter 10

2004

2016

Heat transfer

AGITATED VESSEL HEAT TRANSFER

Carpenter, K.J.

DOI:
10.1615/AtoZ.a.agitated_vessel_heat_transfer

N_{js} (Just Suspended Speed)
Brown et al., “Solid-Liquid Mixing”, Chapter 10

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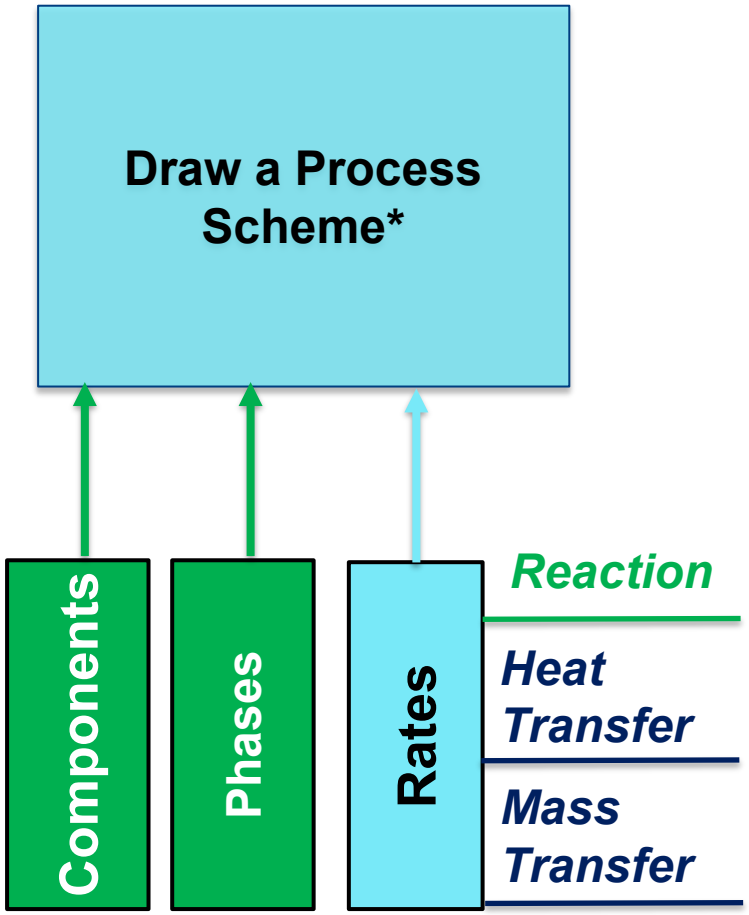
Step 2: Know Your Process!

Components are	**SCALE-INDEPENDENT**
Phases are	**SCALE-INDEPENDENT**
Reaction Kinetics are	**SCALE-INDEPENDENT**
Heat Transfer Rate is	**SCALE-DEPENDENT**
Bulk Mass Transfer Rate is	**SCALE-DEPENDENT**



*Dynochem, Scale-up Suite 2.1, Mettler Toledo, Dublin, Ireland, 2022

Great Process Development Quotes

It's all about the mass balance

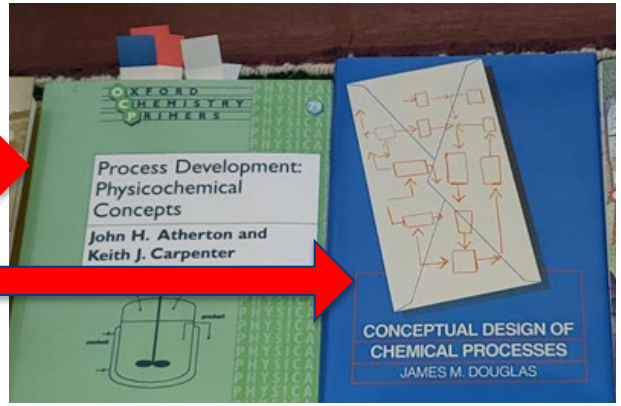
It depends . . .

It's too early to draw a process scheme

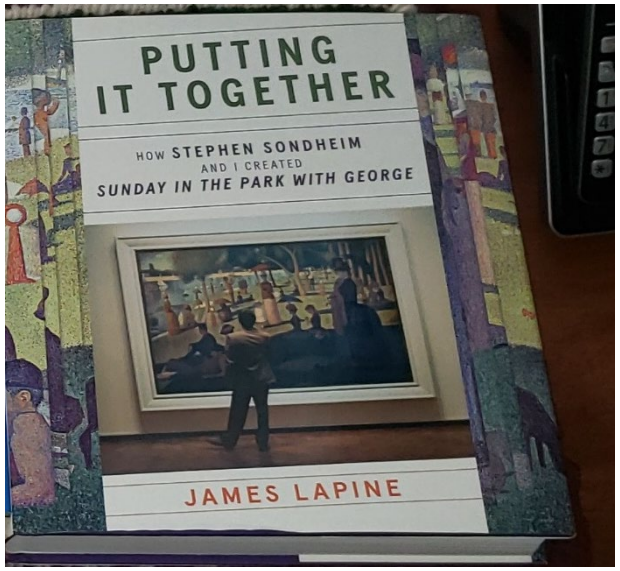
measure kinetics

do a cost estimate

And the corollary to the latter: why haven't you done a cost estimate?

