Process Systems Engineering (PSE)

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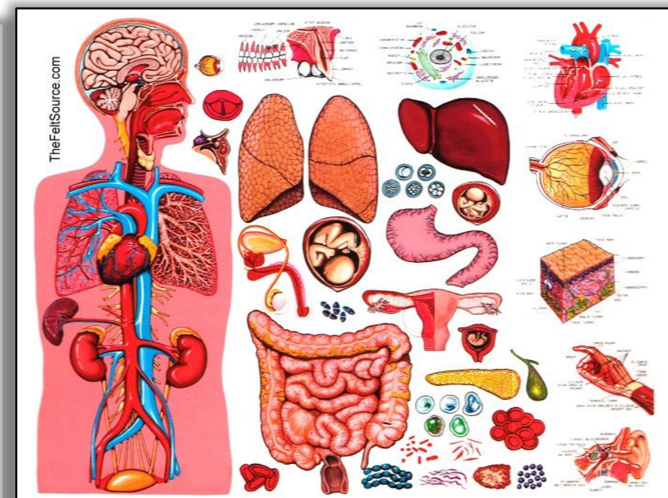
What is a System?

A set of interrelated components organized to achieve certain goals

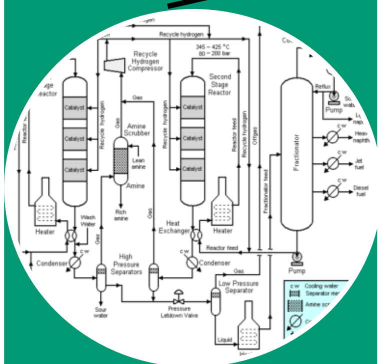
- Emphasize the performance **as a whole**
- Understand **the interrelationships** among the components

The whole is more than the sum of its parts: Aristotle

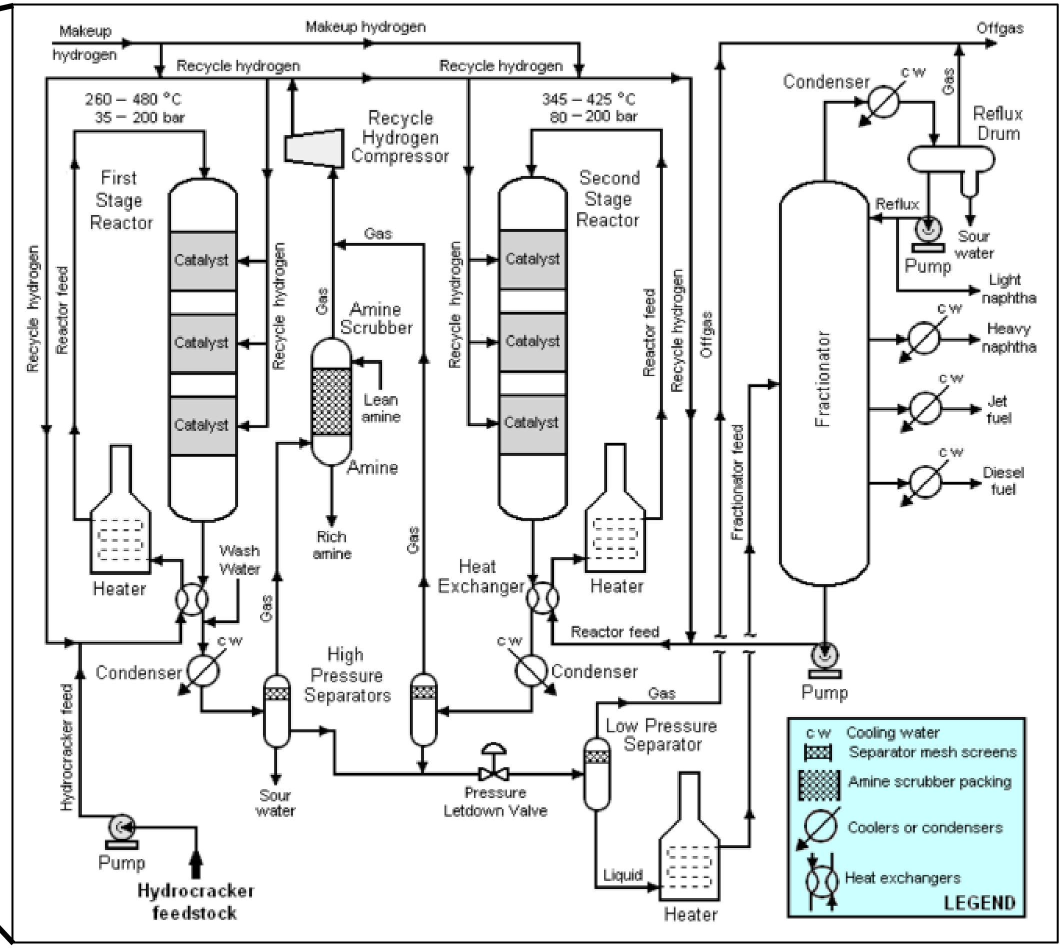
Reductionism Vs Holism



Examples of a “system”



Chemical processes, process plants



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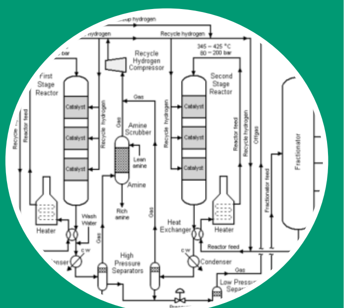

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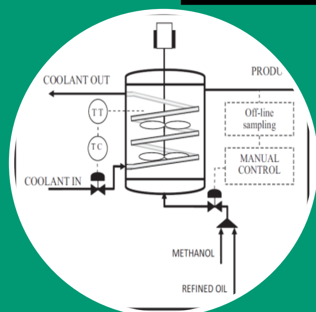
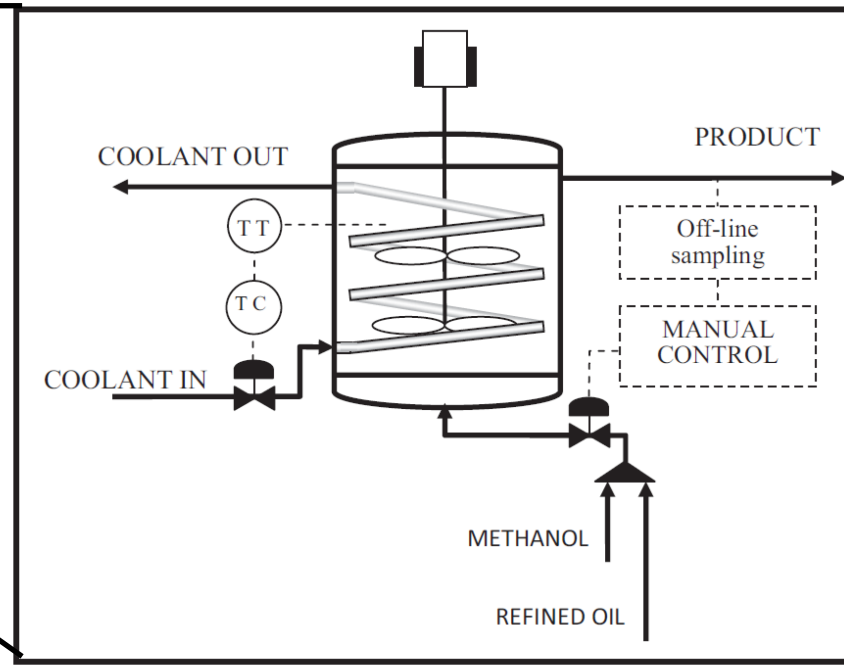


Reactor; Distillation column



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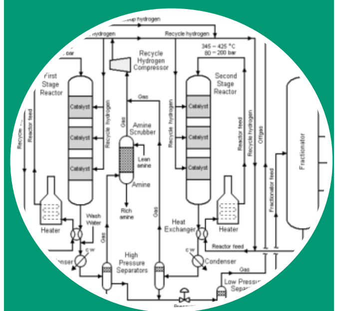

