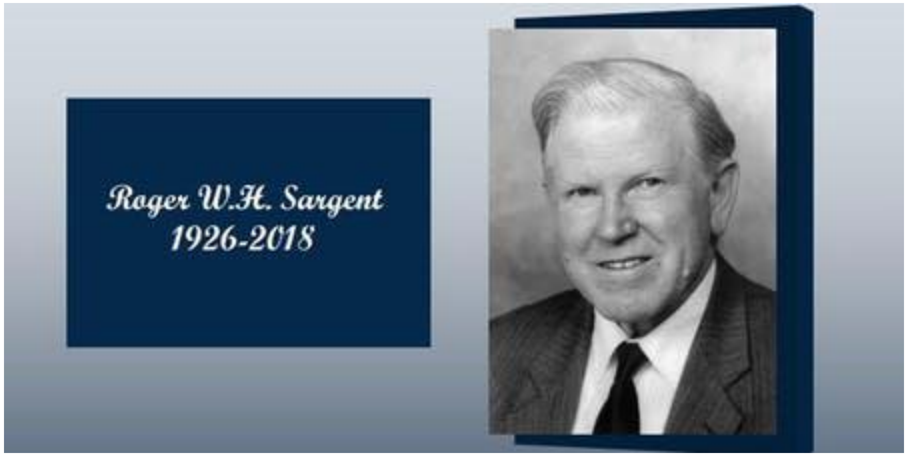
The Professor Roger Sargent Medal
IChemE Webinar

Stratos Pistikopoulos PhD FIChemE FAIChE FREng
Dow Chemical Chair
Director, Texas A&M Energy Institute

- Professor Roger Sargent – a tribute



Vision – ‘Ahead of Time’

- ***Shaping the future*** in flow-sheeting, modelling, control, optimization, design, synthesis, scheduling, physical properties/molecular systems …

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Vision - 'Ahead of time'

Engineering science - or scientific engineering?
A new SQP algorithm for large-scale nonlinear programming
Optimal control
Optimal control of inequality constrained DAE systems
Implementation of linear and nonlinear optimal control techniques in a CO2 absorption/desorption plant
Boundary conditions for flow with dispersion
A functional approach to process synthesis and its application to distillation systems
TRENDS IN THE DEVELOPMENT OF PROCESS-CONTROL
ADVANCES IN MODELING AND ANALYSIS OF CHEMICAL PROCESS SYSTEMS
FLOWSHEETING
A NEW ALGORITHM FOR PROCESS FLOWSHEETING
DEVELOPMENT OF FEED CHANGEOVER POLICIES FOR REFINERY DISTILLATION
OPTIMUM DESIGN OF MULTIPURPOSE CHEMICAL-PLANTS
OPTIMUM DESIGN OF CHEMICAL-PLANTS WITH UNCERTAIN PARAMETERS
OPTIMUM DESIGN OF HEAT-EXCHANGER NETWORKS
SELECTION OF MEASUREMENTS FOR OPTIMAL FEEDBACK-CONTROL
CALCULATION OF OPTIMAL CONTROLS OF SPECIFIED ACCURACY
EFFICIENT IMPLEMENTATION OF LEMKE ALGORITHM AND ITS EXTENSION TO DEAL WITH UPPER AND LOWER BOUNDS
OPTIMAL MEASUREMENT POLICIES FOR CONTROL PURPOSES
DESIGN OF AN ON-LINE CONTROL SCHEME FOR A TUBULAR CATALYTIC
THEORETICAL PREDICTIONS OF EQUILIBRIUM PROPERTIES AND DIFFUSIVITIES OF CARBON DIOXIDE
DIFFUSION OF CARBON DIOXIDE IN TYPE-5A MOLECULAR
APPLICATIONS OF LINEAR ESTIMATION THEORY TO CHEMICAL PROCESSES - FEASIBILITY STUDY
COMPUTATIONAL EXPERIENCE WITH QUADRATICALLY CONVERGENT MINIMISATION
A GENERAL ALGORITHM FOR SHORT-TERM SCHEDULING OF BATCH-OPERATIONS .1. MILP FORMULATION
COMPUTATIONAL EXPERIENCE WITH QUADRATICALLY CONVERGENT MINIMISATION METHODS
SOLUTION OF A CLASS OF MULTISTAGE DYNAMIC OPTIMIZATION PROBLEMS .1. PROBLEMS WITHOUT PATH

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Academic Leadership

- **Established field of Process Systems Engineering**
- **Unparalleled Academic Tree (over 1500+ & growing ..)**
- https://titan.engr.tamu.edu/Sargent_tree/
- **PSE's 'Patriarch' – CPSE Founder**
- **Scientific Chemical Engineering**
- **PSE - 'glue' to Chemical Engineering & beyond**

Process Systems Engineering - *Generation Next*

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Acknowledgements

"Process Systems Engineering - The Generation Next?"

Pistikopoulos, E. N.; Barbosa-Povoa, A.; Lee, J. H.; Misener, R.; Mitsos, A.; Reklaitis, G. V.; Venkatasubramanian, V.; You, F.; Gani, R. *(Computers & Chemical Engineering; on-line/in print)*

CPSE (at Imperial College & UCL)

PSE Ltd (A Siemens Company)

Professor Ignacio Grossmann

Professor Rafiqul Gani

Professor John Perkins

Professor George Stephanopoulos

[The late] Professor Christodoulos Floudas

Texas A&M Energy Institute & especially Professor Mahmoud El-Halwagi

Shell – Cyp Van Rijn, Johan Grievink, Jan Van Schijndel, Joe Powell, …

AUTh – especially Professor Iacovos Vasalos

EPSRC, ERC/EU, bp, Shell, Dow, Air Products, NSF, DoE/RAPID, DoE/CESMII ….

Parametric Optimization & Control Research Group (70+ PhD students, 20+ Post-Docs, ..)

Colleagues & Friends ..

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Outline

- *Professor Roger Sargent – a tribute*
- Multi-Scale Process Systems Engineering
  - *Core PSE*
  - *Domain & application-driven PSE*
- What is next for PSE? ***Generation Next***

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Process Systems Engineering

Professor Sargent (1983)

“Process systems engineering is all about the *development of systematic techniques* for process modelling, design and control”.

“*Some formulate their synthesis, design and/or control problem, or some useful simplification of it, in precise mathematical terms, and then seek to exploit the mathematical structure to obtain an effective algorithm, while others seek insight on the problem structure from physical intuition*’

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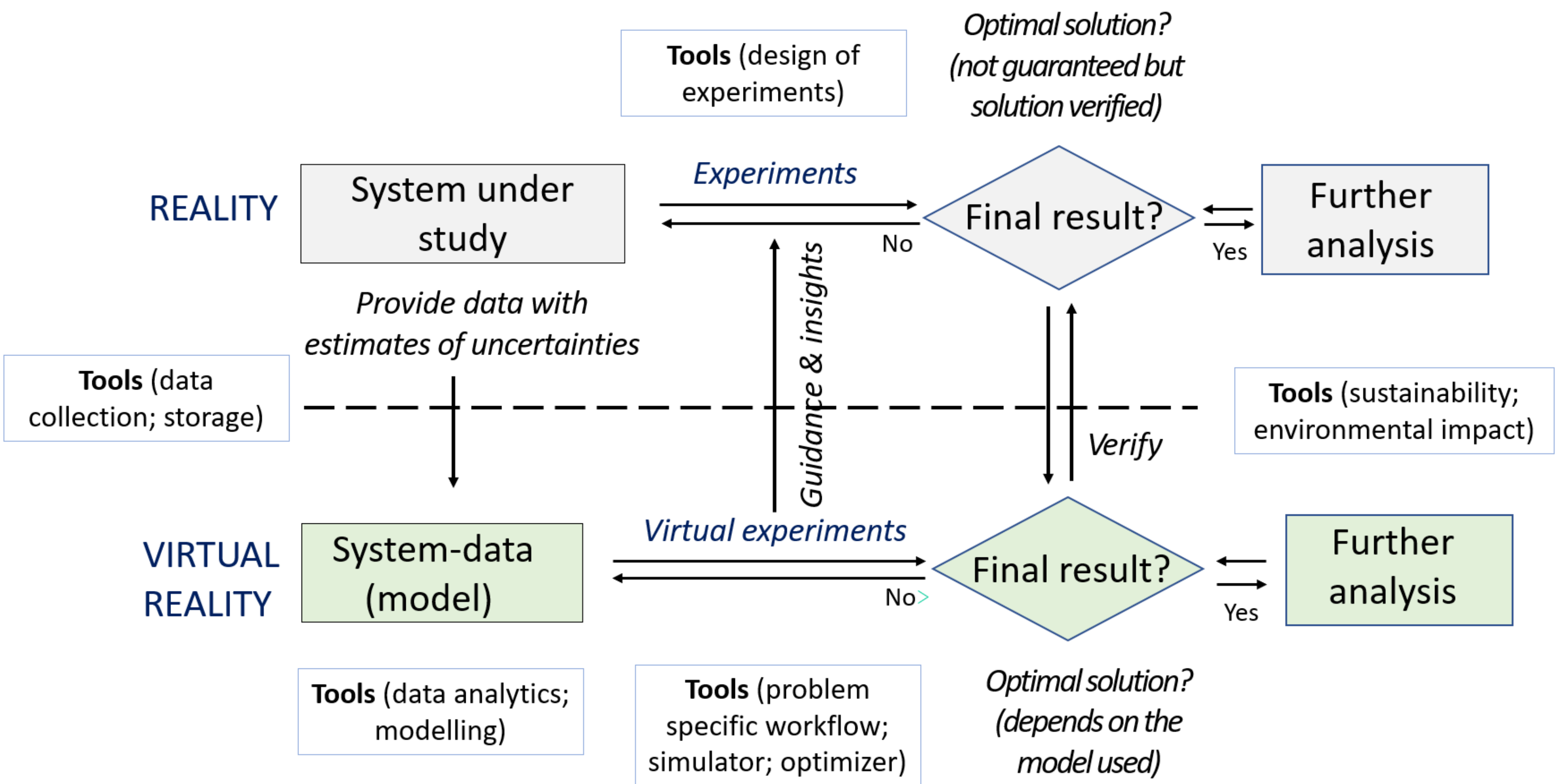
Process Systems Engineering thinking & practice



(Gani)

‘Traditional’ Process Systems Engineering

- **PSE Core**
  - Mathematical Modelling & Simulation
  - Process Synthesis
  - Product & Process Design
  - Process Operations
  - Process Control
  - Numerical Methods & Software Tools

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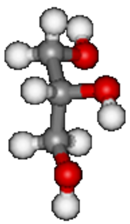
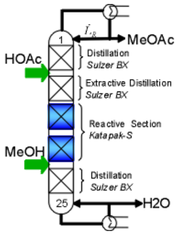
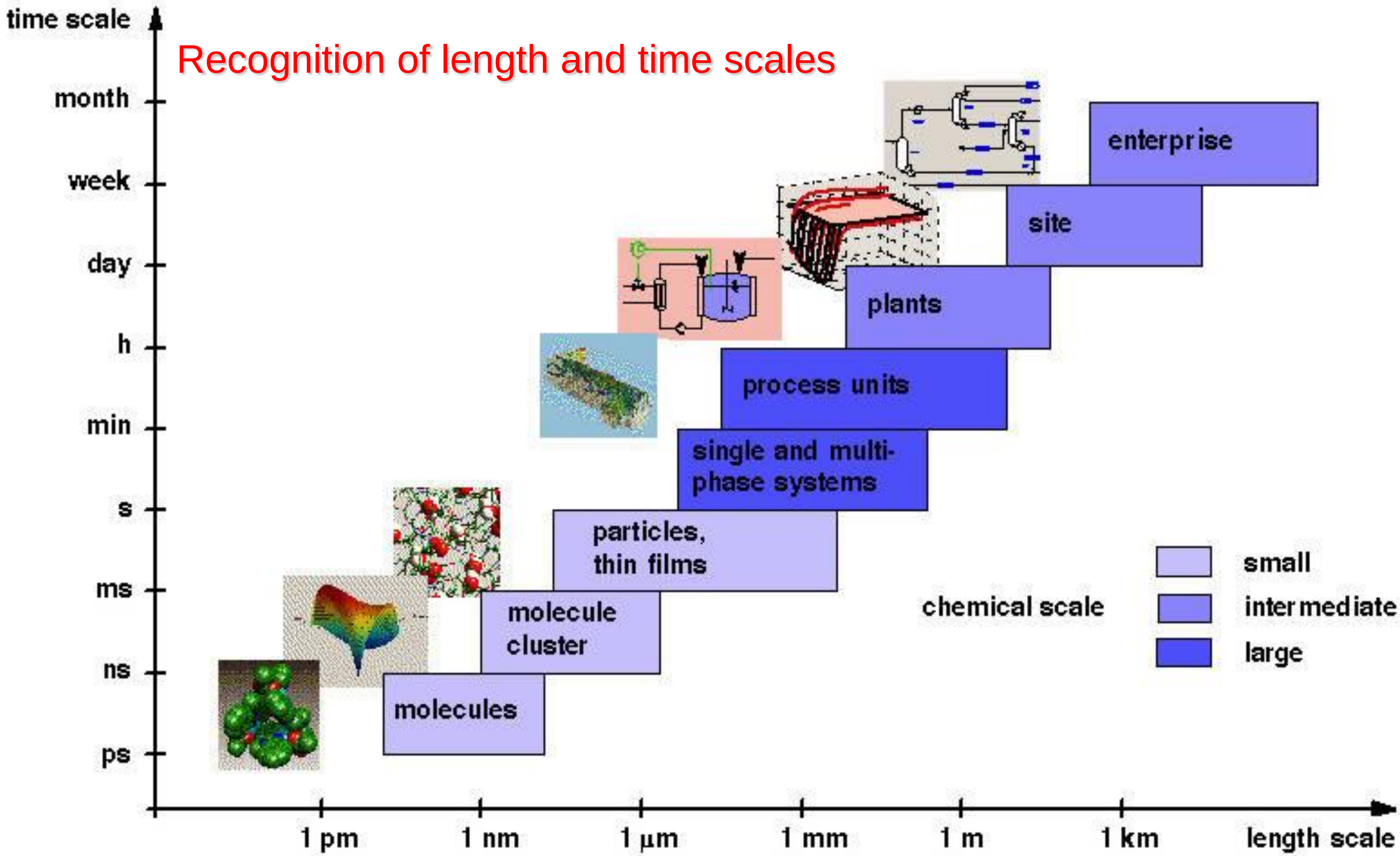
Process Systems Engineering evolution ..





