Introduction to Process Systems Engineering

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Lesson **1** of “Process Systems Engineering” – Master Degree in Chemical Engineering – Politecnico di Milano

Definition of Process Systems Engineering

- PSE has traditionally been concerned with the understanding and development of systematic procedures for the design, control and operation of chemical process systems (Sargent, 1991).

Systematic: having, showing, or involving a system, method, or plan
- Dictionary.com

Definition of Process Systems Engineering

- PSE is an academic and technological field related to methodologies for chemical engineering decisions. Such methodologies should be responsible for indicating how to plan, how to design, how to operate, how to control any kind of unit operation, chemical and other production process or chemical industry itself (Takamatsu, 1983).

Definition of Process Systems Engineering

- PSE is concerned with the understanding and development of systematic procedures for the design and operation of chemical process systems, ranging from microsystems to industrial-scale continuous and batch processes (Grossmann & Westerberg, 2000).

Definition of Process Systems Engineering

- PSE is the field that encompasses the activities involved in the engineering of systems involving physical, chemical, and/or biological processing operations (Stephanopoulos & Reklaitis, 2011).

Definition of Process Systems Engineering

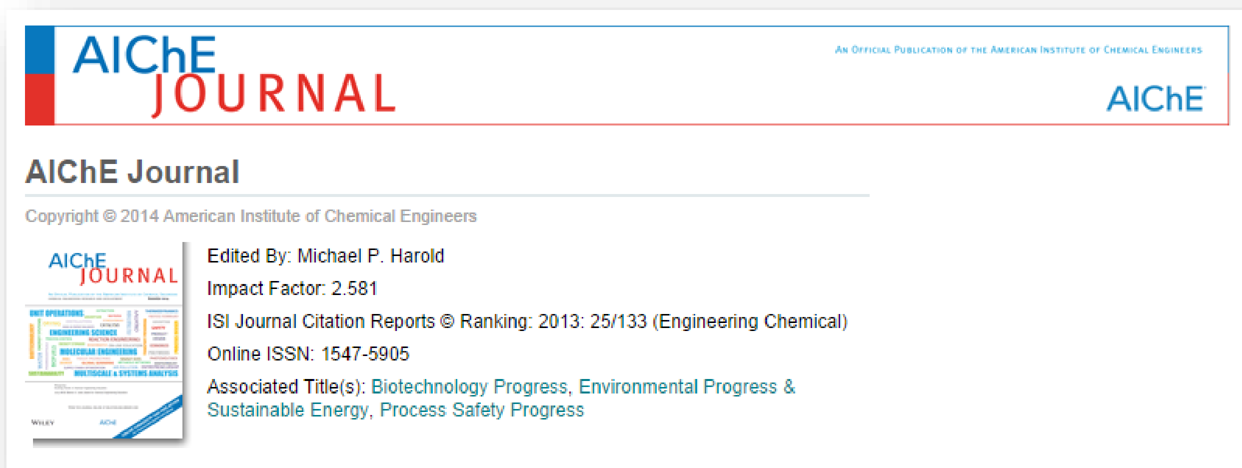
- PSE is a largely mature and well-established discipline of chemical engineering.
- The systems approach has been successfully adapted and refined to address the needs of designing, controlling and operating chemical process systems in a **holistic** manner.
- PSE has been evolving into a specialized field at the interface between chemical engineering, applied mathematics and computer science with specific model-based methods and tools as its core competencies to deal with:
  - the **inherent complexity** of chemical processes
  - the **multi-objective nature** of decision-making during the lifecycle of the manufacturing process of chemical products.
- PSE has been successfully implemented as a discipline in its own right in research, industrial practice as well as in chemical engineering education (Klatt & Marquardt, 2009).

Holistic: relating to or concerned with wholes or with complete systems rather than with the analysis of, treatment of, or dissection into parts

- Merriam Webster Encyclopedia

Definition of Process Systems Engineering

- Process Systems Engineering is the field that encompasses the activities involved in the **engineering of systems** with physical, chemical, and/or biological processing operations.
- PSE classification according to AIChE:
  - Process Modeling, Simulation and Optimization
  - Process Design/Synthesis and Product Design
  - Process Identification, State estimation and Control
  - Process Operations: Optimization, Monitoring, and Fault Diagnosis