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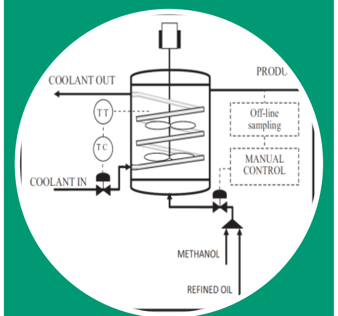

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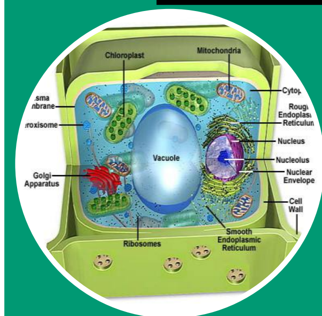
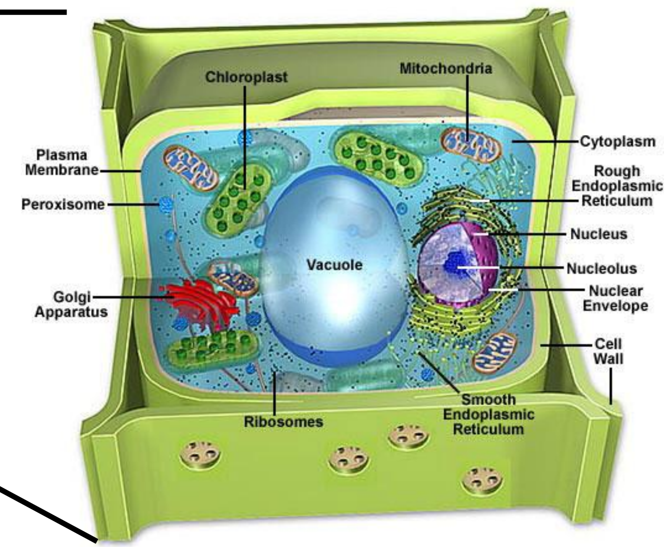
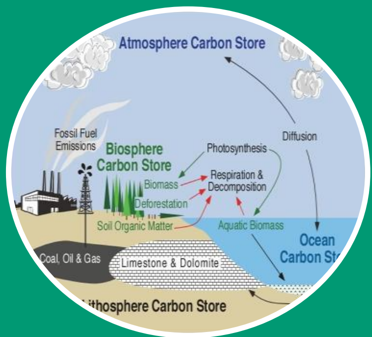


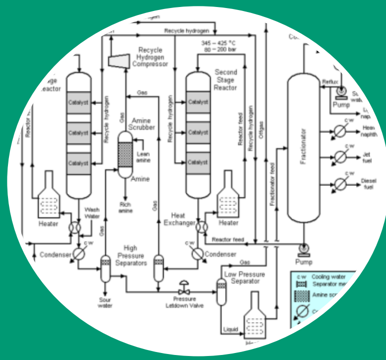
Plant cell wall; Nano-catalyst structure



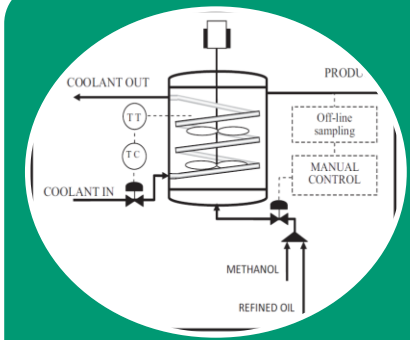
Examples of a "system"