- **Recognition of length and time scales**
  - From nano-scale (molecular)
    to micro-scale (particles, crystals)
    to meso-scale (materials, equipment, products)
    to mega-scale (supply chain networks, environment)

Multi-Scale Modelling



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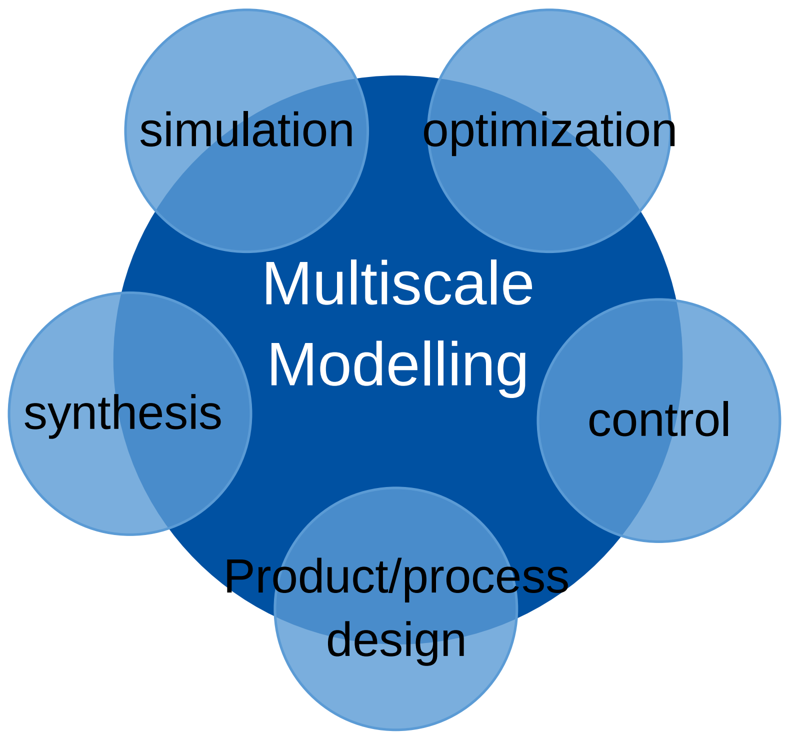
PSE evolution ... *from Core to …*



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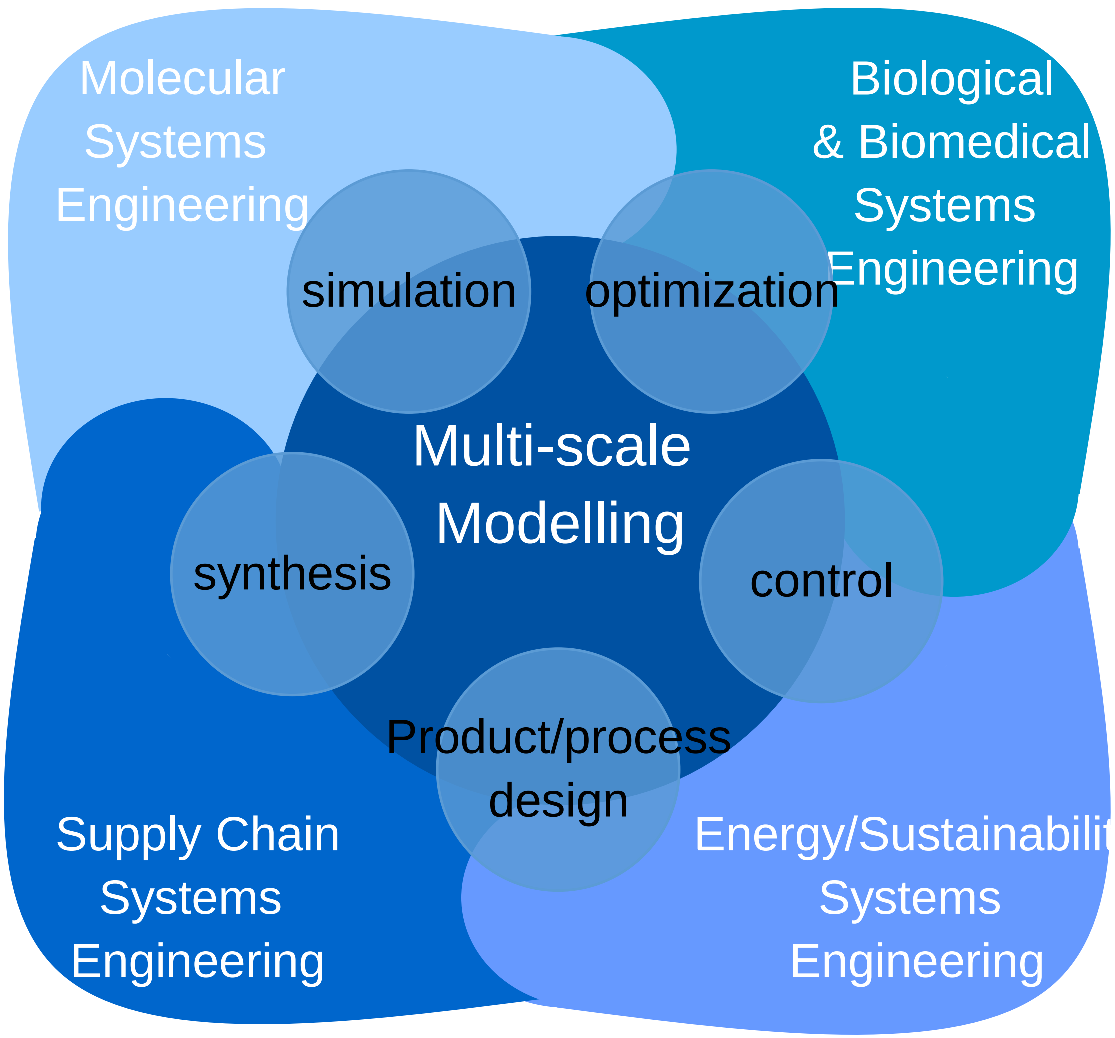
Multi-Scale Process Systems Engineering



Multi-Scale Process Systems Engineering

- PSE Core
- Domain-driven PSE
- Problem-centric PSE

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PSE Core

- Multi-scale Modelling
- Multi-scale Optimization
- Product & Process Design
- Process Operations
- Control & Automation
- Software Tools

Domain-driven PSE

- Molecular Systems Engineering
- Materials Systems Engineering
- Biological Systems Engineering
- Healthcare Systems Engineering
- Energy Systems Engineering

Problem-centric PSE

- Environmental systems engineering - sustainability
- Safety systems engineering
- Manufacturing supply chains
- Life Science Systems Engineering

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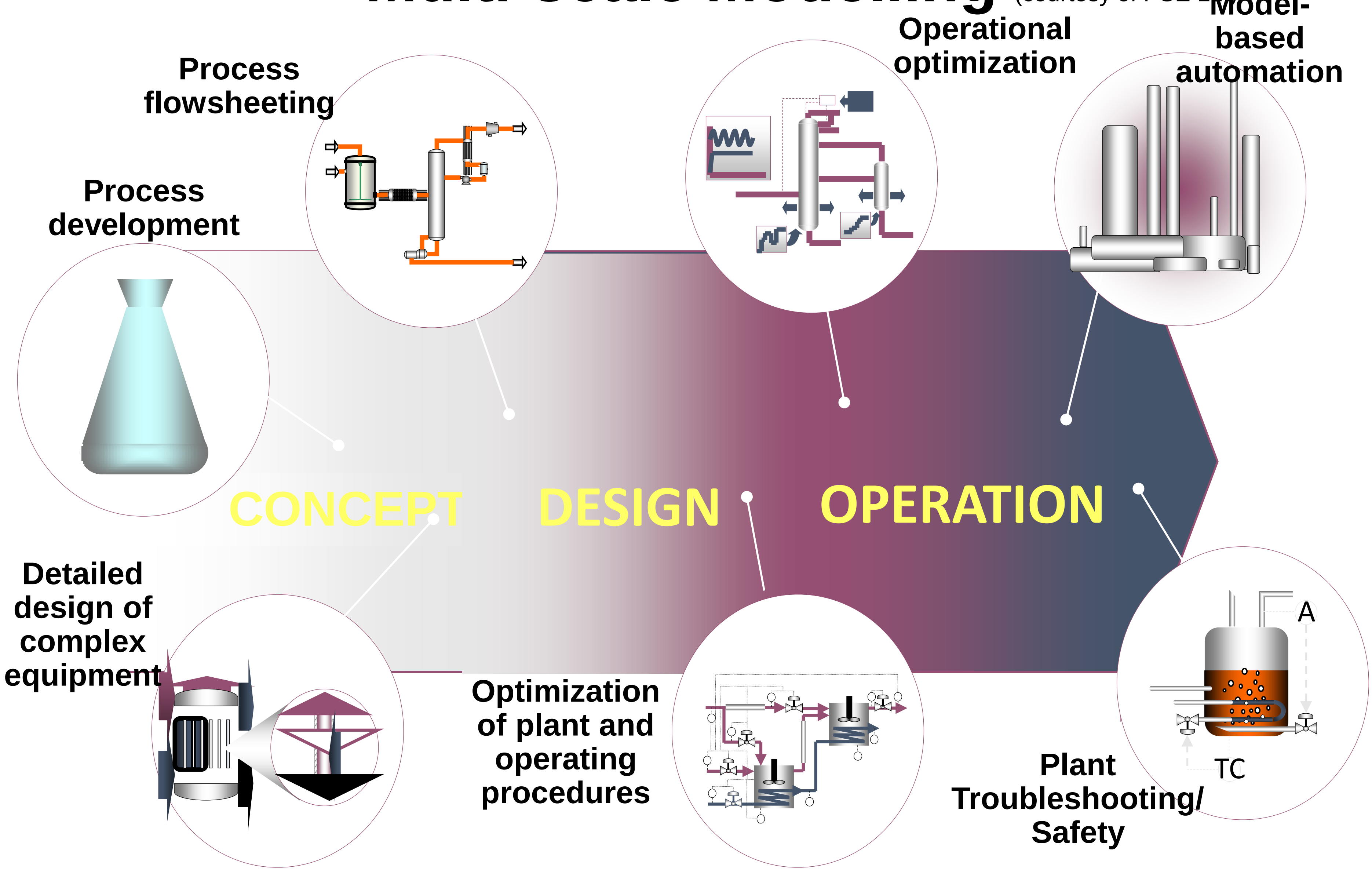
Multi-scale Modelling (courtesy of PSE Ldt)