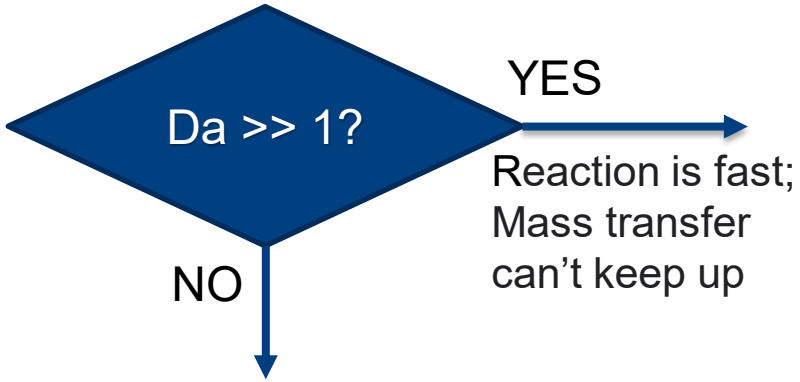


Step 3 Put it All Together!



Assess fit of chemistry/process and existing equipment using the Damkohler number, defined for reactors as the quotient of

$$\frac{\text{Chemical Reaction Rate}}{\text{Mass Transfer rate (Diffusion or Convection)}}$$



Use correlations (previous slide) for Da denominator

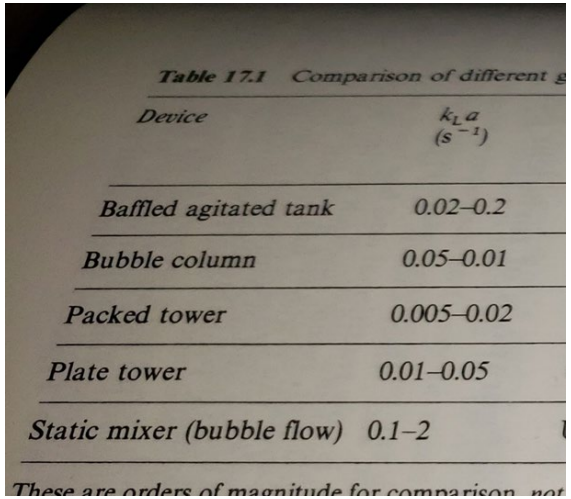


Table 17.1 Comparison of different g

Device	$k_L a$ (s^{-1})
Baffled agitated tank	0.02–0.2
Bubble column	0.05–0.01
Packed tower	0.005–0.02
Plate tower	0.01–0.05
Static mixer (bubble flow)	0.1–2

These are orders of magnitude for comparison, not

"Gas Dispersion and Mixing", J.C. Middleton, Chapter 17, Mixing in the Process Industries, N. Harnby et al., Buttersworth, 1985

Challenge: extend approach to

- other multiphase reactions
- non-reacting systems
- single phase reactions

Reframe DA

$$\frac{\text{Kinetic Process Rate}}{\text{Limiting Transfer Rate}}$$

Current State: ”Reducing to Practice” the Approach for RAPID RACER AMPD

- Step 1: Know the Equipment
  - Stirred Vessels (Batch, CSTR) and Tubular Reactors:
    - Liquid-Gas Mass Transfer (kL_as)
    - Liquid-Liquid Bulk Mixing/Blend Time
    - Heat Transfer
    - Solid Suspension
  - Crystallization
  - Solid-Liquid Separation
- Step 2: Know the Process
  - Count phases, components (get properties!) for 2 chemistries
  - Extract kinetics from AVN process development data

Step 3

Put it all

Together!

Concluding with Great Quotes in Process Development, Unabridged

1. It's all about the mass balance.
2. Everything depends on execution.
3. Why should I listen to you?
4. Now we get to be the adults.
5. Never assume.
6. What happens if I hit this button?
7. Then a miracle happens.
8. We're losing money on every batch, but we'll make it up in volume.
9. It depends . . .
10. I do not think you know what that word means.
11. If you didn't have the solubility limit, how much could you get into solution?
12. Kinjal made a batch in the lab, so we plan on going commercial in two months.
13. I know it when I see it.
14. I love solids.
15. I just want to go into the lab and run experiments.
16. Make it work!
17. We have all the responsibility and none of the control.

Which of these wasn't said to me?

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THANK YOU!