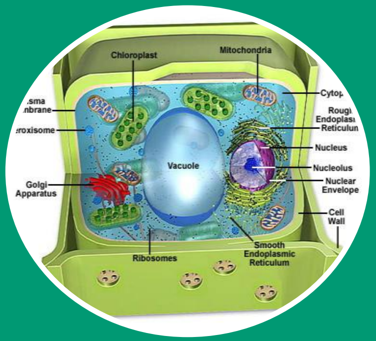
Carbon cycle; Product supply chain



Chemical processes, process plants



Reactor; Distillation column

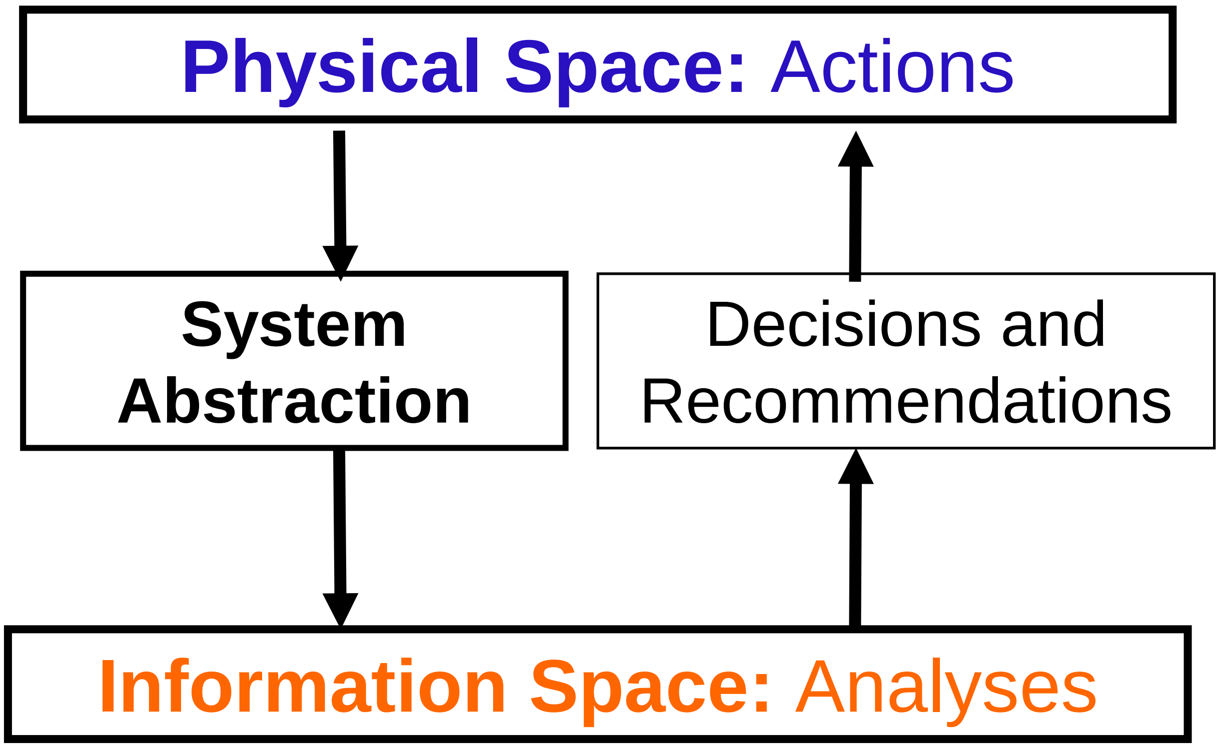


Plant cell wall; Nano-catalyst structure

Increasing spatial and temporal scale

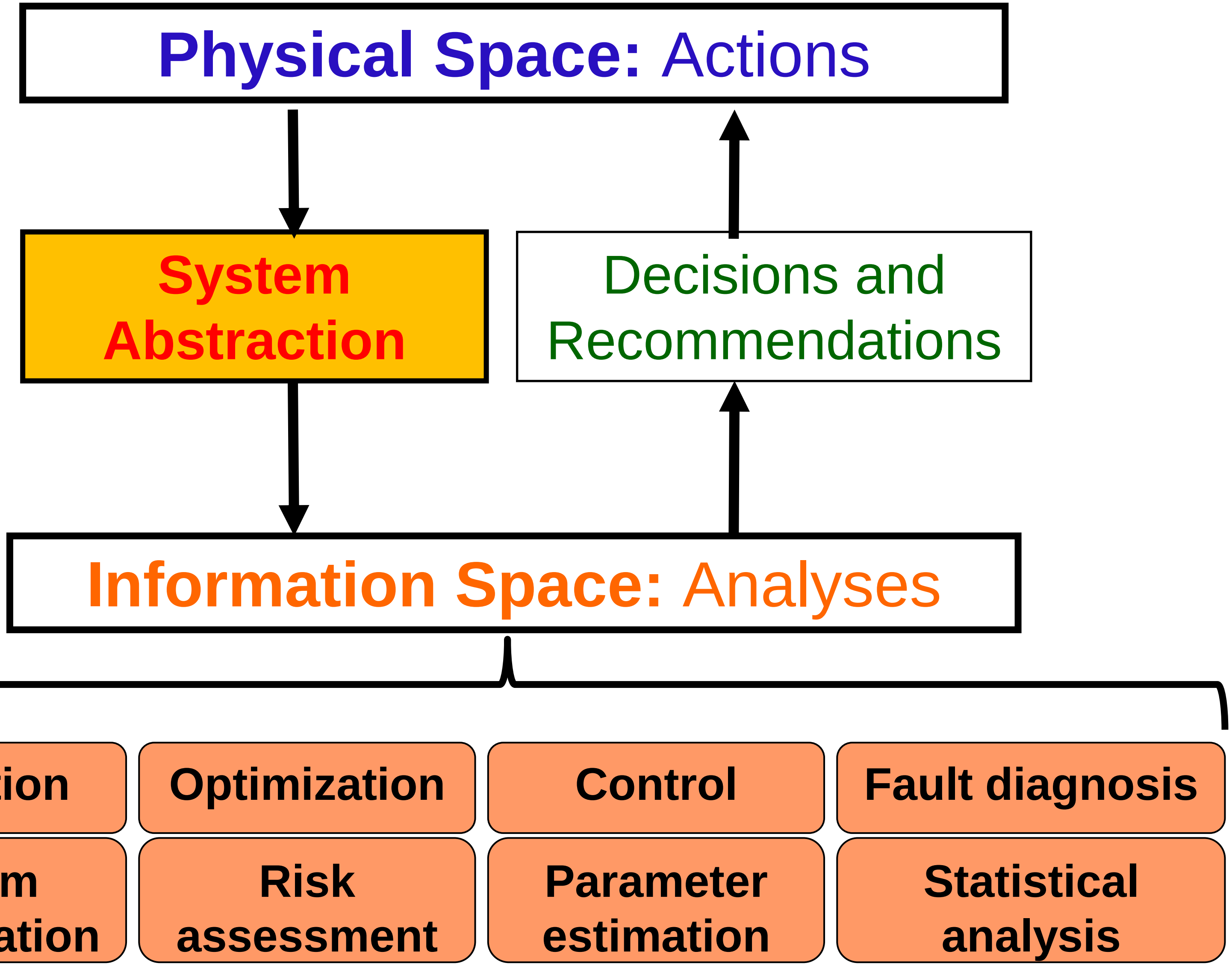
- Each system consists of multiple components (sub-systems)
- Each component is a system in itself

What is Systems Engineering?



System Abstraction or Modeling a Necessary Step

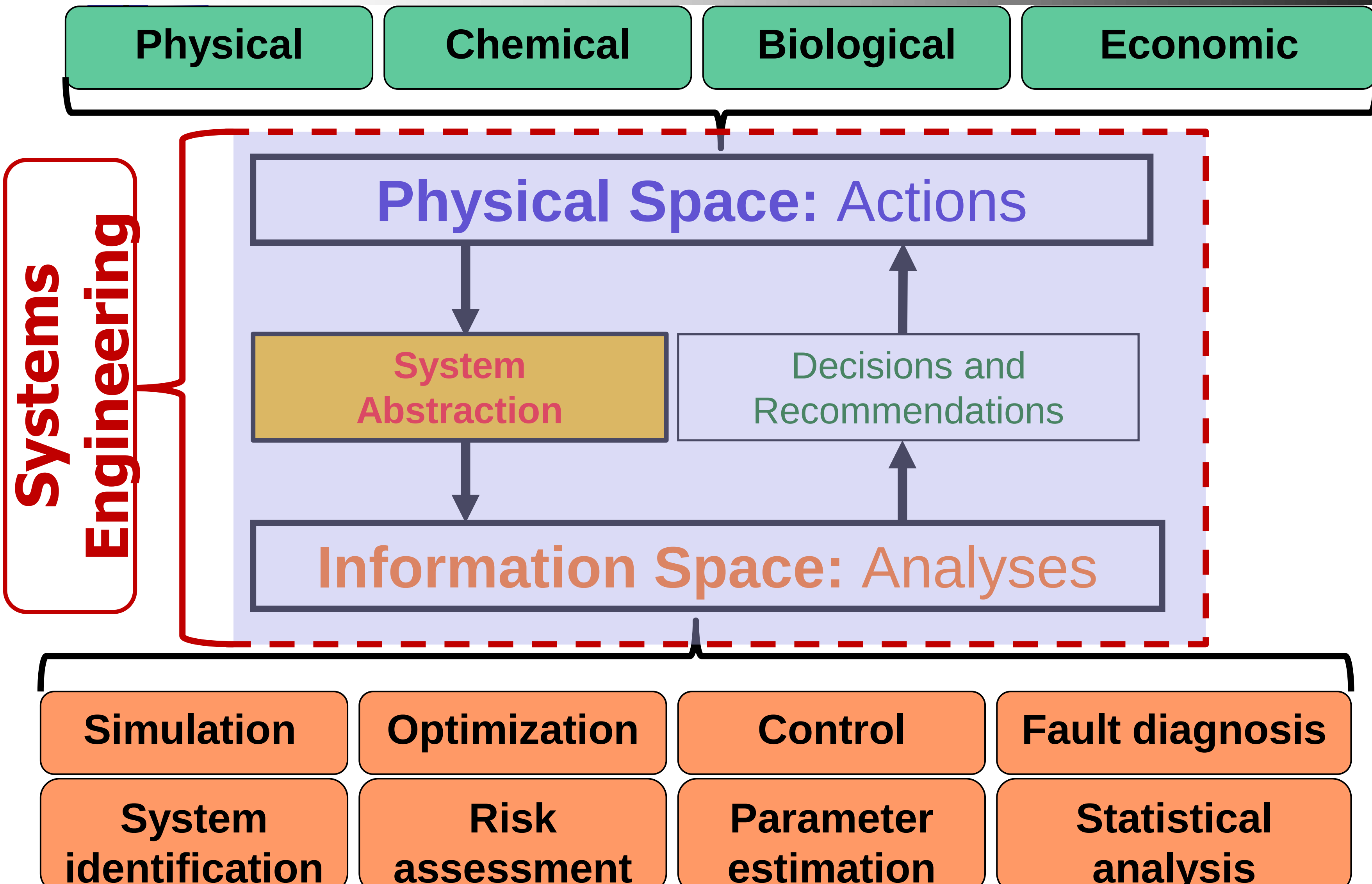
What is Systems Engineering?



What is Process Systems Engineering?