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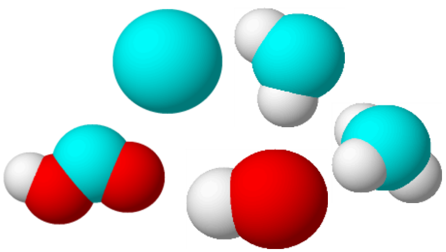
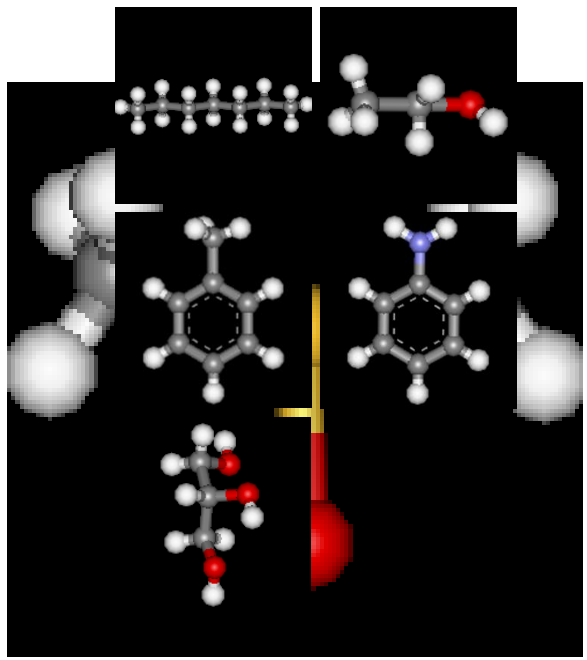
Molecular Systems Engineering



$$Property = \sum_i n_i Property_i + const$$

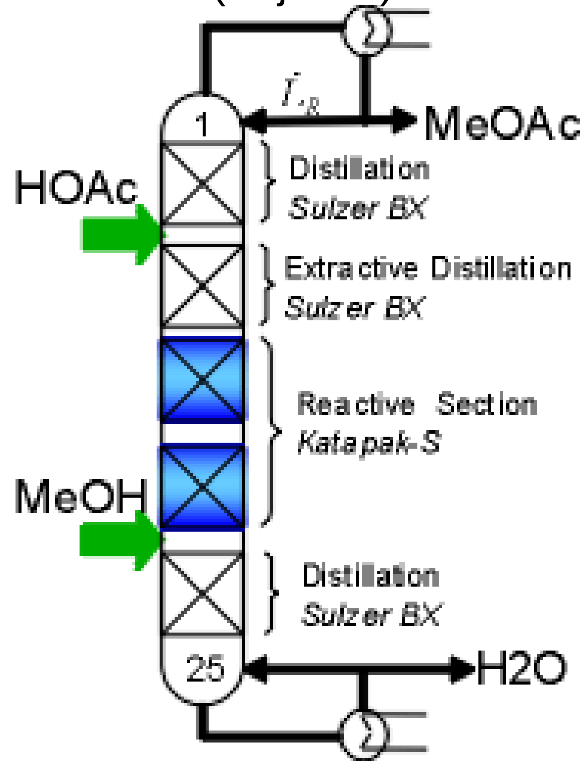
$$\log k = \log k_0 + s(S + d\delta) + aA + bB + h\delta_H^2/100$$

Building blocks



Solvents and reactions

(Adjiman)



Chemical process

nanoscale → microscale → macroscale

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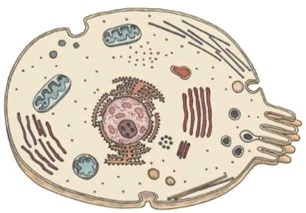
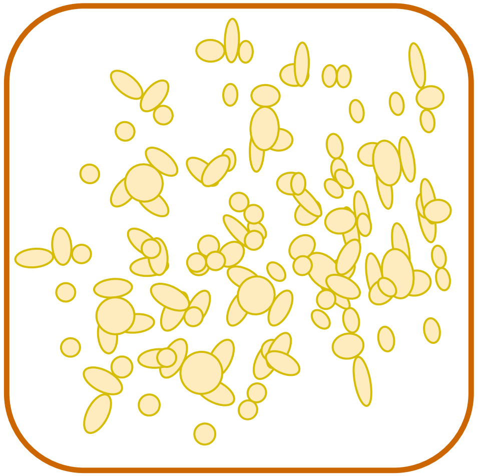
Biological Systems Engineering

(Mantalaris *et al*)



Individual cells



Cell population

Bioreactor

microscale → mesoscale → macroscale

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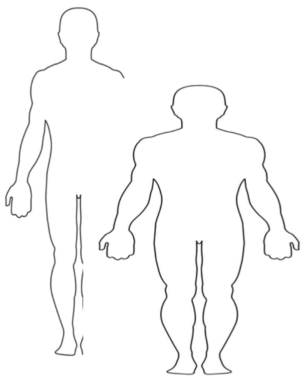
Life Sciences Systems Engineering

(Maria Papathanasiou)



PSE approaches in biomanufacturing

Personalised healthcare modelling

Supply chain optimization in life sciences

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PSE Software Tools

Process Simulator

- Steady state simulation, dynamic simulation, optimization - **Aspen**
- Steady state simulation, optimization - **Chemstations**
- Steady state-dynamic simulation, optimization – **gPROMS/PSE**
- Steady state simulation, optimization **- PRO/II**
- Steady state simulation-modelling **- ProMax**
- Steady state -dynamic simulation, optimization **- UNISIM**

Integrated Systems

- Modeling, simulation, optimization - **IDAES**
- Superstructure-based optimization - **Super-O**
- Integrated tool for process control - **ProCACD**
- Process synthesis, design, intensification - **ProCAFD**
- Product synthesis-design - **OptCAMD**
- Process synthesis – **PyoSIN**
- Product synthesis-design – **ProCAPD**
- Model-based process control & optimization – **PAROC**
- Model-based risk analysis - **TECSMART**

Equation Solving

- DAE solver **– ACADO, CasADi, DAEPACK, Dyos, PyoMO-dae**

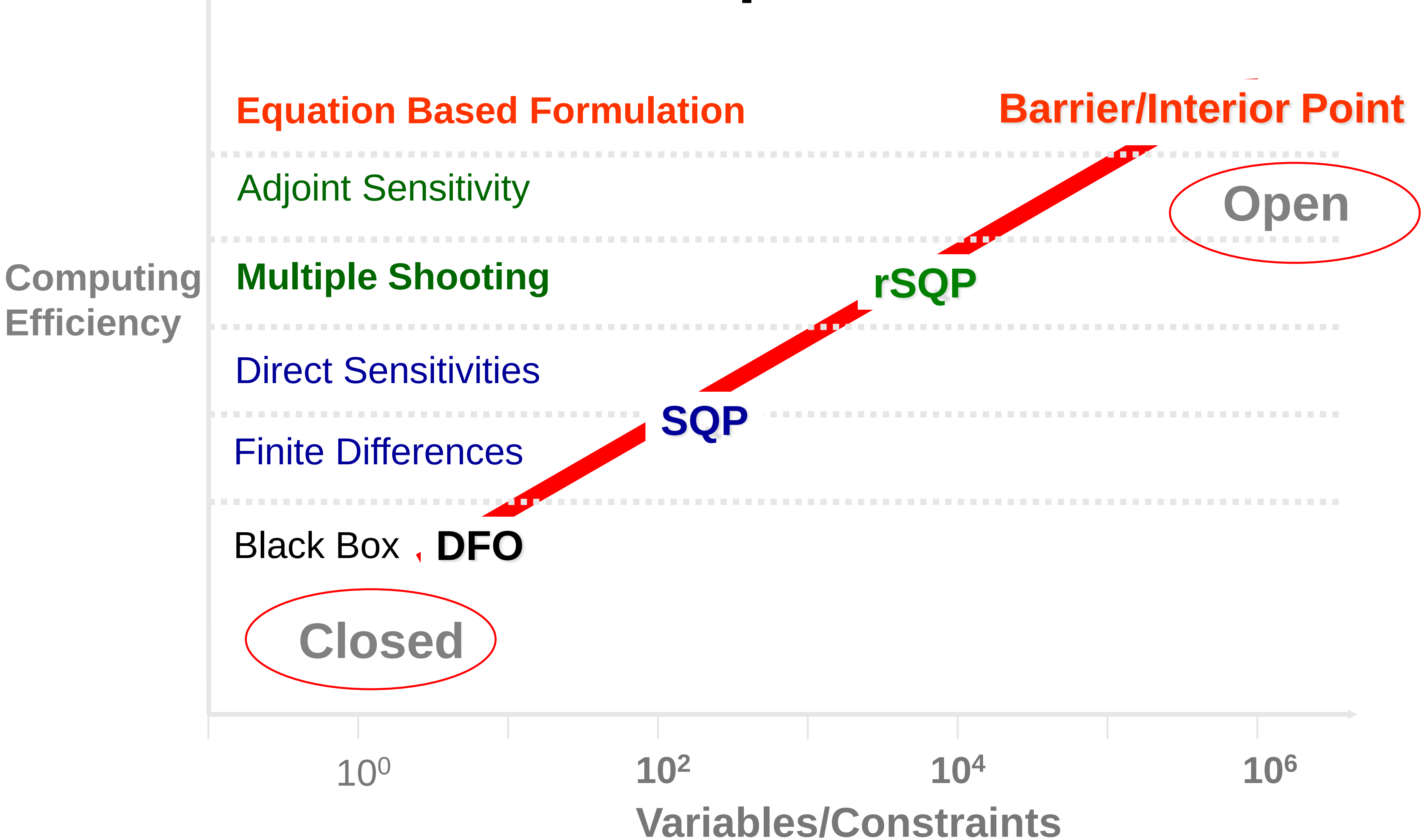
Optimization Solvers

- Auxiliary Variable – **Antigone, BARON, GloMIQO, SCIP**
- Convex MINLP – **DICOPT, SHOT, αECP**
- Factorable programming –**EAGO, MAiNGO**
- NLP- **iPOPT**
- Parametric optimization toolbox - **POP**
- αBB – **OCTERACT, αBB**

Modeling

- Modeling, equation-solver, optimization - **ALAMO, ARGONAUT, Aspen Custom Modeller, GAMS, gPROMS, JuMP, Matlab, MoT, Simulink, Pyomo**
- 3D modeling software - **ANSYS-Fluent, COMSOL**

Multi-scale Optimization (Biegler)



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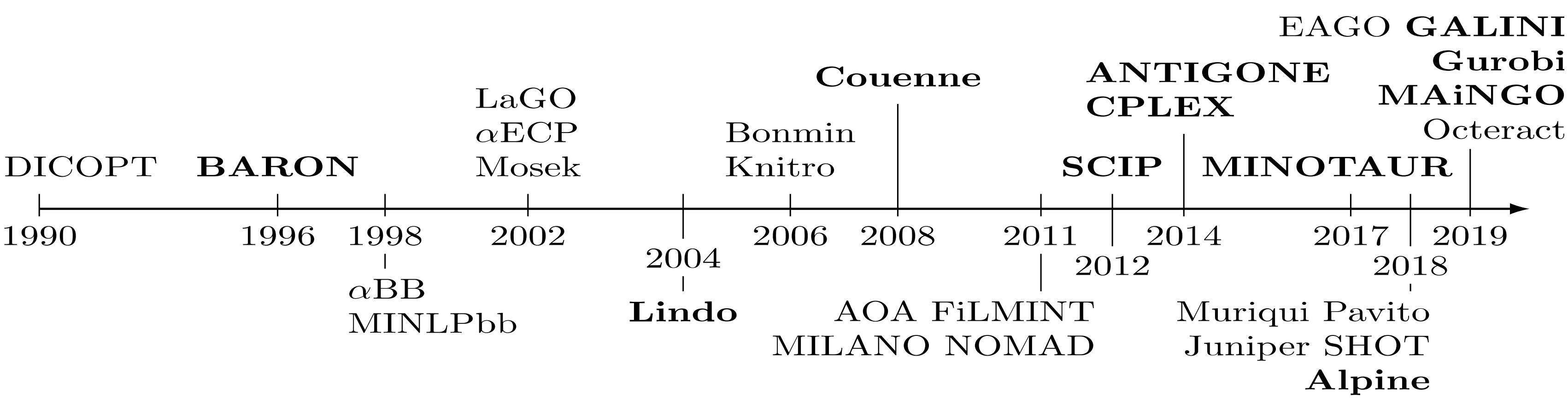
Global Optimization (Misener)

