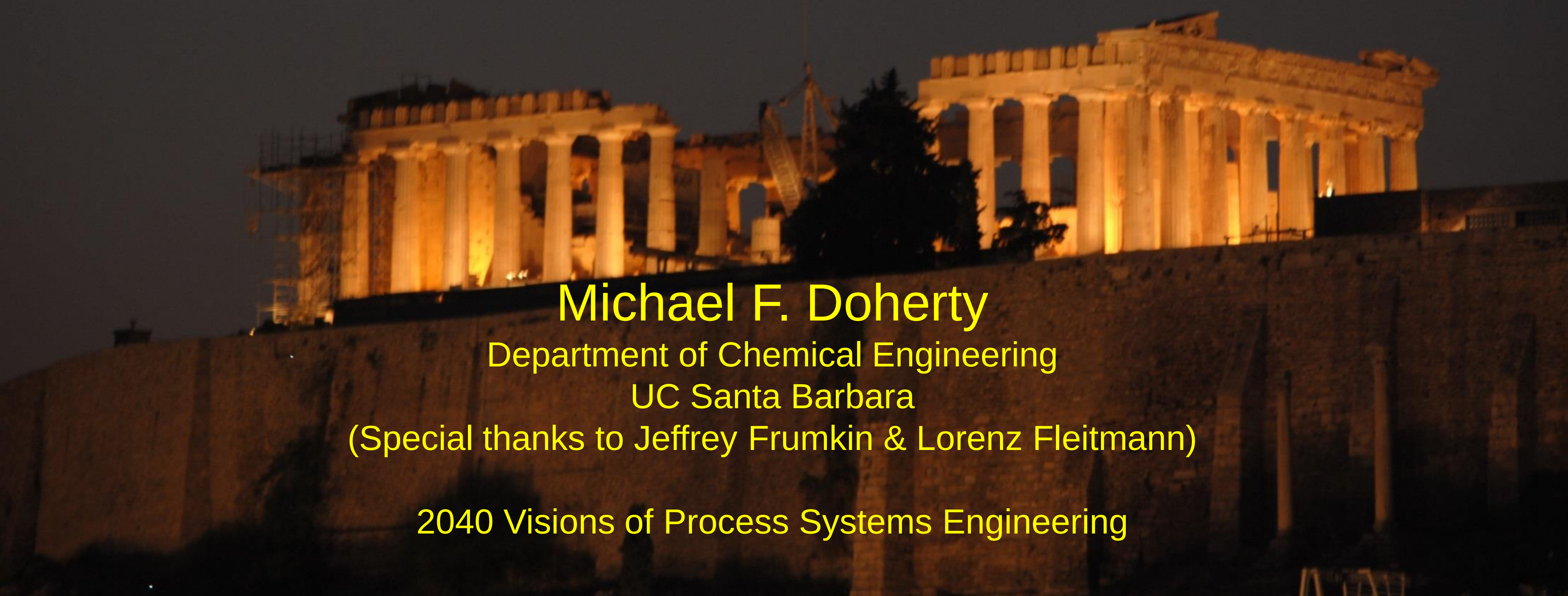
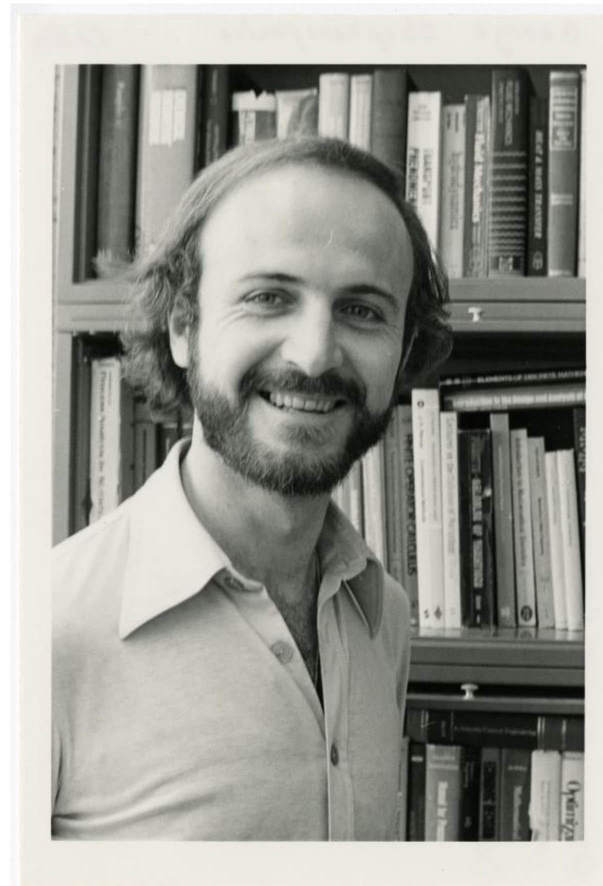
The Paradigm After Next: 50 Years On