…field that encompasses the activities involved in the ***engineering*** of ***systems*** involving *physical*, *chemical*, and/or *biological* processing operations

Process Systems Engineering



Decisions and Recommendations

Process design:
- Product/molecular design
- Reactor design
- Flow sheet synthesis
- Supply chain networks
- Sensor network design

Process control:
- Online control strategies

Process Operations:
- Management and operational strategies

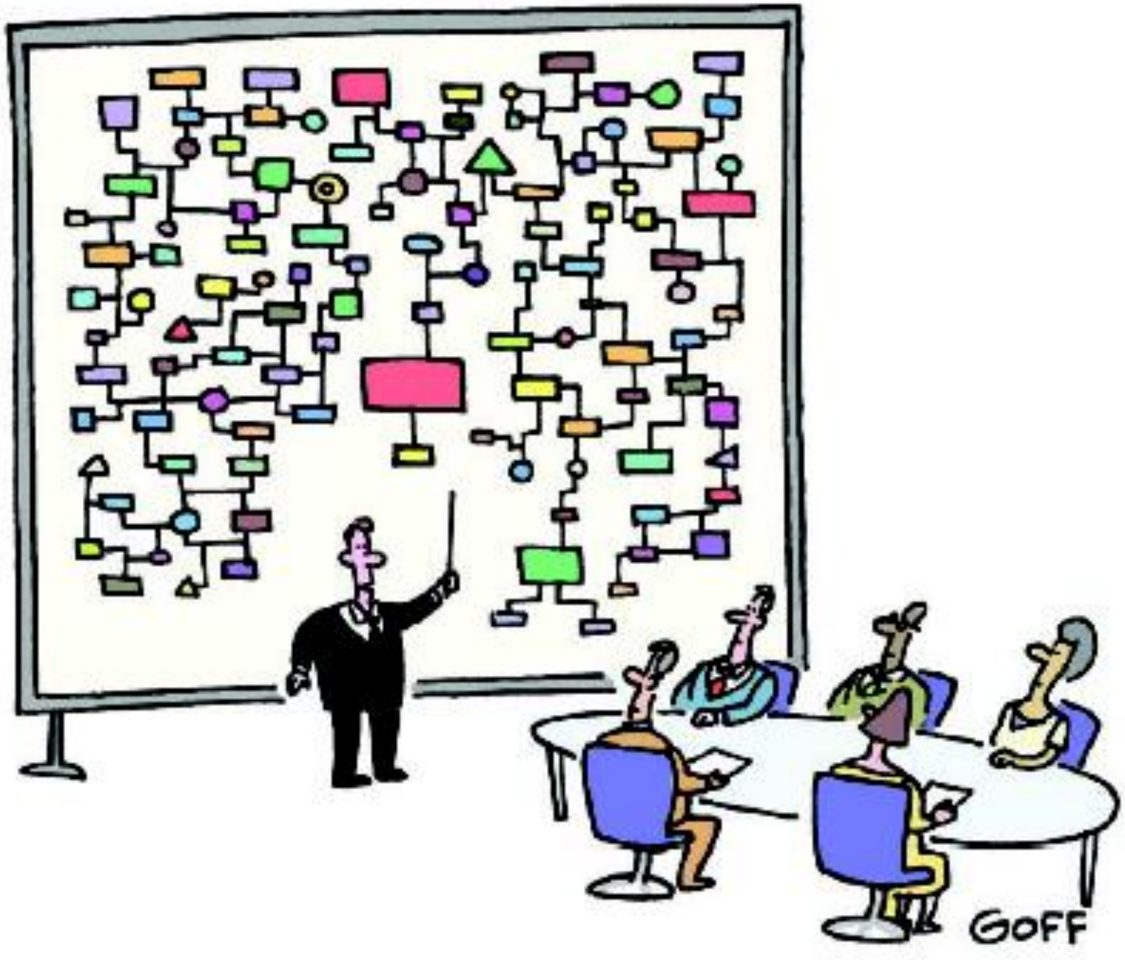
Novel methodological contributions:
- Optimization algorithms
- Control approaches/strategies
- Informatics and statistical methods

Evolution of PSE: 1860s – to date

Ernest Solvay: The First Process Engineering

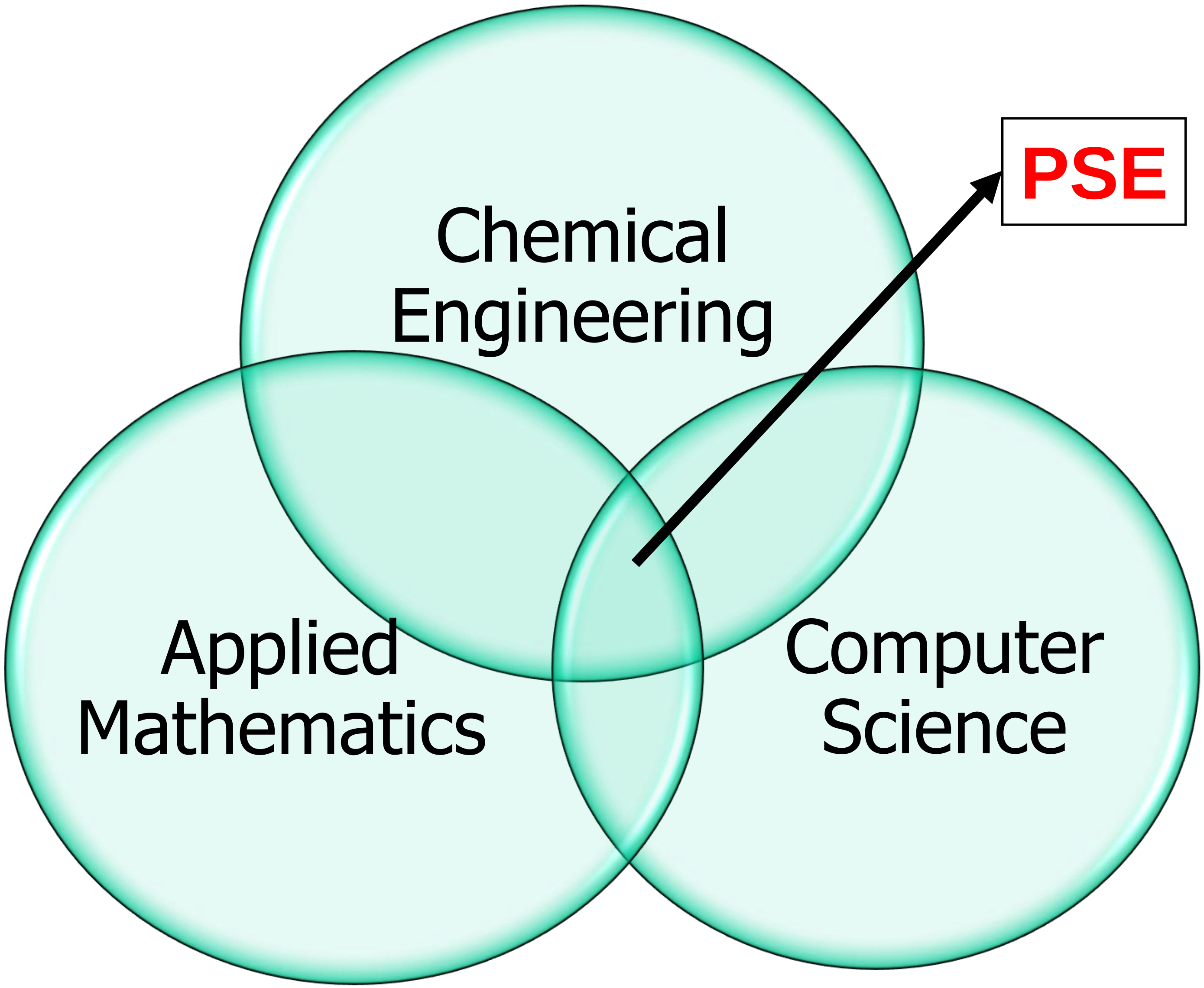
- **Formative period (1860s-1920s)**
  - Ammonia based soda production process by Solvay (1872)
  - Haber-Bosch process for ammonia production
- **Waiting period (1920s – 1960s):**
  - Developments in applied mathematics, numerical methods, control and optimization theory
- **Explosion period (1960s – to date):**
  - Process design and synthesis, process control, process optimization, and planning and scheduling

Growing Importance of Computing and Informatics



"And that's why we need a computer."