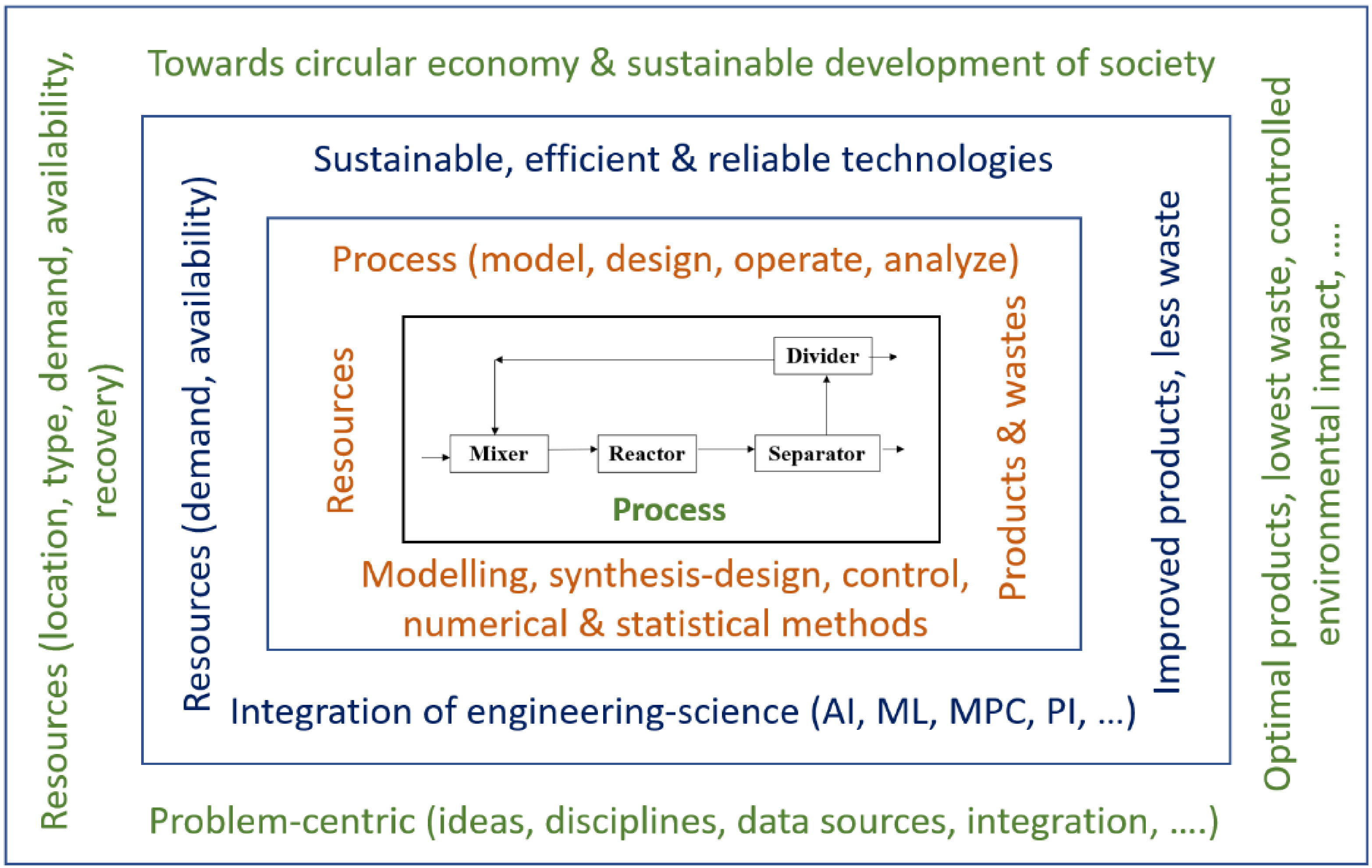
Wide range of available solver software (commercial software Gurobi & CPLEX)



Outline

- *Professor Roger Sargent – a tribute*
- Multi-Scale Process Systems Engineering
  - *Core PSE*
  - *Domain & application-driven PSE*
- **What is next for PSE?** ***The 'Generation Next'***

The multi-layered view of Process Systems Engineering (Gani)



The Generation Next

… *expanding/consolidating* the scope of Process Systems Engineering …

- *Towards enhanced 'Hybrid Modeling' capabilities & tools*
    - Models, 'meta-models' & Big Data Analytics, Digital Twins
    - Bridging the multiple-scales
- **'Smart Manufacturing' - CESMII**
- **'Modular Process Intensification' - RAPID**
- Food-Energy-Water-Nexus Systems Engineering
- Future Energy Systems – **Multi-scale Energy Systems Engineering**
- Life Science Systems Engineering
- Resilience & Sustainability in integrated energy/manufacturing networks
- **Circular Economy Systems Engineering**

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U.S. DEPARTMENT OF ENERGY
Energy Efficiency & Renewable Energy

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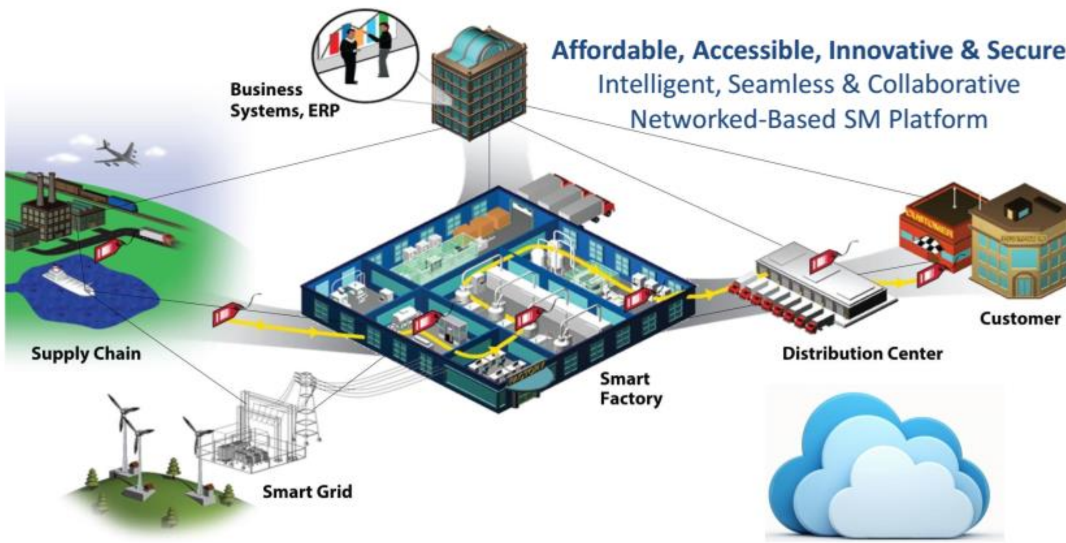
Manufacturing USA



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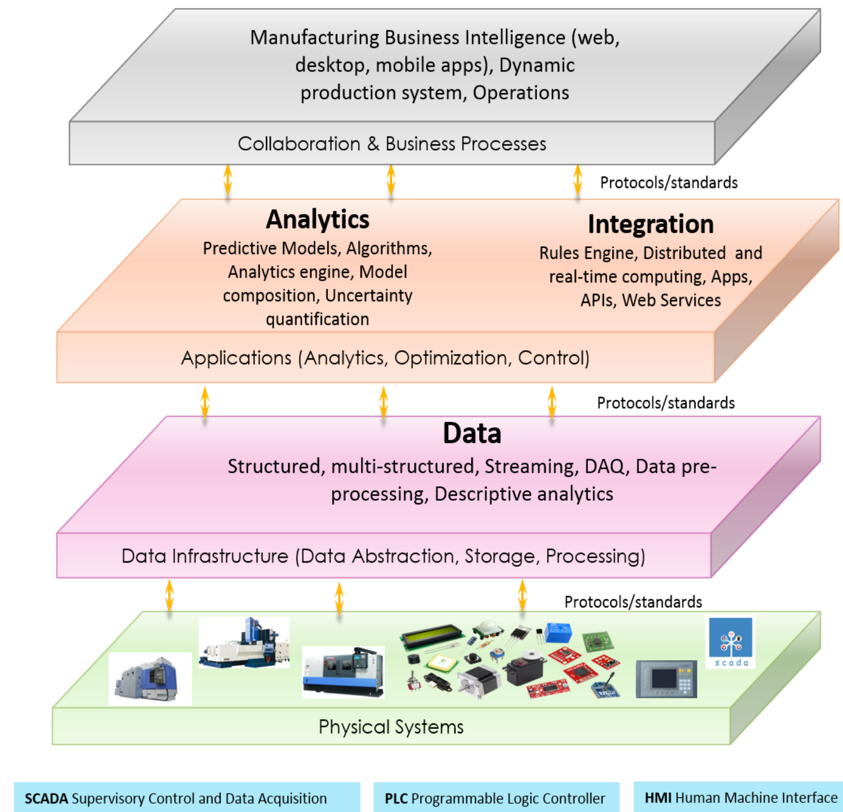
Smart Manufacturing

- **Advanced High Fidelity Modeling**
  - Predictability
  - Uncertainty evaluation
- **Data Infrastructure**
  - Advanced Sensors
  - Industry Testbeds
- **Connectivity**
  - Software and Communication Platforms
  - Application Toolkits for SM Deployment
- **Control and Automation**
  - Real-Time Data Analytics
  - Real-Time Optimization



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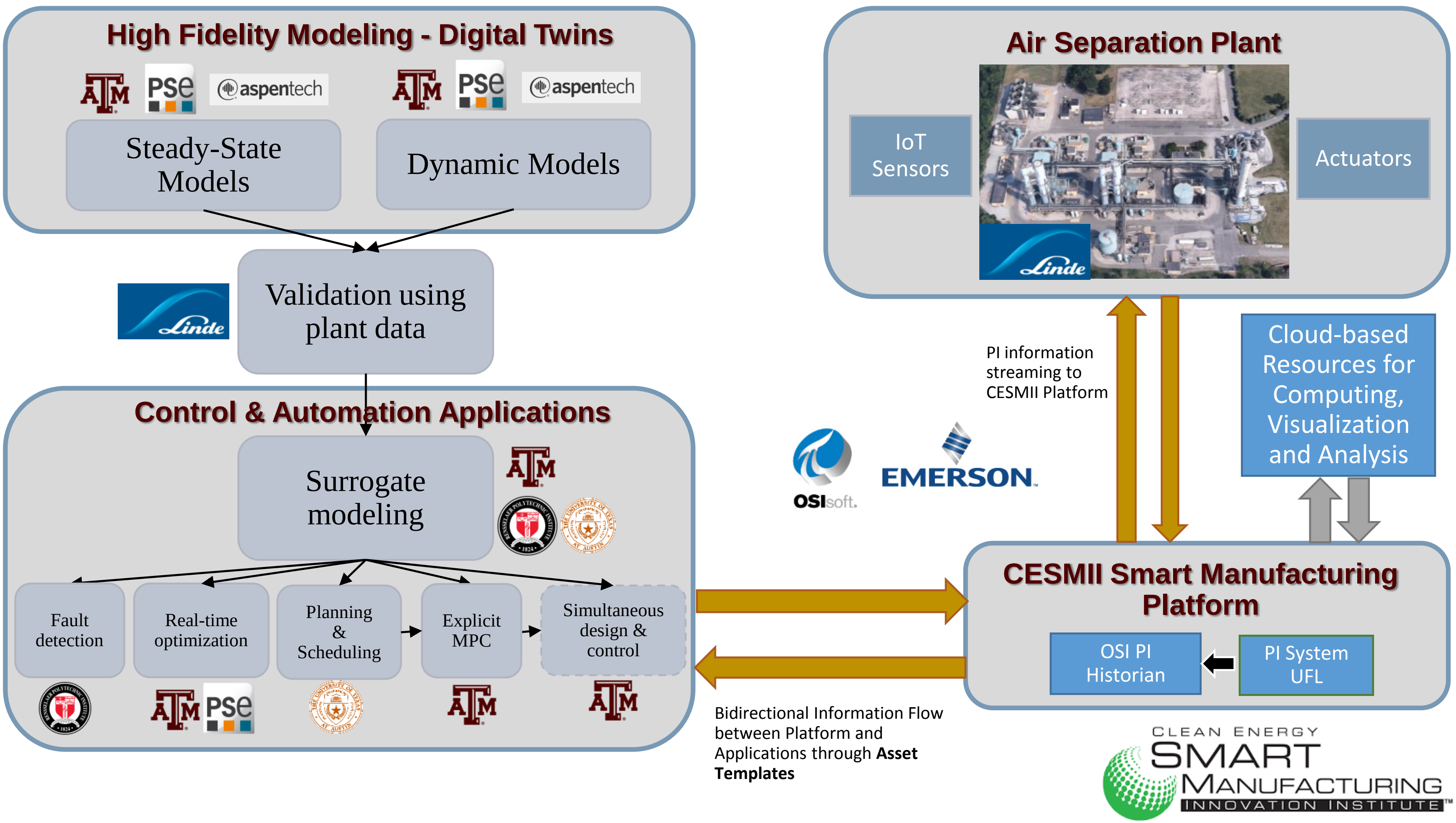
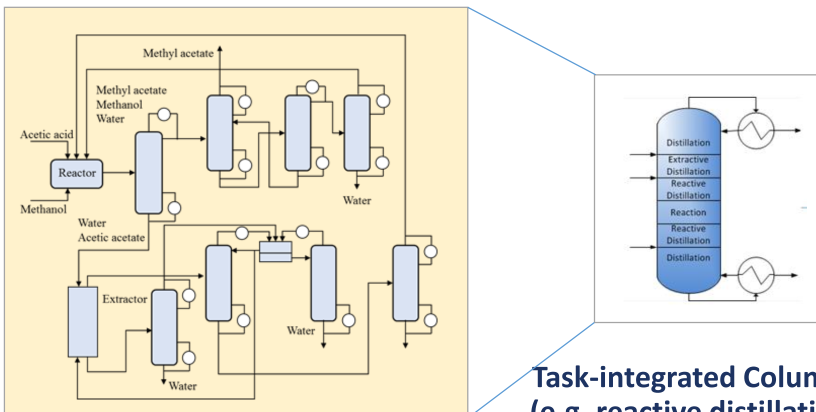
Smart Manufacturing – Air Separation System