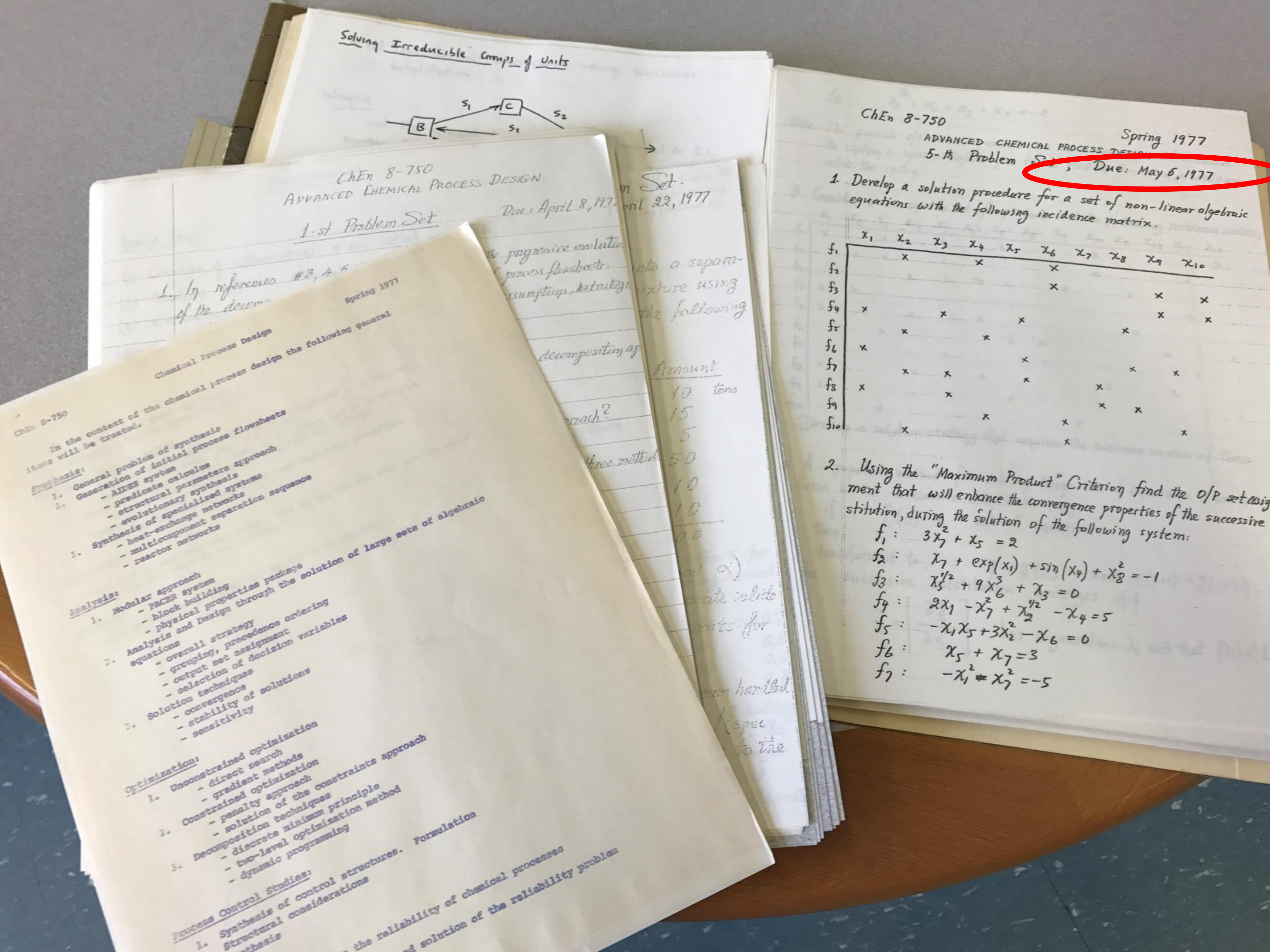


Michael F. Doherty
Department of Chemical Engineering
UC Santa Barbara
(Special thanks to Jeffrey Frumkin & Lorenz Fleitmann)

2040 Visions of Process Systems Engineering

Circa 1976 Minnesota CEMS





Solving Irreducible Groups of Units
ChEn 8-750
ADVANCED CHEMICAL PROCESS DESIGN
Due: April 8, 1977
1-st Problem Set
ChEn 8-750
Spring 1977
ADVANCED CHEMICAL PROCESS DESIGN
5-th Problem Set, Due: May 6, 1977
1. Develop a solution procedure for a set of non-linear algebraic equations with the following incidence matrix.
2. Using the "Maximum Product" Criterion find the O/P set assignment that will enhance the convergence properties of the successive substitution, during the solution of the following system:
$f_1: 3x_7^2 + x_5 = 2$
$f_2: x_7 + \exp(x_1) + \sin(x_4) + x_8^2 = -1$
$f_3: x_5^{1/2} + 9x_6^3 + x_3 = 0$
$f_4: 2x_1 - x_7^2 + x_2^{1/2} - x_4 = 5$
$f_5: -x_1x_5 + 3x_2^2 - x_6 = 0$
$f_6: x_5 + x_7 = 3$
$f_7: -x_1^2 + x_7^2 = -5$
ChEn 8-750
Spring 1977
Chemical Process Design
In the context of the chemical process design the following general items will be treated.
Synthesis:
1. General problem of synthesis
2. Generation of initial process flowsheets
- AIDES system
- predicate calculus
- structural parameters approach
- evolutionary synthesis
3. Synthesis of specialized systems
- heat-exchange networks
- multicomponent separation sequence
- reactor networks
Analysis:
1. Modular approach
- PACER system
- block building
- physical properties package
2. Analysis and Design through the solution of large sets of algebraic equations
- overall strategy
- grouping, precedence ordering
- output set assignment
- selection of decision variables
3. Solution techniques
- convergence
- stability of solutions
- sensitivity
Optimization:
1. Unconstrained optimization
- direct search
- gradient methods
2. Constrained optimization
- penalty approach
- solution of the constraints approach
3. Decomposition techniques
- discrete minimum principle
- two-level optimization method
- dynamic programming
Process Control Studies:
1. Synthesis of control structures. Formulation
Structural considerations