PSE: A Confluence of Three Disciplines



Major PSE Research Activities in the Department of Chemical Engineering

PSE Faculty in the Department of Chemical Engineering, IIT Bombay

Core Faculty

- Arun Moharir
- Kannan Moudgalya
- Mani Bhushan
- Ranjan Malik
- Ravindra Gudi
- Sachin Patwardhan
- Sharad Bhartiya
- Yogendra Shastri

Associated Faculty

Sanjay Mahajani
K.V. Venkatesh
Santosh Noronha
Pramod Wangikar
Sandip Roy
Chandra Venkataraman
Abhijit Chatterjee

K. P. Madhavan (Professor Emeritus)

Modelling and Simulation: "What – if" Analysis

$$y = f(x, u, \theta)$$

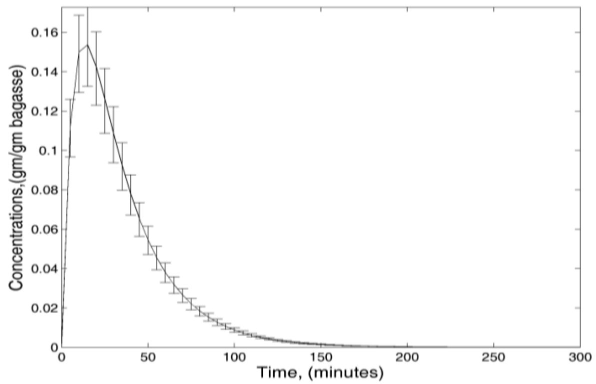
- Mechanistic Vs Data based (regression)
- Static Vs Dynamic
- Linear Vs Non-linear
- Distributed Vs Lumped parameter
- Deterministic Vs Stochastic
- Quantitative Vs. Qualitative

All models are wrong, only some are useful!

.... George E.P. Box

Different modeling approaches are being used

- **Modeling**
- **Optimization**
- **Control**
- **Fault diagnosis**
- **Parameter estimation**
- **Statistical analysis**
- **Risk assessment**
- **System identification**

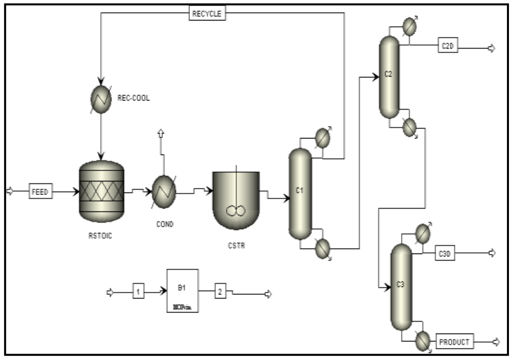


$$\frac{d[C_{Ai}]}{dt} = -k_{1i}[C_{Ai}]$$

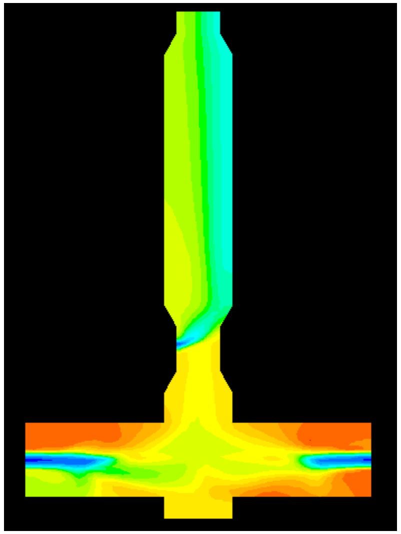
$$k_{ji} = A_{ji} \times C_{Acid}^{n_{ji}} \times e^{\left(\frac{E_{ji}}{RT}\right)}$$

Batch reactor modeling using reaction kinetics

Flowsheet modeling for process simulation (ASPEN Plus)



Computational Fluid Dynamics (CFD) modeling using distributed parameter approach



Challenges and Opportunities in Modeling

Modeling

Optimization

Control

Fault diagnosis

Parameter estimation

Statistical analysis

Risk assessment

System identification

- Multi-scale modeling
- Modeling of uncertain systems
- Modeling for sustainability

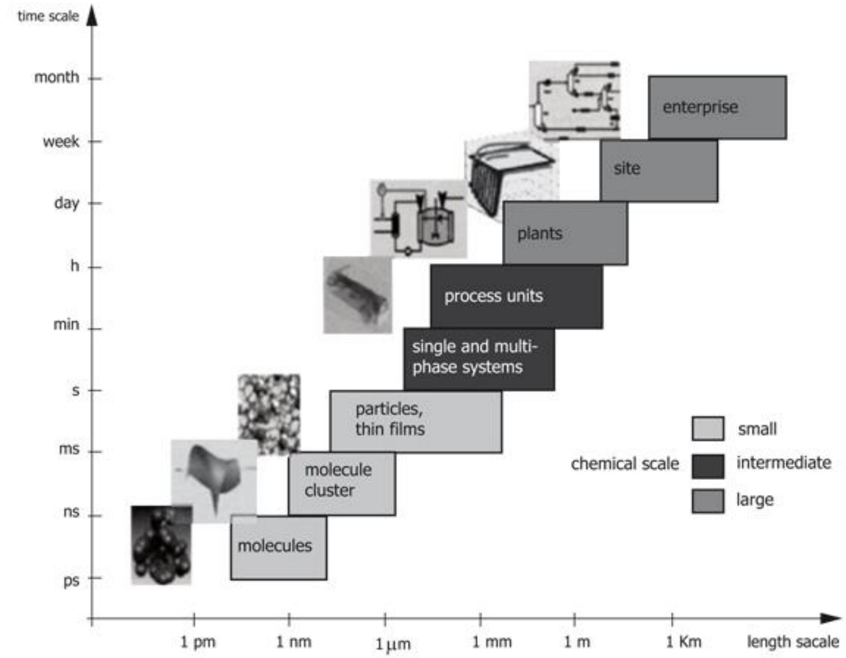


Figure 1. Chemical supply chain (Grossman & Westberg, 2000)

Faculty involved: All of us!

Optimization

- What is the best solution among multiple potential solutions?
- How to find that solution using minimum time and maximum accuracy?
- A widely used tool in different fields

"...and that, in simple terms, is my idea on how to increase factory optimization. any questions?"

Example: Synthesis of an Optimal Algal Biorefinery

- Modeling
- **Optimization**
- Control
- Fault diagnosis
- Parameter estimation
- Statistical analysis
- Risk assessment
- System identification

Raw material / Resources → Algal growth and harvesting → Algal oil upgradation → Product distribution