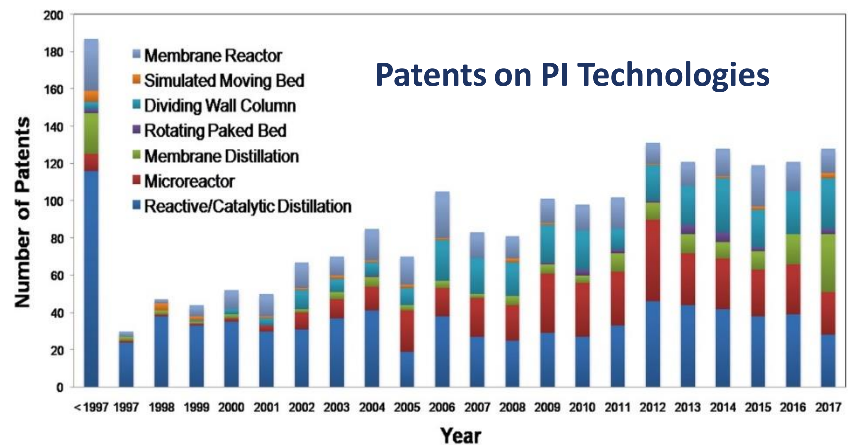


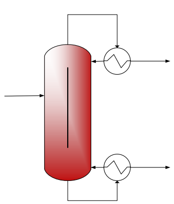
Process Intensification

Substantially decreasing *equipment volume, energy consumption, or waste formation*; ultimately leading to *cheaper, safer, sustainable* technologies

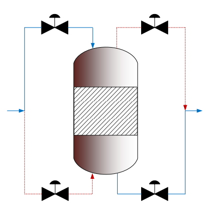


Task-integrated Columns (e.g. reactive distillation)

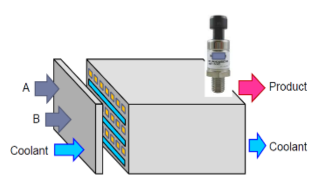




Divided-wall Column



Reverse Flow Reactor



Micro-Reactor

Tian, Demirel, Hasan, and Pistikopoulos. "An Overview of Process Systems Engineering Approaches for Process Intensification: State of the Art", Chemical Engineering and Processing: Process Intensification (2018), 133, 160-210.

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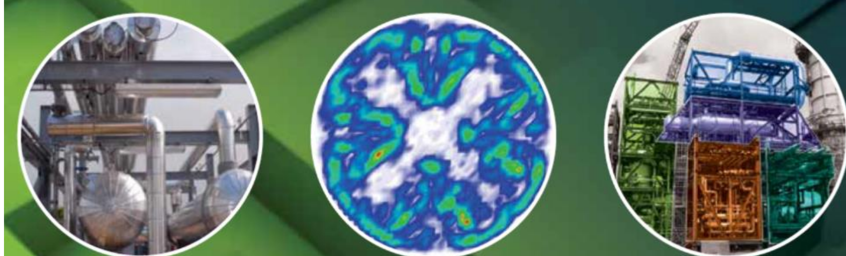
SPECIAL SECTION:
PROCESS INTENSIFICATION



Process Intensification: Its Time is Now

For more than 40 years, process intensification (PI) efforts in the U.S. have lagged behind those in other parts of the world. Europe has invested heavily in

opportunities — the majority of which lie in high-grade, specialty chemicals rather than in the commodity sector. They look at viable opportunities available to chemical

Realize the Potential of Process Intensification

JAMES BIELENBERG
RAPID MANUFACTURING INSTITUTE
MICHELLE BRYNER
AIChE

With a history that dates back to the 1970s, process intensification (PI) is not a new concept. Several developments have moved PI forward, but realizing PI's full potential will require the concerted efforts of industry, academia, and government.

Process intensification aims to dramatically improve manufacturing processes through the application of novel process schemes and equipment. These novel

ogy space at an early point in its technical and commerc development

- limited understanding of design and operation

Modularization in Chemical Processing

MICHAEL BALDEA
THOMAS F. EDGAR
THE UNIV. OF TEXAS AT AUSTIN
BILL L. STANLEY
VENTECH
ANTON A. KISS
THE UNIV. OF MANCHESTER

Most high-margin growth opportunities lie in high-grade specialty chemicals. To realize these opportunities, manufacturers are looking to distributed modular production facilities. Process intensification could help to enable these new technologies.

Two fundamental tenets have driven chemical engineering over the last century. The first is economy of scale — which reasons that constructing larger chemical plants improves capital efficiency and resource utilization, thereby reducing operating costs and product price, as

attention in the past two decades. The objective of PI is to design substantially smaller plants, while improving operational safety, environmental performance, and energy efficiency. The Rapid Advancement in Process Intensification Deployment (RAPID) Manufacturing Institute, sup-

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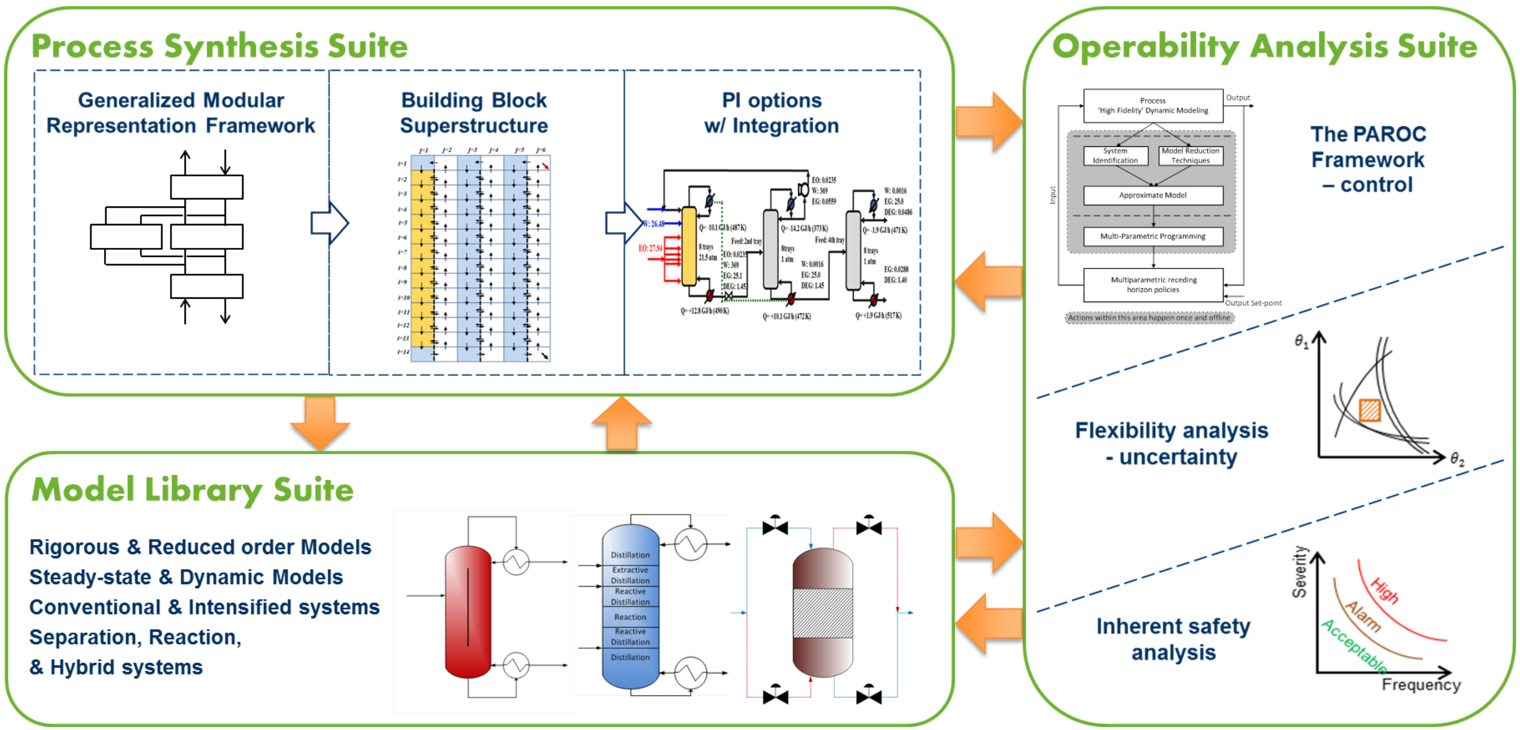
Process Intensification

SYNthesis of Operable ProcesS Intensification Systems (SYNOPSIS)



RAPID Transforming Process Industries

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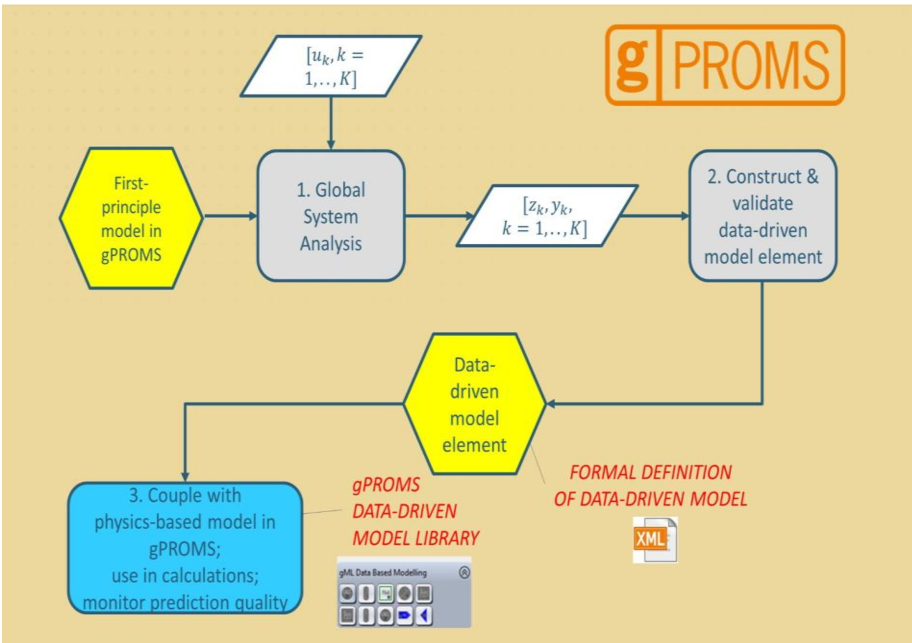
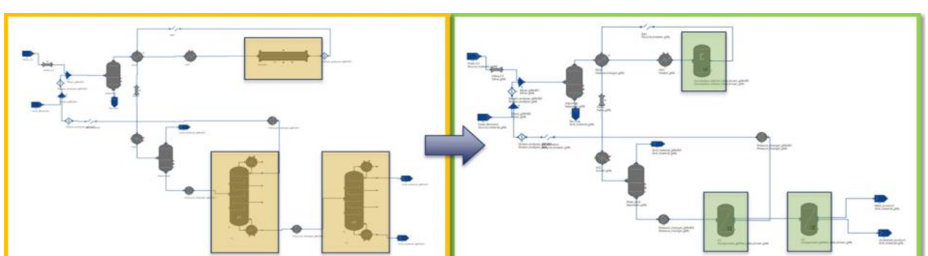
Process Intensification - *SYNOPSIS*





- **Surrogate model generation**
  - Comparison of algorithms
  - Identify most promising to implement
- **Hybrid model library**
  - Couple surrogate/data-driven and first principle models in flowsheets

PSE
A Siemens Business

RAPID
Transforming Process Industries

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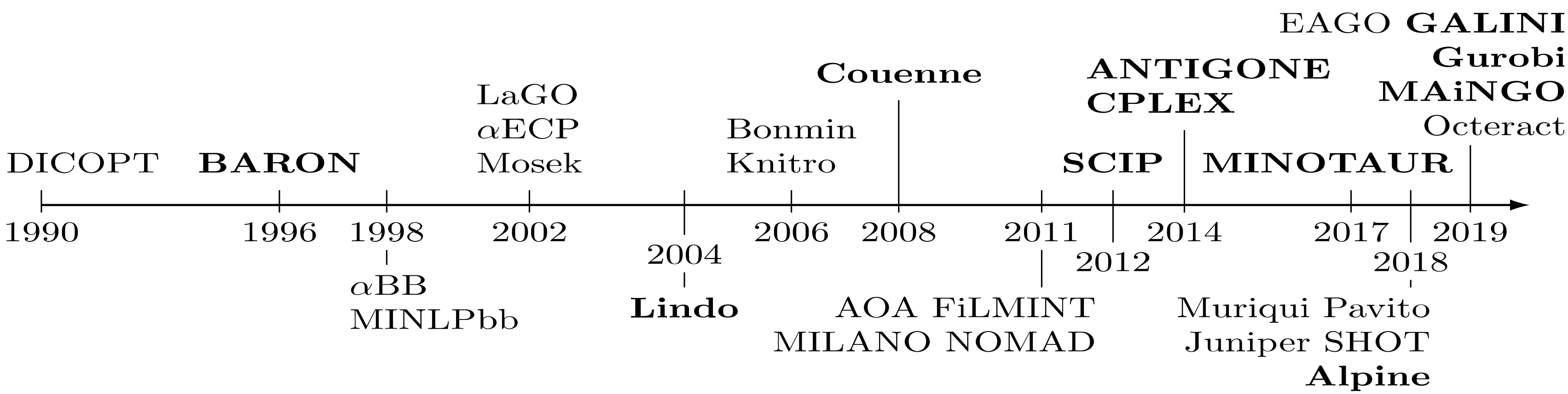
Global Optimization (Misener)