May 1977

ChEn 6-750 Chemical Process Design Spring 1977

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My Theme: Conceptual Design

You can't understand the process if you don't understand the chemistry

Mavrovouniotis & Stephanopoulos 1989-1992

Synthesis of Reaction Mechanisms Consisting of Reversible and Irreversible Steps. 1. A Synthesis Approach in the Context of Simple Examples

Michael L. Mavrovouniotis*

Department of Chemical Engineering and Systems Research Center, A. V. Williams Building, University of Maryland, College Park, Maryland 20742

George Stephanopoulos

Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

The analysis of pseudo-steady states of a chemical system can be aided by the identification of mechanisms responsible for overall reactions, from a known set of elementary steps that involve overall reactants and products as well as reaction intermediates. In the context of examples of catalytic synthesis of ammonia and methanol, an alternative approach for the construction of mechanisms from steps is presented. The approach is based on successive processing and elimination of reaction intermediates which should not appear in the net stoichiometry of the overall reactions accomplished.

Introduction

Consider a given set of elementary reaction steps which are feasible in a system, and the species involved in these steps. Following Happel and Sellers (1982, 1983, 1989), Happel (1986), Sellers (1984, 1989), and Happel et al. (1990)—this set of references is hereafter referred to as H&S—species can be classified as either *intermediates*, which occur in very small amounts, or *terminal* species which can occur in significant amounts and constitute the raw materials and products of the process. An *overall* ...

the accumulation term in the mass balance for an intermediate to zero. *Overall* reactions can thus be defined as the set of net transformations permissible under the pseudo-steady-state assumption, while *overall* mechanisms are the combinations of steps that accomplish this. This article focuses on the *synthesis of reaction mechanisms*, the systematic identification of sets of mechanism steps that accomplish net reactions involving only terminal species.

One is particularly interested in *direct* mechanisms (Milner, 1964), which are the smallest possible physically

2040 and Beyond

The future of chemical engineering
is in prediction not correlation

Why Modeling?

"If you can't model your process, you don't understand it. If you don't understand it, you can't improve it. And, if you can't improve it, you won't be competitive in the 21st century."

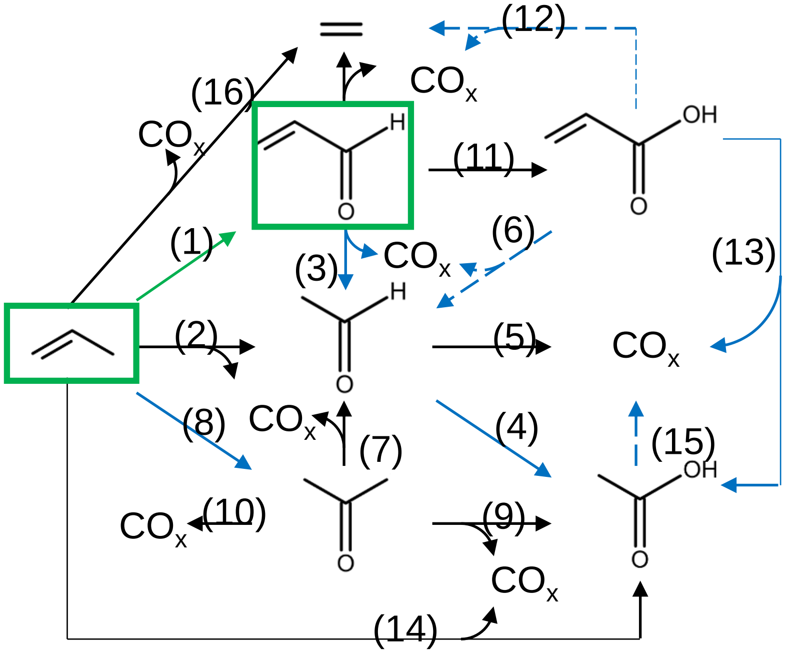
Jim Trainham, DuPont

Perspectives

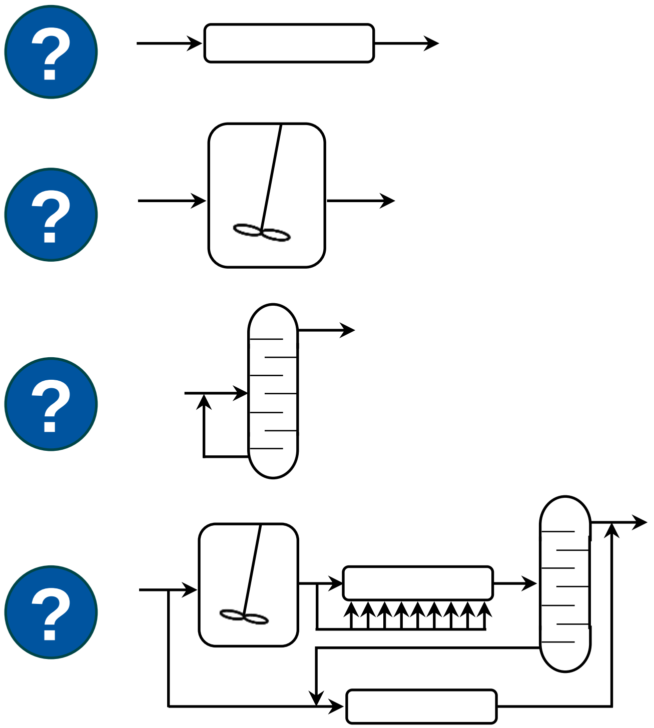
- Engineers believe that their models approximate nature
- Scientists believe that nature approximates their models
- Mathematicians don’t give a damn either way