Strain
Sunlight
CO_2
Water
Nutrients

Integrated Biorefinery

Biochemical
Thermochemical
Anaerobic digestion
Combustion
Microbial fuel cells

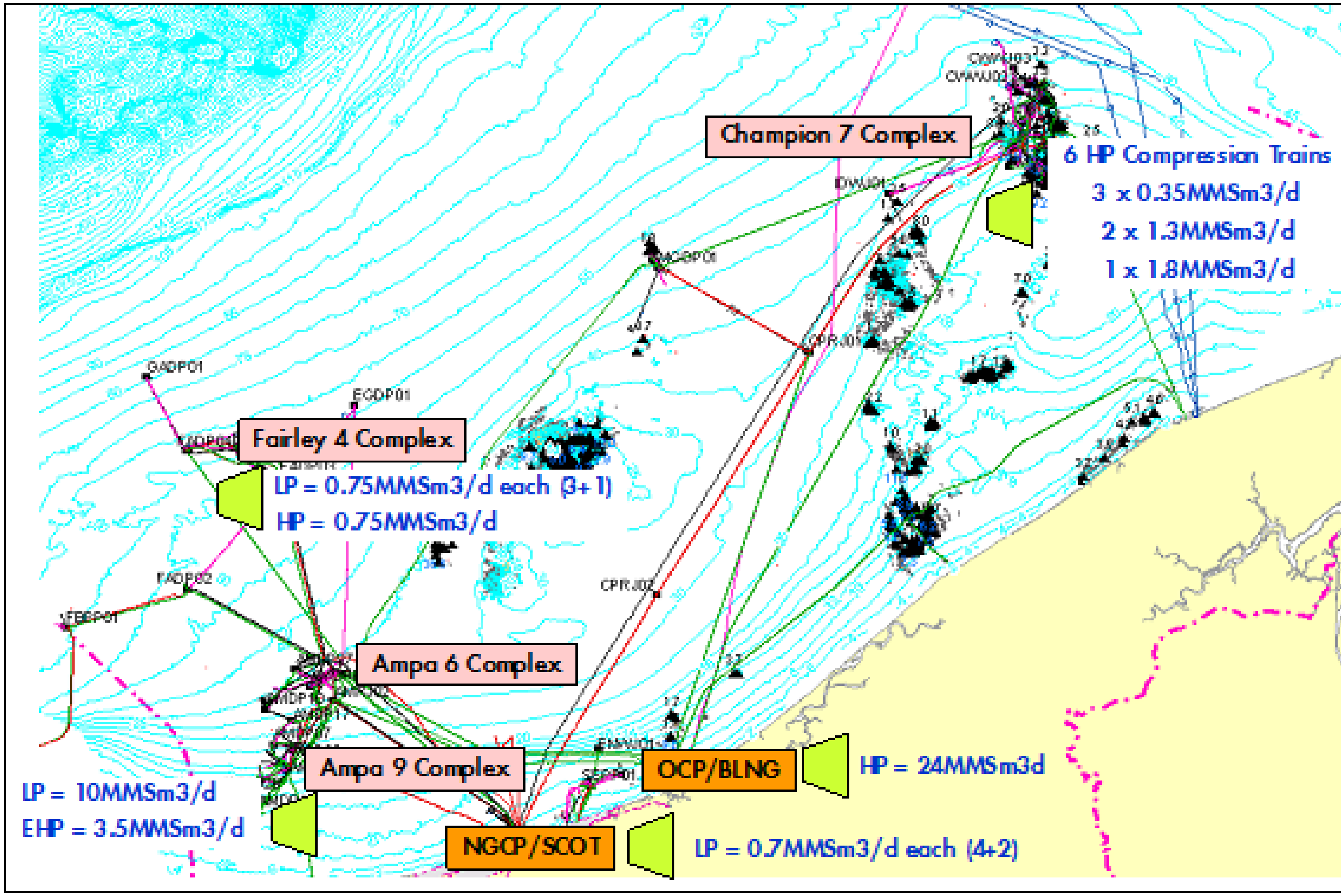
Products

Biodiesel
Ethanol
Heat/power
Neutraceuticals
Methane
Bioplastics

Integrated biorefinery an important element of the proposed approach

Optimization of Gas Production Network

- Modeling
- **Optimization**
- Control
- Fault diagnosis
- Parameter estimation
- Statistical analysis
- Risk assessment
- System identification



Production scheduling and supply chain optimization

Major Challenges in Optimization

- Modeling
- **Optimization**
- Control
- Fault diagnosis
- Parameter estimation
- Statistical analysis
- Risk assessment
- System identification

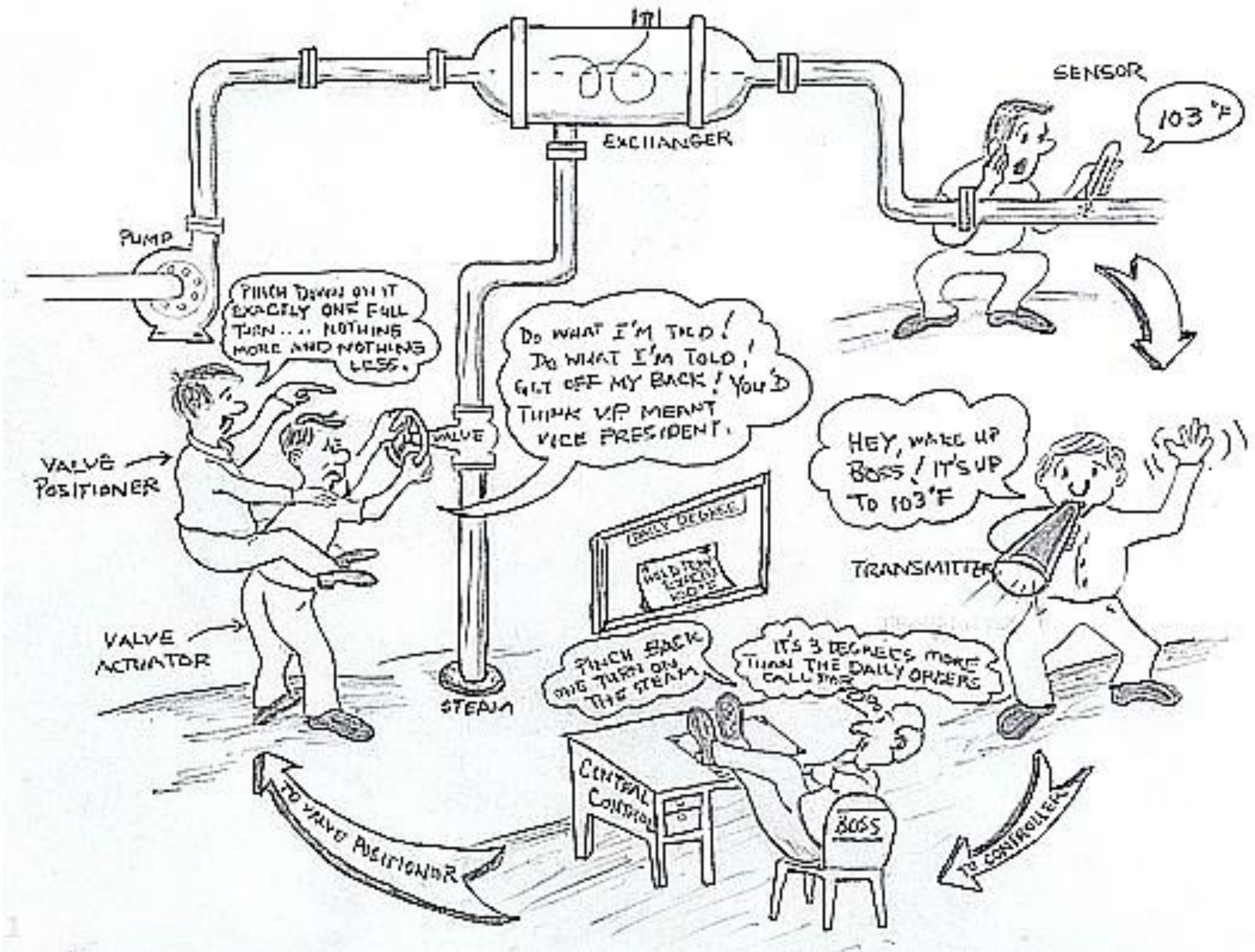
- Nonlinear problems
- Stochastic problems
- Non-convex problems (global optimization)
- Mixed integer linear/nonlinear problems
- Large scale problems (decomposition)

Faculty involved:

- Ravindra Gudi
- Yogendra Shastri
- Sharad Bhartiya

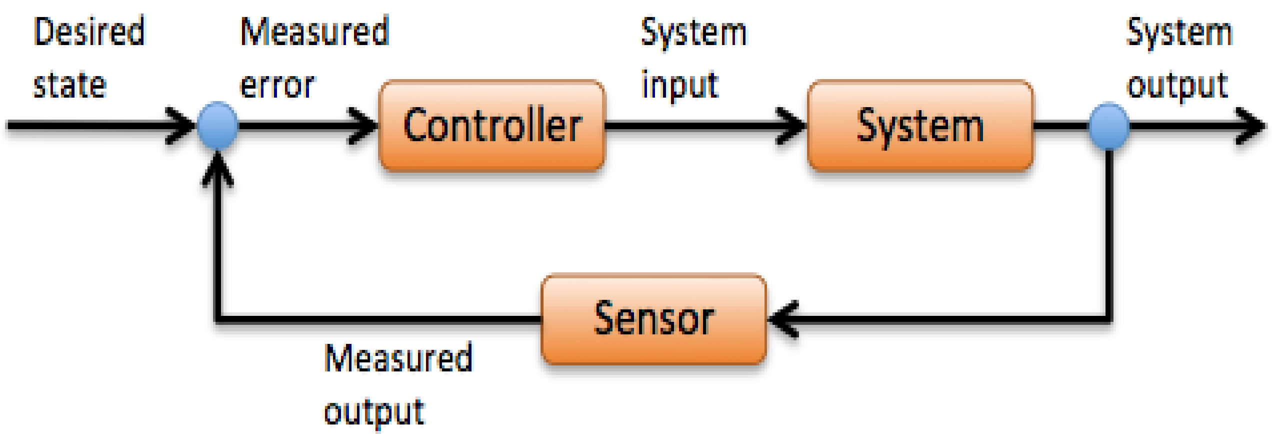
Process Control

- Modeling
- Optimization
- **Control**
- Fault diagnosis
- Parameter estimation
- Statistical analysis
- Risk assessment
- System identification