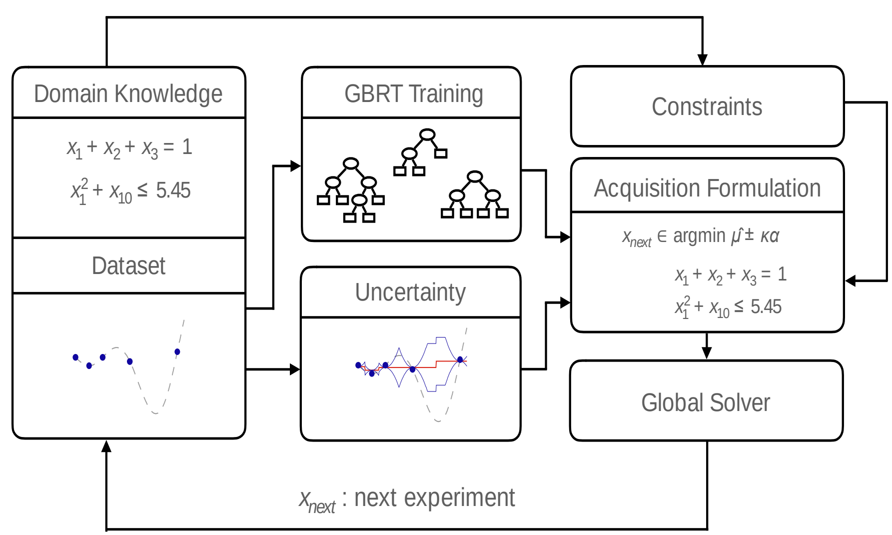


Research trends

- Exploiting special structure for engineering problems
- Machine learning to expedite solvers
- Incorporating aspects of both mechanistic & data-driven models into optimization problems

  ALAMO (CMU/GATech), ARGONAUT (TAMU), ENTMOOT (Imperial), MeLON (RWTH)

ENTMOOT



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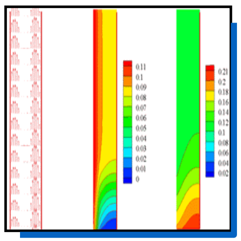
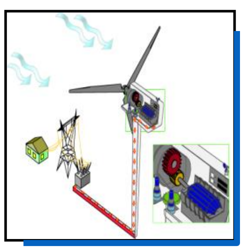
Multi-Scale Energy Systems Engineering

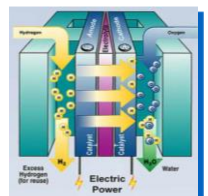


Fuel cell CFD model

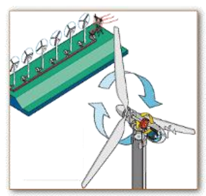


Wind turbine system model

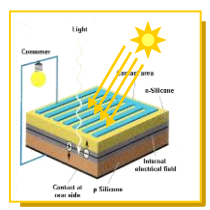
Component models



Fuel cells (SOFC)



Wind turbines



Photovoltaic cells

Power technologies

GB TRANSMISSION GRID

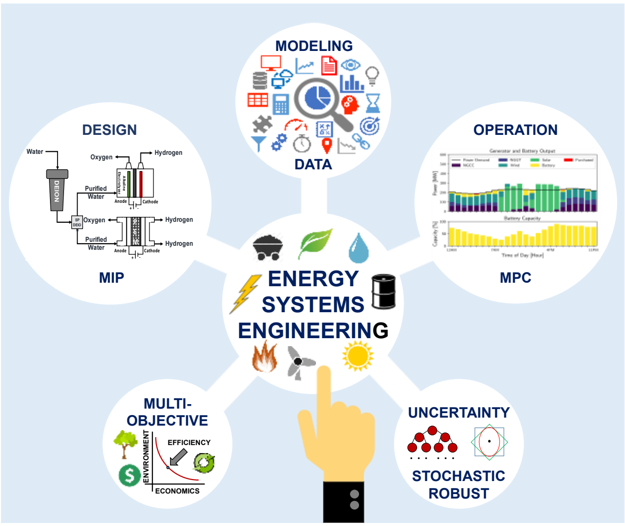
Energy infrastructure

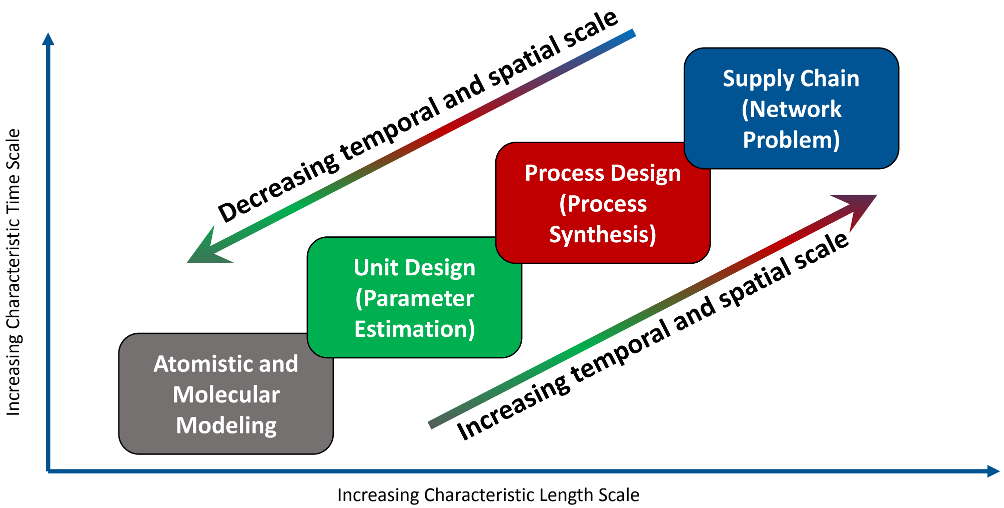
mesoscale

macroscale

megascale

Multi-Scale Energy Systems Engineering





- Significantly improving Energy Efficiency
- Analysing 'Best' Options for technology/resources mix to meet demand/targets
- Delivering cost-effective production strategy to meet energy targets
- Navigating the Energy Transition landscape – scenario analysis

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Multi-Scale Energy Systems Engineering

Methanol
Ammonia
Hydrogen

Reference Case

Traditional fossil fuel-based route

Carbon source: NG

H_2 source: NG

N_2 source: Air

Heat: NG

Electricity: NG

Hybrid Transition Period Case

Fossil Fuels + Renewables + Novel Technologies

Carbon source: NG, biomass, CO_2

H_2 source: NG, biomass, water

N_2 source: Air

Heat: NG, biomass

Electricity: NG, biomass, wind, solar PV

Biomass Options:

- Hardwood
- Switchgrass

Long Range Aim

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Fully Renewable Route
(aim is going carbon neutral)

Carbon source: Biomass, CO_2

H_2 source: Water, biomass

N_2 source: Air

Heat sources: Biomass

Electricity: Wind, solar PV

Biomass Options:

- Hardwood
- Switchgrass
- Municipal Solid Waste

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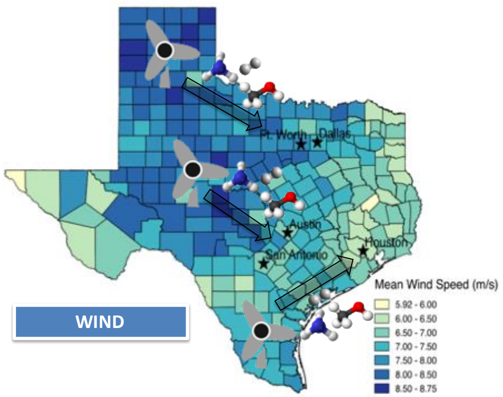
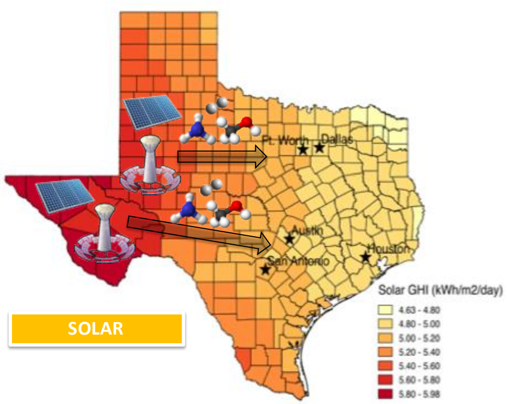
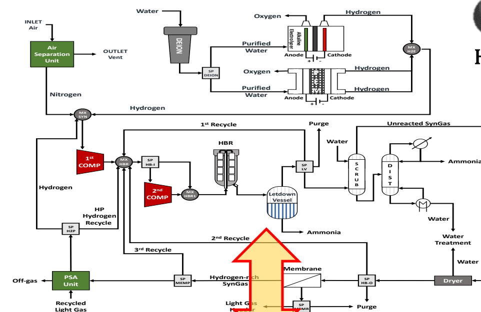


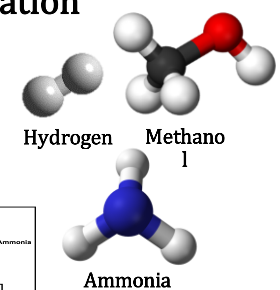


Multi-Scale Energy Systems Engineering

Process Synthesis & Optimization

- Optimal topology for producing energy carriers
- Minimized production cost





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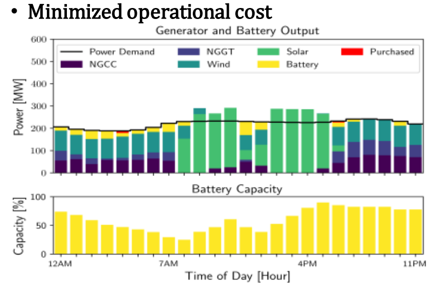
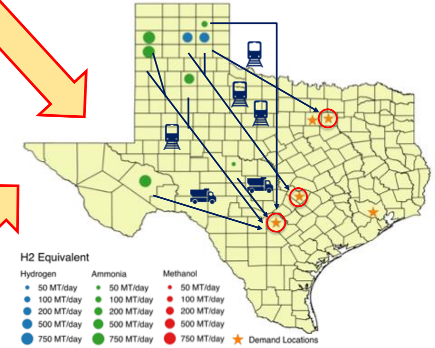
Renewable Power Scheduling

- Optimal operation of energy storage
- Minimized operational cost



Supply Chain Optimization

- Optimal energy carrier supply chain network
- Minimized total cost



The Generation Next

… *expanding/consolidating* the scope of Process Systems Engineering …

- *Towards enhanced **'Hybrid Modeling'** capabilities & tools*
  - Models, 'meta-models' & Big Data Analytics, Digital Twins
  - Bridging the multiple-scales – Multiscale Modeling
- **'Smart Manufacturing' - CESMII**
- **'Modular Process Intensification' - RAPID**
- Food-Energy-Water-Nexus Systems Engineering
- Future Energy Systems – **Multi-scale Energy Systems Engineering**
- Life Science Systems Engineering
- Resilience & Sustainability in integrated energy/manufacturing networks
- **Circular Economy Systems Engineering**

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Toward Circular Economy Systems Engineering