Process design for a complex reaction network

Production of Acrolein[1]



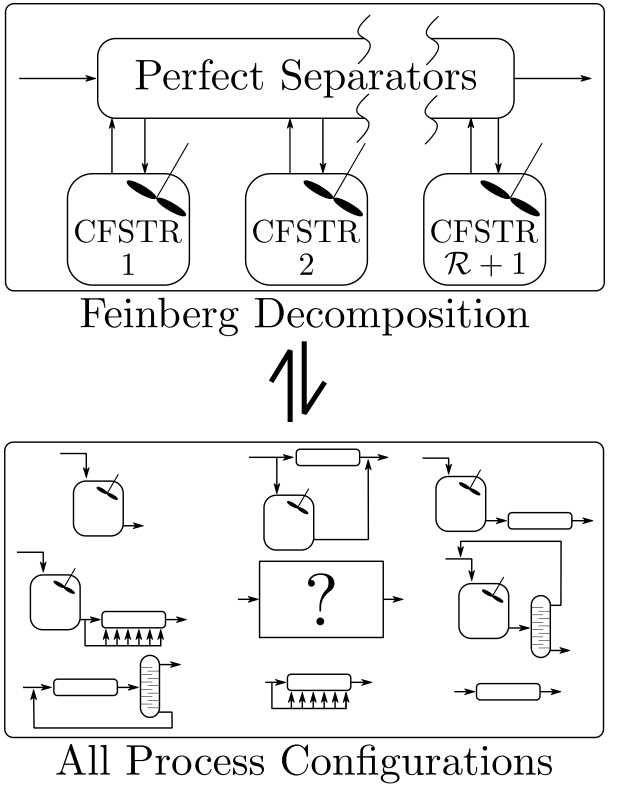
What is the process design with the highest selectivity?



$$\text{Selectivity} = \frac{\text{Product produced}}{\text{Limiting reactant consumed}}$$

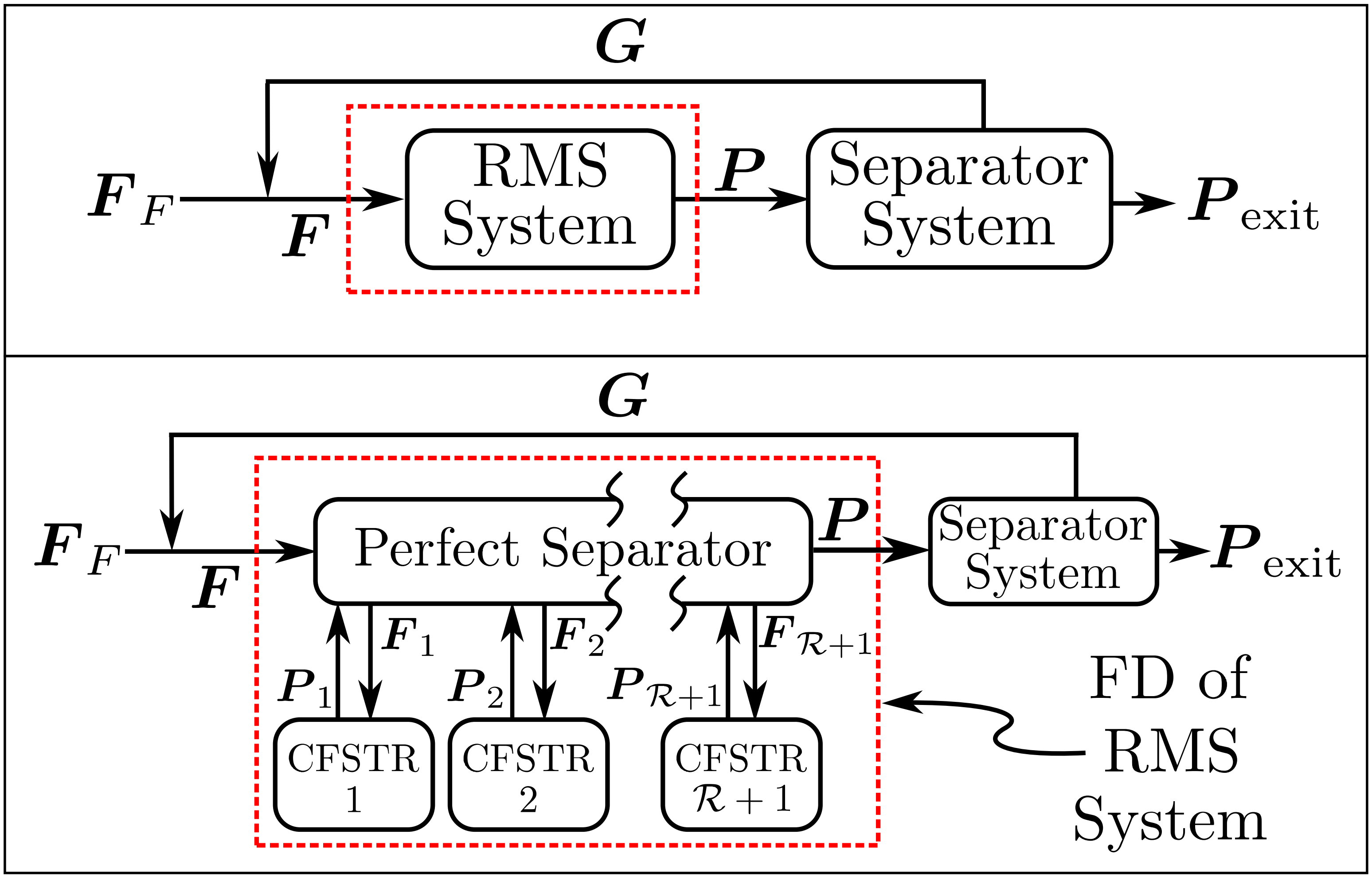
[1] Bui, Chakrabati & Bhan, *ACS Catalysis*, 6(10), 6567-6580, 2016