Basic Feedback Control Structure

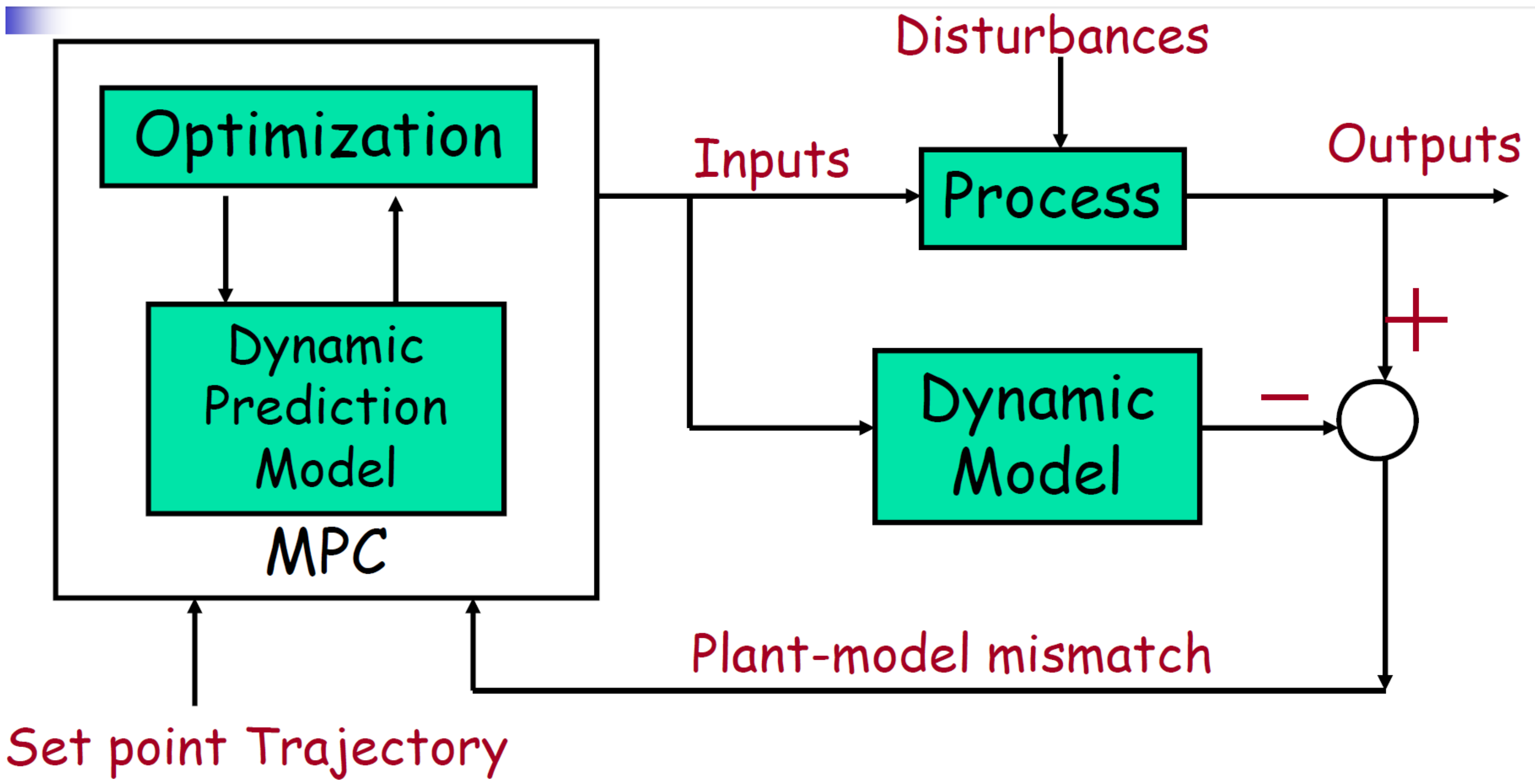
Modeling
Optimization
Control
Fault diagnosis
Parameter estimation
Statistical analysis
Risk assessment
System identification



- Traditional approach: P/PI/PID controllers
- Advanced control: Necessary for nonlinear processes and accurate control
- Advanced model based control: Model predictive control, optimal control

Model Predictive Control (MPC)

- Improvement over simple feedback (P/PI) control
- Uses process model to optimize control input



Major Challenges in Advanced Control

- Economic model predictive control
- Distributed/plant-wide control
- Fault tolerant model predictive control
- MPC of multi-rate systems
- Stochastic control

Faculty involved:
- Sharad Bhartiya
- Sachin Patwardhan
- Mani Bhushan
- Ravindra Gudi
- Kannan Moudgalya

Fault Detection and Diagnosis

Modeling

Optimization

Control

Fault diagnosis

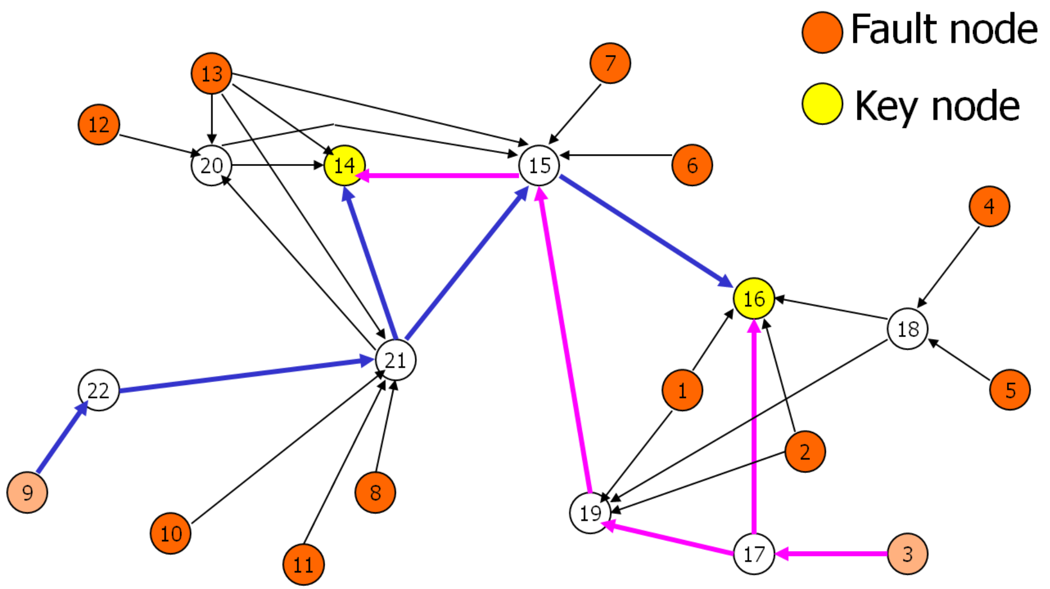
Parameter estimation

Statistical analysis

Risk assessment

System identification

- Fault detection: Is there a fault in the system?
- Fault diagnosis: What is the fault?