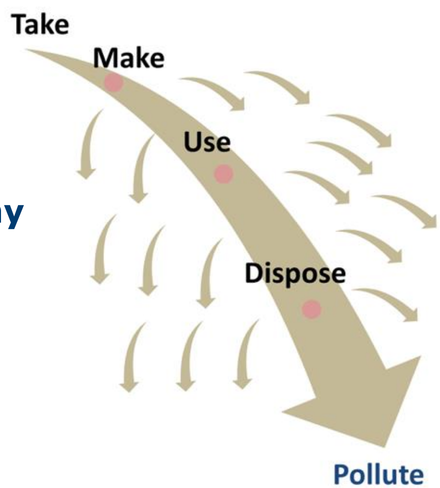
30% of Food is Wasted

Cars sit Unused 92% of their life

Offices are used 50-65% of the time

86% of Plastic Package is Not Recycled

Linear Economy



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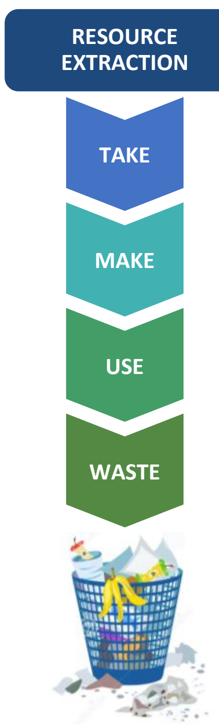
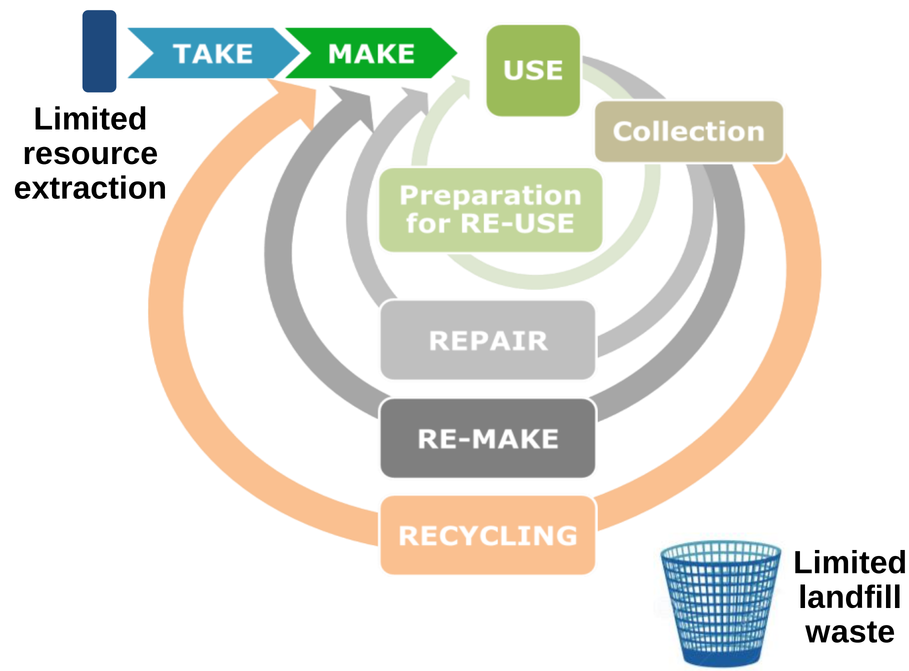
Linear Economy



Circular Economy



Toward Circular Economy Systems Engineering

- Rising populations put huge stresses on the natural resources
- Wastes have a negative impact on the environment
- Successful Circular Economy would contribute to all dimensions of sustainable development:
  - Economic
  - Environmental
  - Social

- A more politically/socially accepted term?

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Toward Circular Economy Systems Engineering

China Circular Economy Promotion Law

Benefits of a Circular Economy in South Australia
Government of South Australia
Green Industries SA

Roadmap for the Circular Economy
Let's be in the loop, let's change model
Liberté • Égalité • Fraternité
RÉPUBLIQUE FRANÇAISE

European Commission
CIRCULAR ECONOMY
Closing the loop
AN AMBITIOUS EU CIRCULAR ECONOMY PACKAGE

TORONTO
GM28.29
REPORT FOR ACTION
Implementation Plan and Framework for Integrating Circular Economy Approaches into City Procurement Processes to Support Waste Reduction and Diversion

Unilever

U.S. CHAMBER OF COMMERCE FOUNDATION
Sustainability and Circular Economy Program

A Circular Economy in the Netherlands by 2050
Government-wide Programme for a Circular Economy

bp

LUXEMBOURG AS A KNOWLEDGE CAPITAL AND TESTING GROUND FOR THE CIRCULAR ECONOMY

CIRCULAR GLASGOW

PHILIPS

CE is currently promoted by several national governments and businesses around the world

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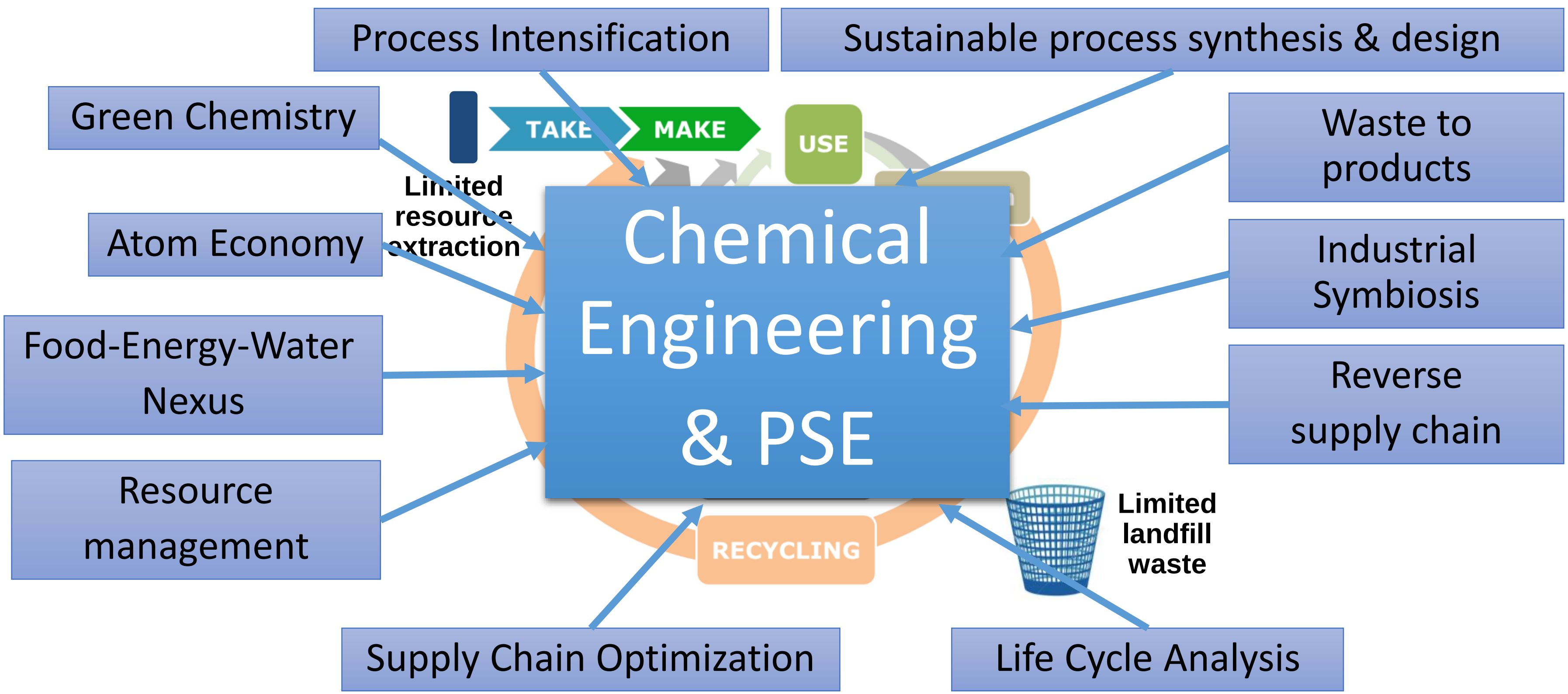
Toward Circular Economy Systems Engineering



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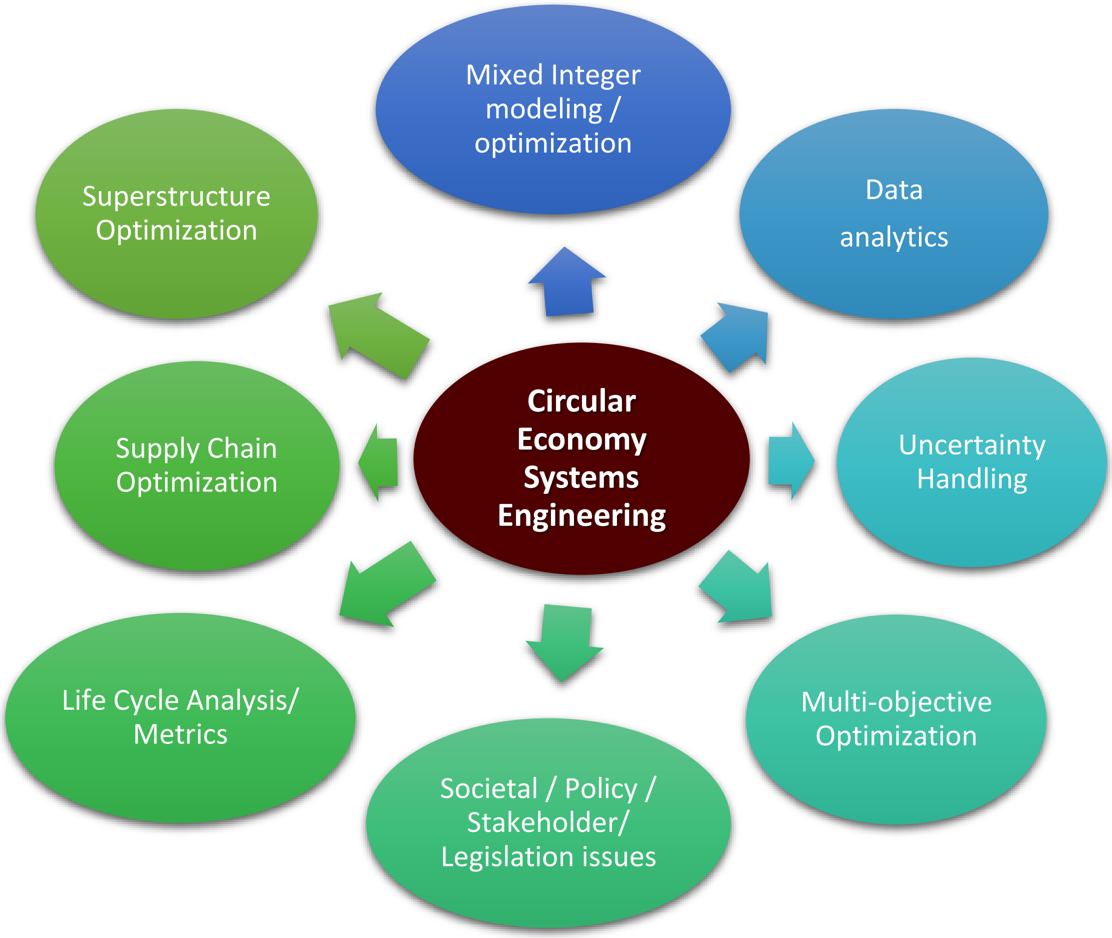
Circular Economy Systems Engineering

(Avraamidou et al; Circular Economy - a challenge and an opportunity for Process Systems Engineering, 2020, CACE)

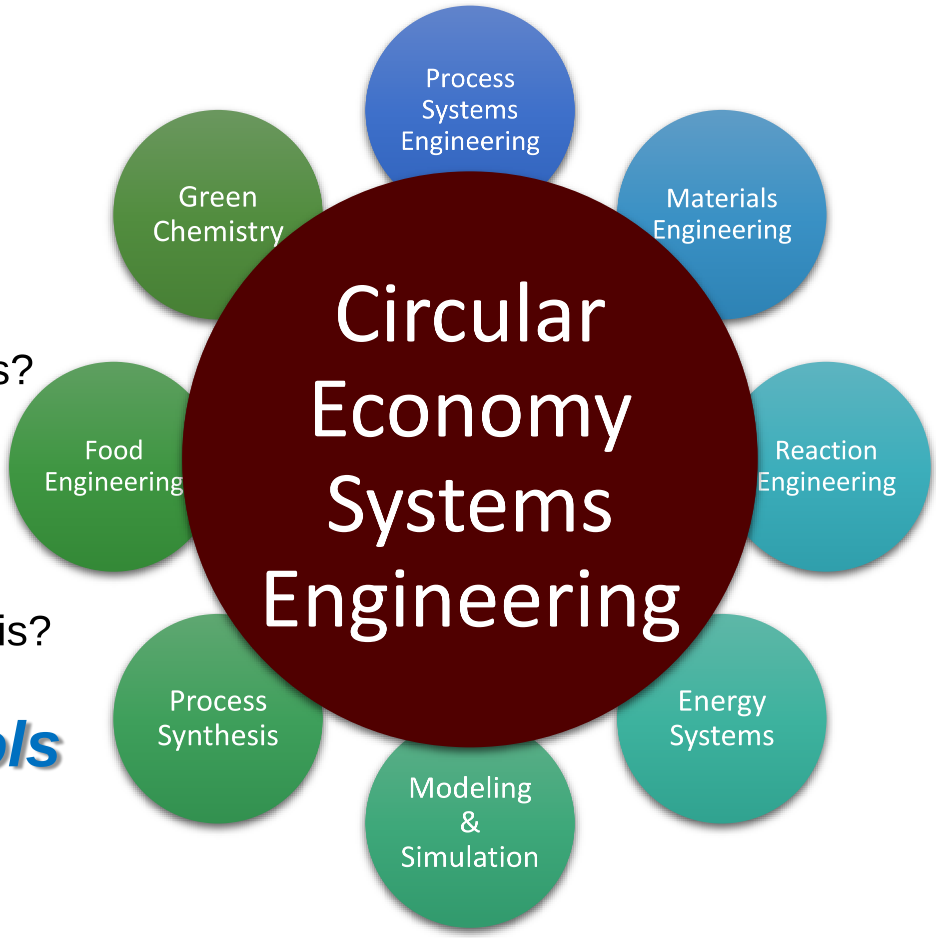


Circular Economy Systems Engineering

Open Research Questions

1. Metric to compare 'circular' alternatives - a 'circular index' ?
2. Uniqueness of a circular system? Robustness?
3. At which scale? Centralized? Decentralized?
4. Policy & regulation issues?
5. Resource utilization & novel pathways analysis?