Feinberg Decomposition

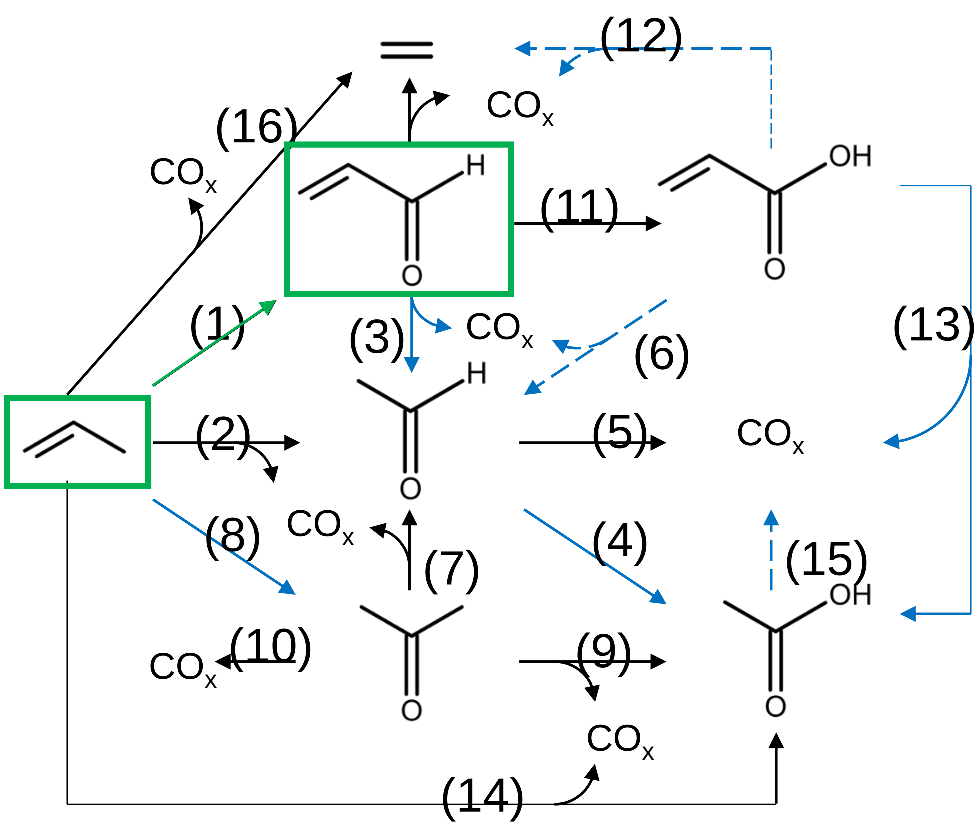


Martin Feinberg and Phillipp Ellison. General Kinetic Bounds on Productivity and Selectivity in Reactor-Separator Systems of Arbitrary Design: Principles, *Industrial & Engineering Chemistry Research*, 40, 3181–3194 (2001)

The Overall PFD Structure



Production of acrolein by partial oxidation of propylene at 350°C [1]



LR = propylene

All reaction irreversible with following kinetics, e.g.:

$$\hat{r}_1 = k_1\, p_{C_3H_6} \qquad (\longrightarrow)$$

$$\hat{r}_8 = k_8\, p_{C_3H_6}\, p_{H_2O} \qquad (\longrightarrow)$$

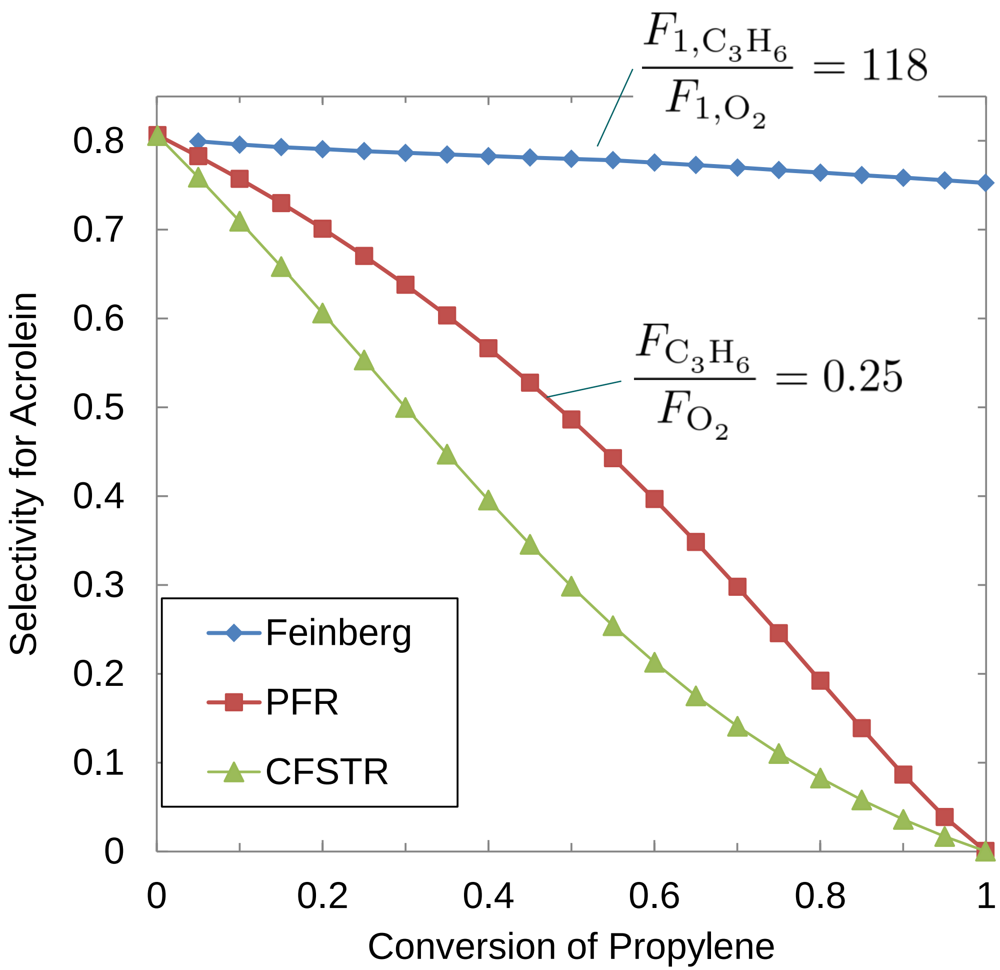
$$\hat{r}_{15} = k_{15}\, \frac{p_{CH_3COOH}}{p_{H_2O}} \qquad (\dashrightarrow)$$

All rates independent of oxygen partial pressure!

$$\boldsymbol{F} = \begin{array}{cc} \begin{bmatrix} 5\% \\ 20\% \\ 75\% \end{bmatrix} & \begin{array}{r} C_3H_6 \\ O_2 \\ N_2 \end{array} \end{array}$$

 [1] Bui, Chakrabati & Bhan, *ACS Catalysis*, 6(10), 6567-6580, 2016

Results: Maximum selectivity to acrolein



- For given feed:

  More complex processes than PFR and CFSTR only required

- Feinberg Decomposition:

  No inerts and only as little oxygen as necessary (separate air)

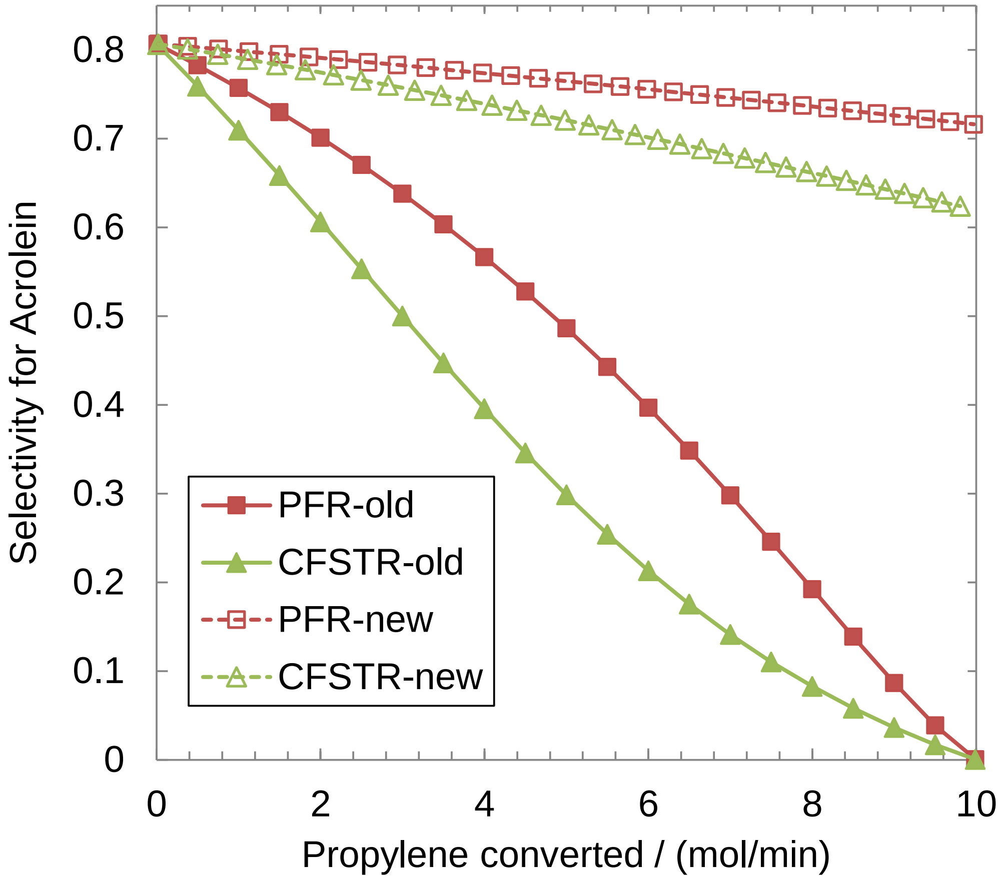
  → high molar ratio

  → increase rate for production of acrolein $(\hat{r}_1 = k_1\, p_{C_3H_6})$

Higher selectivity for excess of propylene, not oxygen

Improve existing design!