Faculty involved:

- Mani Bhushan

State Estimation

Modeling

Optimization

Control

Fault diagnosis

Parameter estimation

Statistical analysis

Risk assessment

System identification

Problem: Predict the current or future states of the system using previous output and input variables

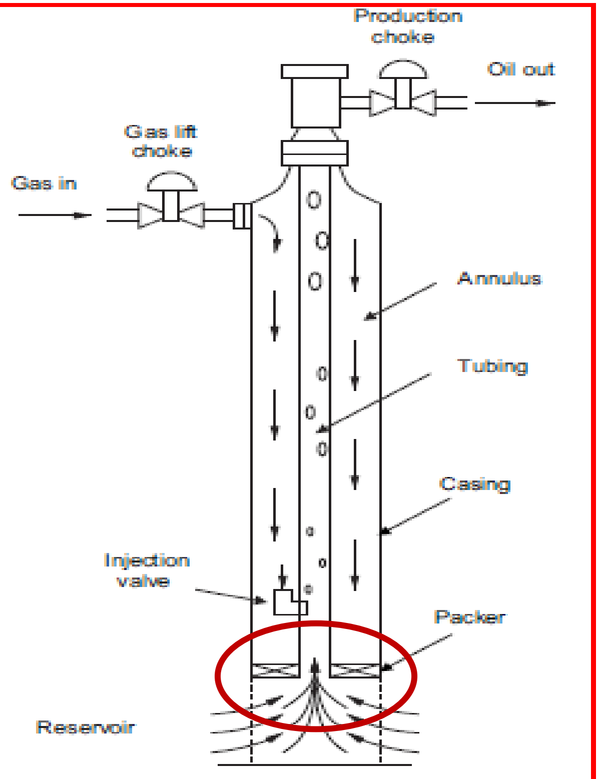
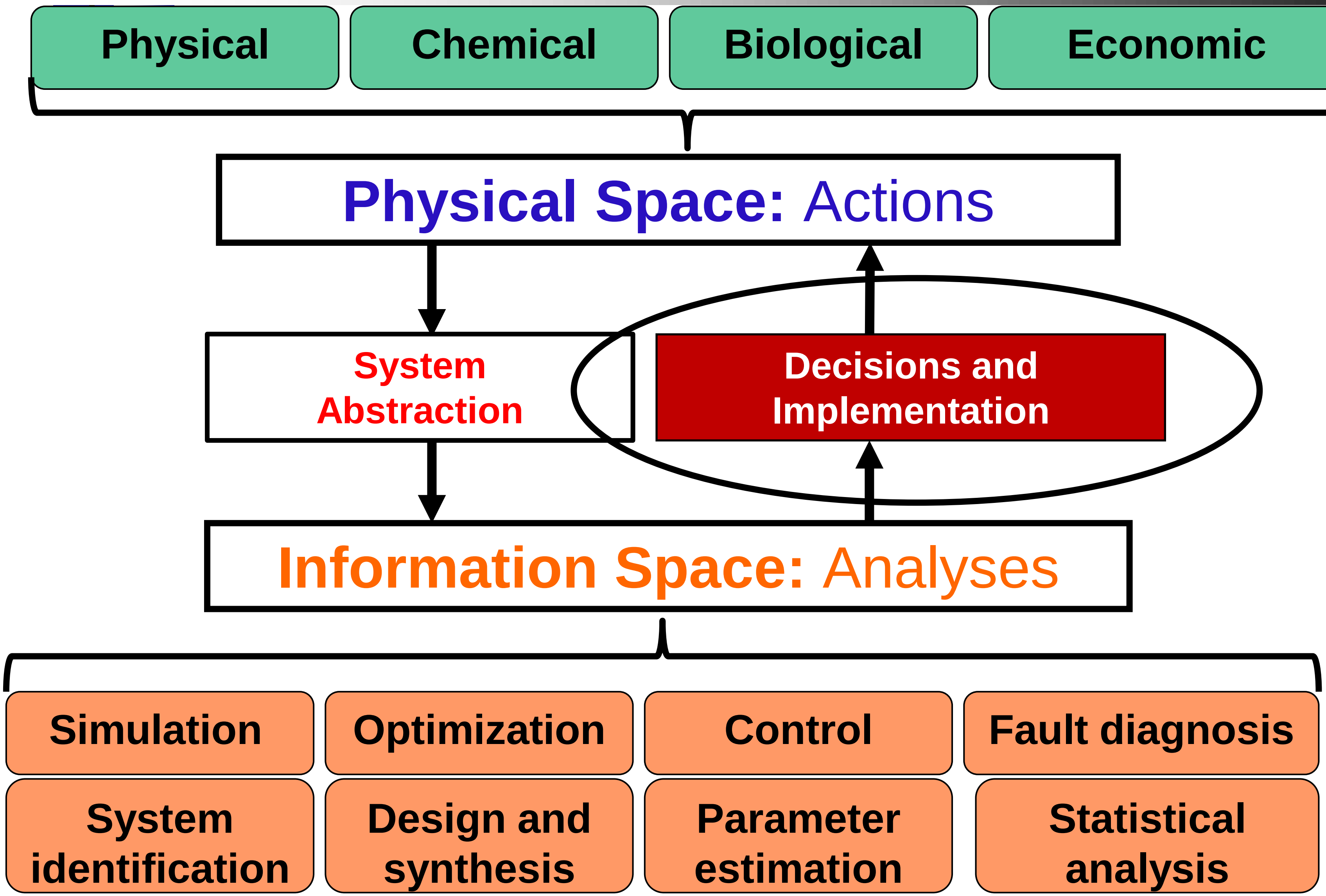


Figure 1.1: The single gas-lift well.

Faculty involved:

- Sachin Patwardhan
- Mani Bhushan
- Sharad Bhartiya
- Ravindra Gudi

Process Systems Engineering



Open source software, Online educational platform

- ASCEND: Open source flowsheeting system
- OpenFOAM: Open source CFD simulation software
- Web-enabled experimentation
- Online teaching modules

Faculty involved:

- Kannan Moudgalya
- Sachin Patwardhan
- Santosh Noronha

(Relatively) New Frontiers in PSE

- Systems biology
- Complex systems
- Sustainability

Faculty involved:

- K.V. Venkatesh
- Sharad Bhartiya
- Yogendra Shastri
- Pramod Wangikar
- Santosh Noronha

Myths and Opportunities

- Myth 1: PSE is only about clumsy math!
- Myth 2: You need to be math geniuses!
- Myth 3: You can only solve theoretical problems!

- Opportunity 1: Solve high impact problems
- Opportunity 2: Solve inter-disciplinary and multi-disciplinary problems
- Opportunity 3: Diversity of opportunities

Diversity of opportunities is really true!

ELSEVIER Applied Mathematics and Computation 95 (1998) 181–192

APPLIED MATHEMATICS AND COMPUTATION

Love dynamics: The case of linear couples

Sergio Rinaldi [1]

Centro Teoria dei Sist

Abstract

This paper propose
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APPLIED MATHEMATICS AND COMPUTATION

www.elsevier.com/locate/amc

Dynamical models of love with time-varying fluctuations

J. Wauer [a,*], D. Schwarzer [a], G.Q. Cai [b], Y.K. Lin [b]

VOL. 61, NO. 1, FEBRUARY 1988 35

Love Affairs and Differential Equations

STEVEN H. STROGATZ
Harvard University
Cambridge, MA 02138

The purpose of this note is to suggest an unusual approach to the teaching of some standard material about systems of coupled ordinary differential equations. The

Where do IITB students with PSE research go?

- ABB, Honeywell, GE, TCS, Ansys (Fluent), United Phosphorous, Reliance, Shell, P&G, Biocon
- Public Sector Units (ISPAT/HPCL/IOCL)
- External Students (NMRL (DRDO), BARC, IICT, HEPL, ISRO)
- Post-doc (Delaware, Arizona State, UIC, NUS, Washington Univ., Alberta)
- Faculty (IIT Bombay, IIT Delhi, IIT Gandhinagar, IIT Guwahati, IIT Hyderabad, PDPU)

Thank You!

yhastri@iitb.ac.in

Visit my web-page

http://www.che.iitb.ac.in/ys/index.html

for a copy of this presentation and an overview poster on process systems engineering