PSE approach, methods & tools essential! **(ESCAPE-31)**



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The Generation Next

… *expanding/consolidating* the scope of Process Systems Engineering …

... some closing remarks …

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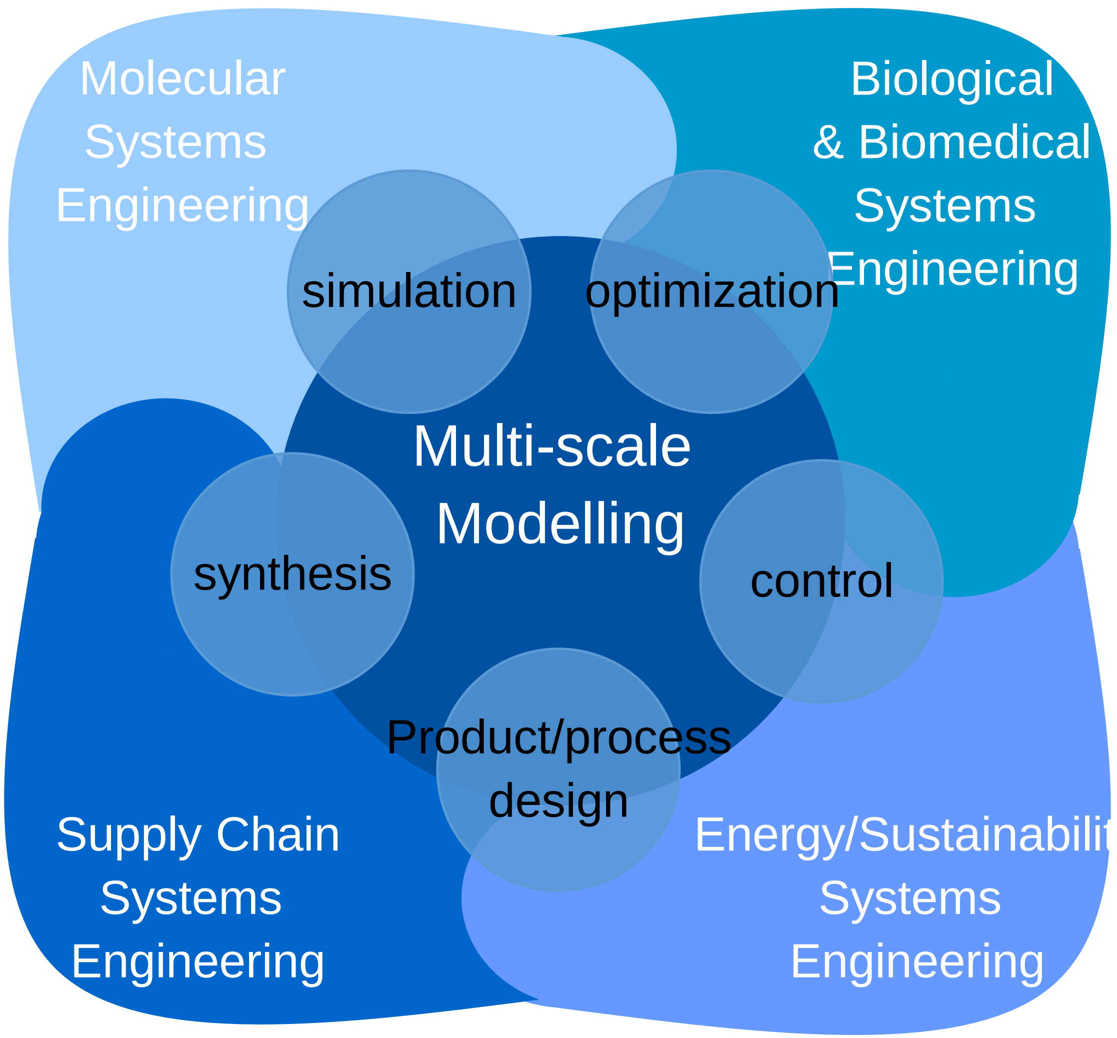
Multi-Scale Process Systems Engineering



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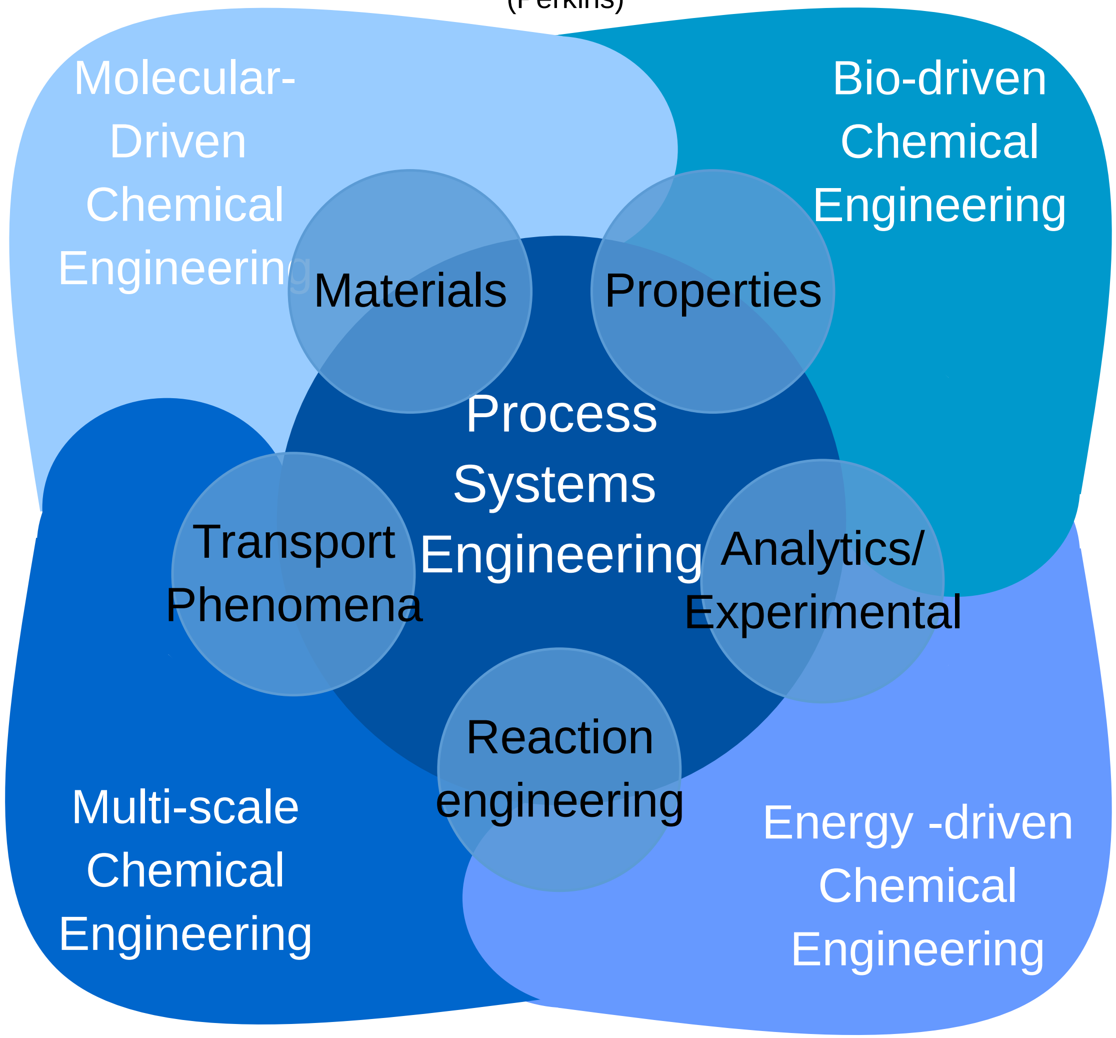
Multi-Scale Process Systems Engineering

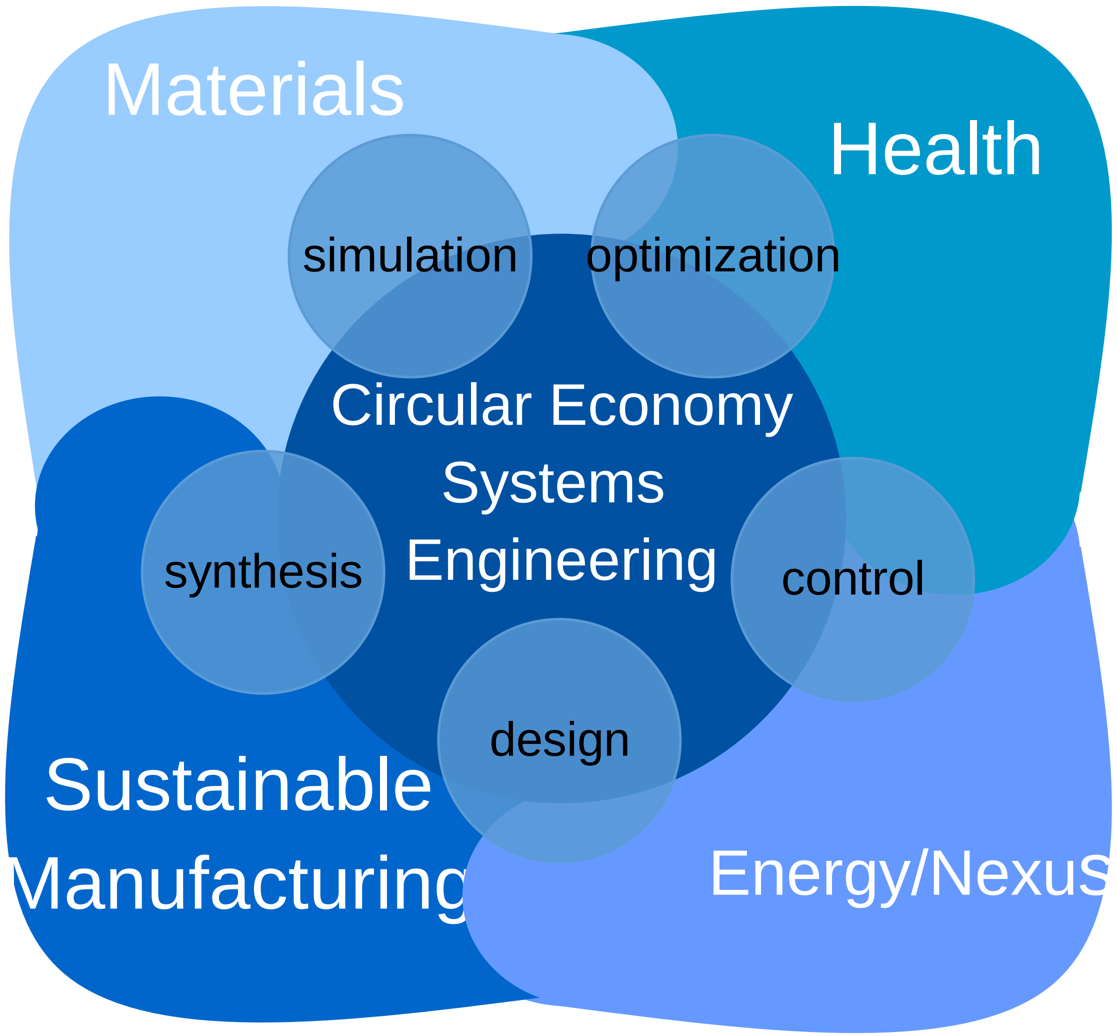
provides the ‘scientific glue’ within chemical engineering

(Perkins)



Process Systems Engineering – The Generation Next

systems thinking & practice *– essential to address* ***societal grand challenges***



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The Professor Roger Sargent Medal
IChemE Webinar

To our parents we owe our being

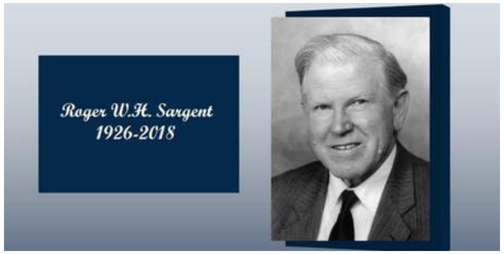
To our teachers (we owe) *our well being*

(Alexander the Great)

THANK YOU ROGER!

… for your inspirational Academic Leadership

& Pioneering Vision



Process Systems Engineering - *Generation Next*

Stratos Pistikopoulos PhD FIChemE FAIChE FREng
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Director, Texas A&M Energy Institute