Improving the process design



New feed: $F_{\text{total}} = 200.5 \text{ mol/min}$

$$F = \begin{bmatrix} 91.5 \\ 22.9 \\ 86.1 \end{bmatrix} \begin{array}{l} \text{mol/min } C_3H_6 \\ \text{mol/min } O_2 \\ \text{mol/min } N_2 \end{array}$$

$$\frac{F_{C_3H_8}}{F_{O_2}} = 4$$

Old feed: $F_{\text{total}} = 200.5 \text{ mol/min}$

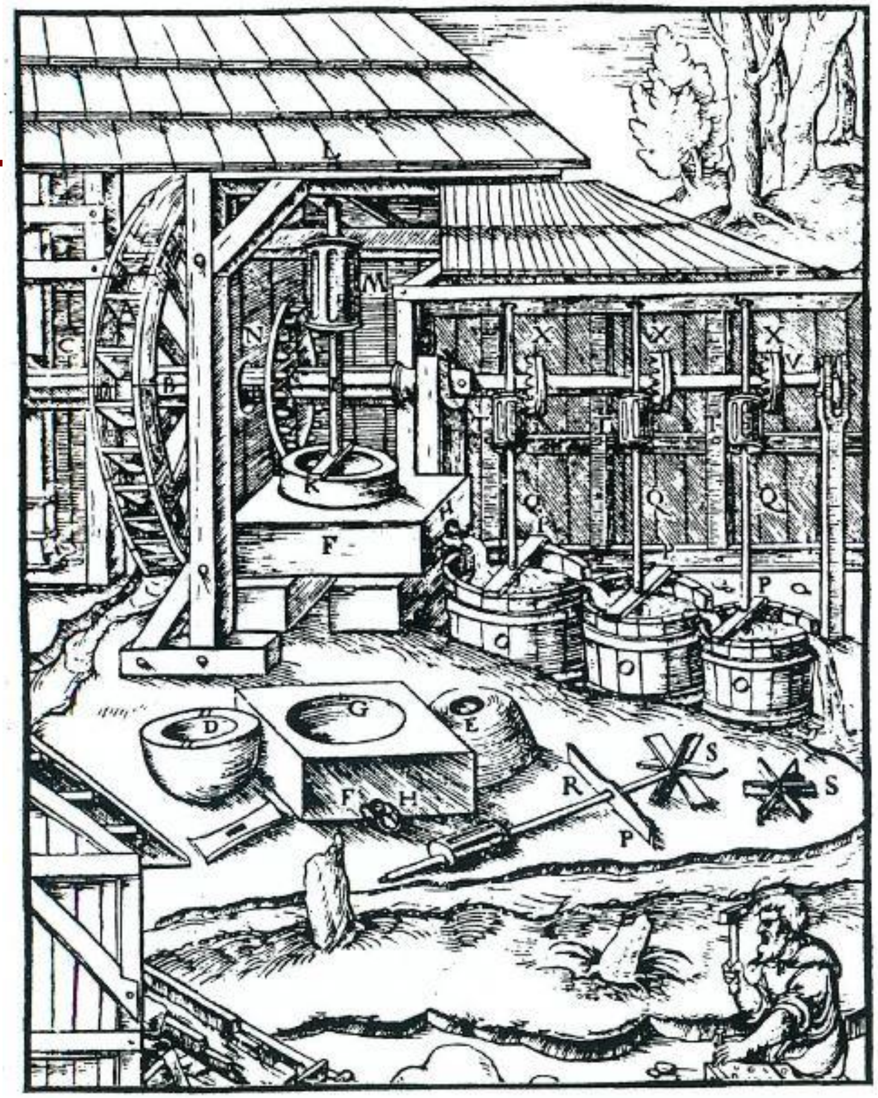
$$F = \begin{bmatrix} 10 \\ 40 \\ 150.5 \end{bmatrix} \begin{array}{l} \text{mol/min } C_3H_6 \\ \text{mol/min } O_2 \\ \text{mol/min } N_2 \end{array}$$

$$\frac{F_{C_3H_8}}{F_{O_2}} = 0.25$$

Significant improvement using the Feinberg results!

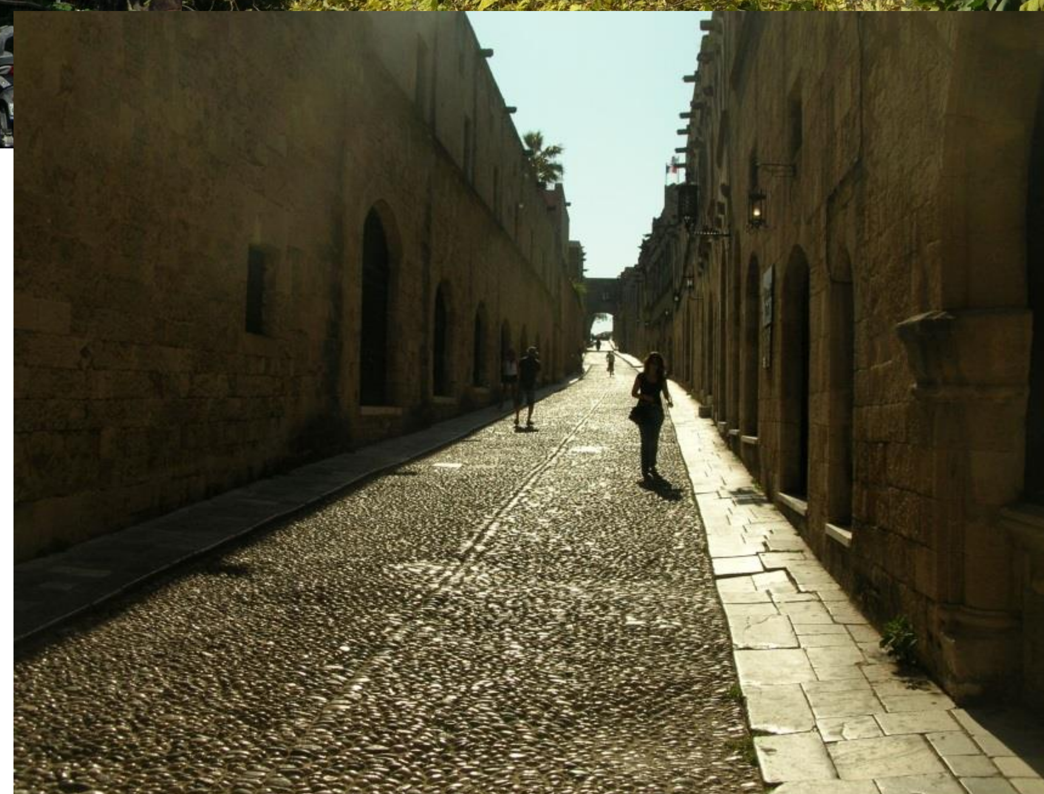
Circa 1556

Let’s not forget what the alchemists knew!



MULTIPURPOSE ORE MILL powered by a single water wheel at the upper left was illustrated in Georgius Agricola's *De re metallica*, published in 1556. Gold ore was processed in the following steps. First the ore was crushed by a cam-lifted stamp (*c*), just visible to the left of the water wheel. Next the crushed ore was ground to a powder in a pair of millstones to the right of the wheel. Two spare dome-shaped upper millstones (*d*, *e*) are on the ground on each side of a spare lower millstone; one of the upper millstones is turned upside down to show the hole that admitted the crushed ore. The outlet for the powdered ore (*h*) in the lower millstone deposited the powder into the first of three settling tubs (*o*). The slurry of powdered ore in the tubs was agitated by paddles driven by cogs (*x*) attached to the axle of the wheel. The agitation separated the heavier gold from the lighter dross, which eventually spilled from the last of the settling tubs.


GRILL

Which Leads to Such Questions as:

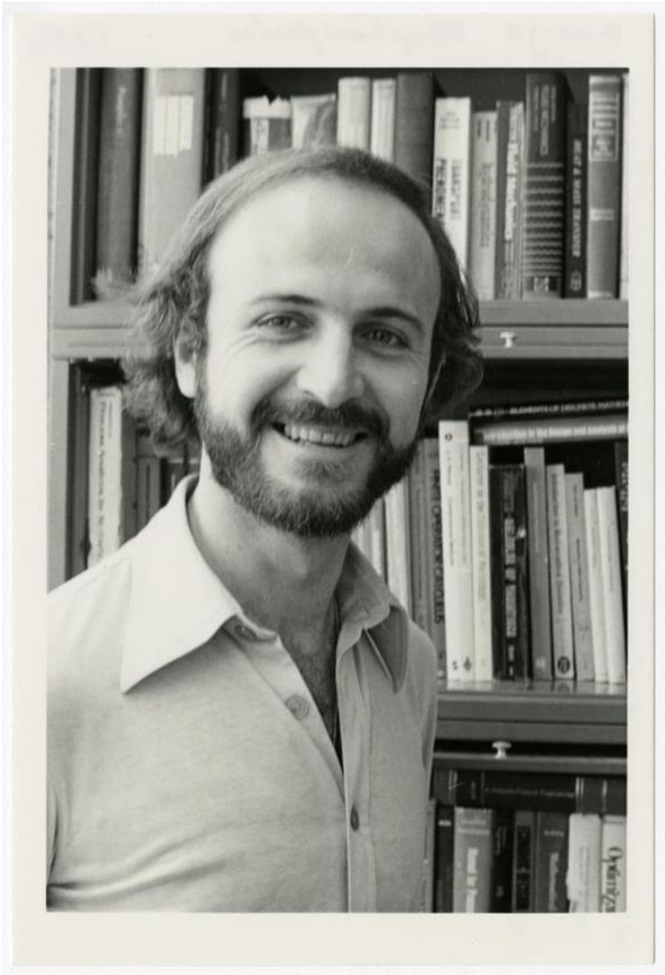
- Does a decomposition exist for reactor systems when thermodynamic constraints are placed on the perfect separation system?

- Does a similar decomposition exist for separation systems (independent from the reactor system)?

- Can an entire process flowsheet be decomposed in a Feinbergian way?

- Does there exist an abstract kinetic/thermodynamic theory of process flowsheets?

40 years on



Shade is Good

50 years on: The Real Paradigm After Next

Stairs & Door in Lindos

Bravo George



C

"These smug pilots have lost touch with regular passengers like us. Who thinks I should fly the plane?"