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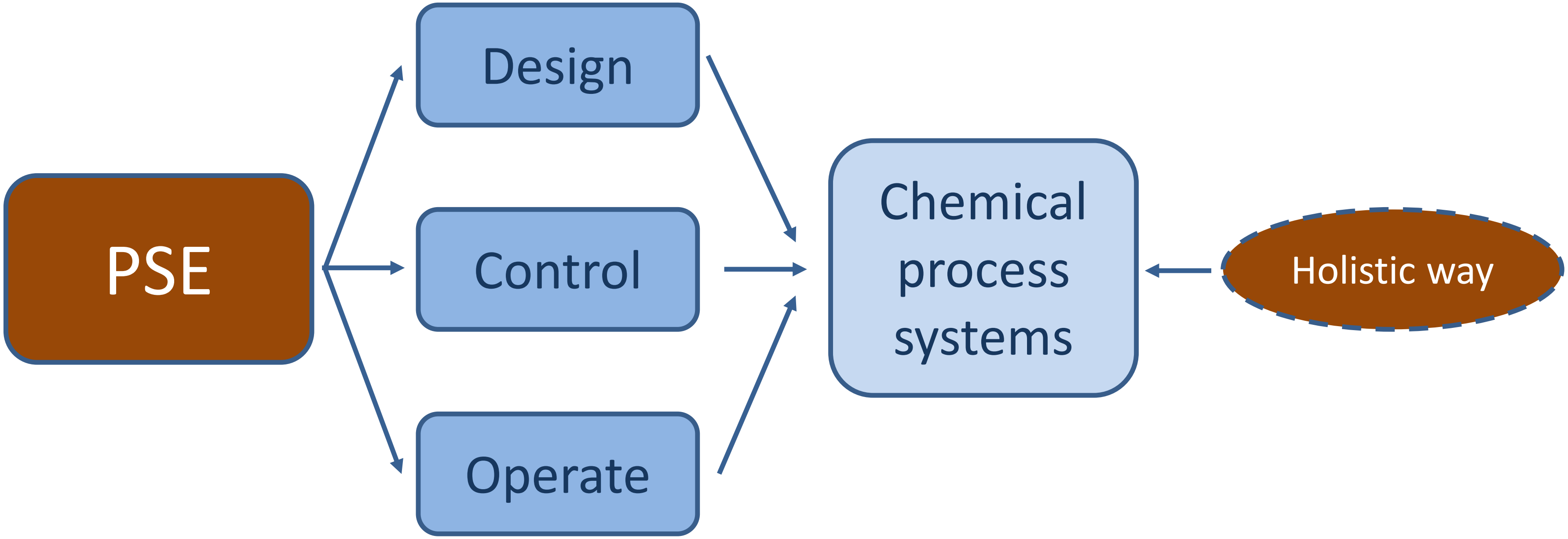
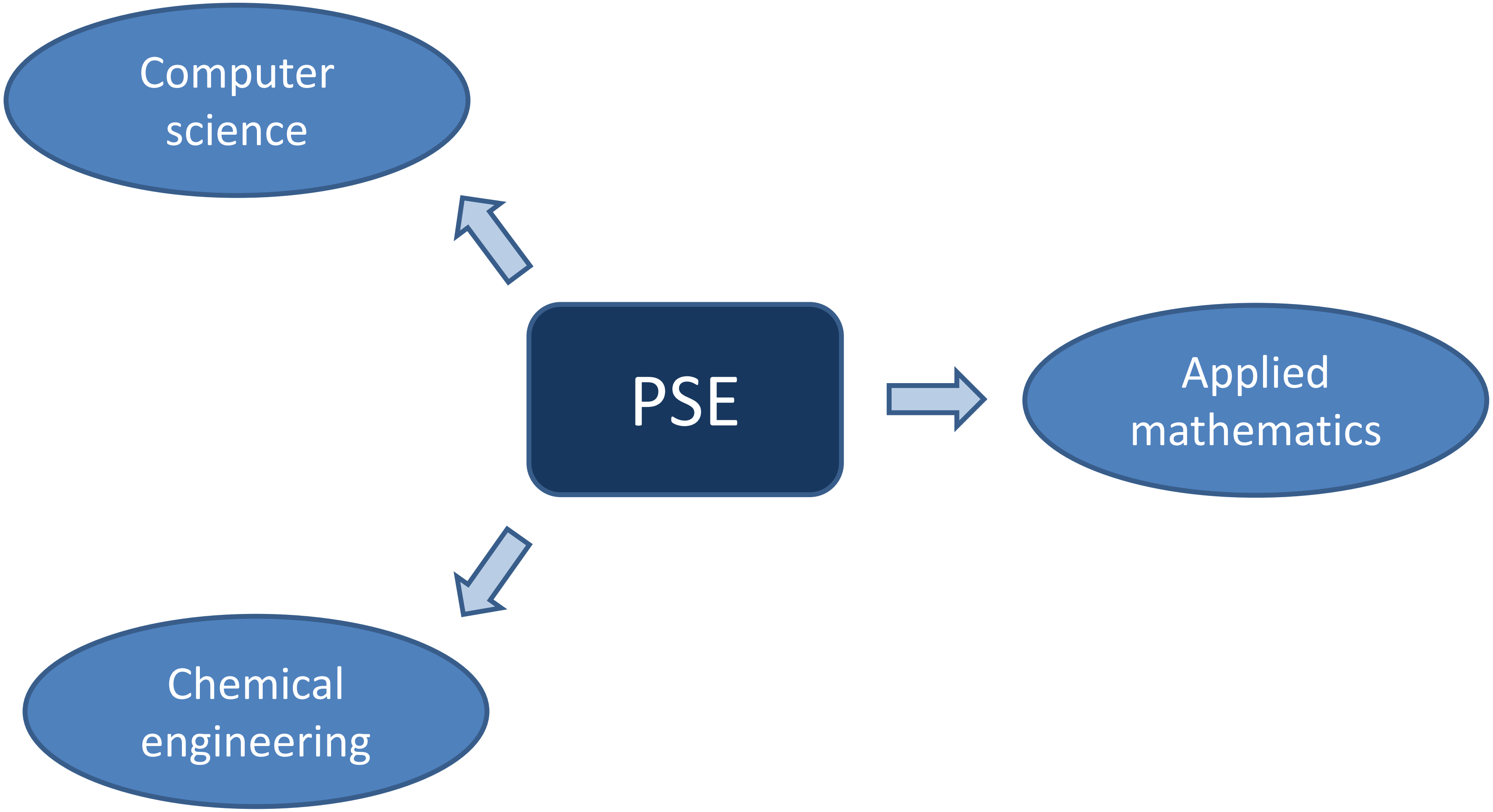
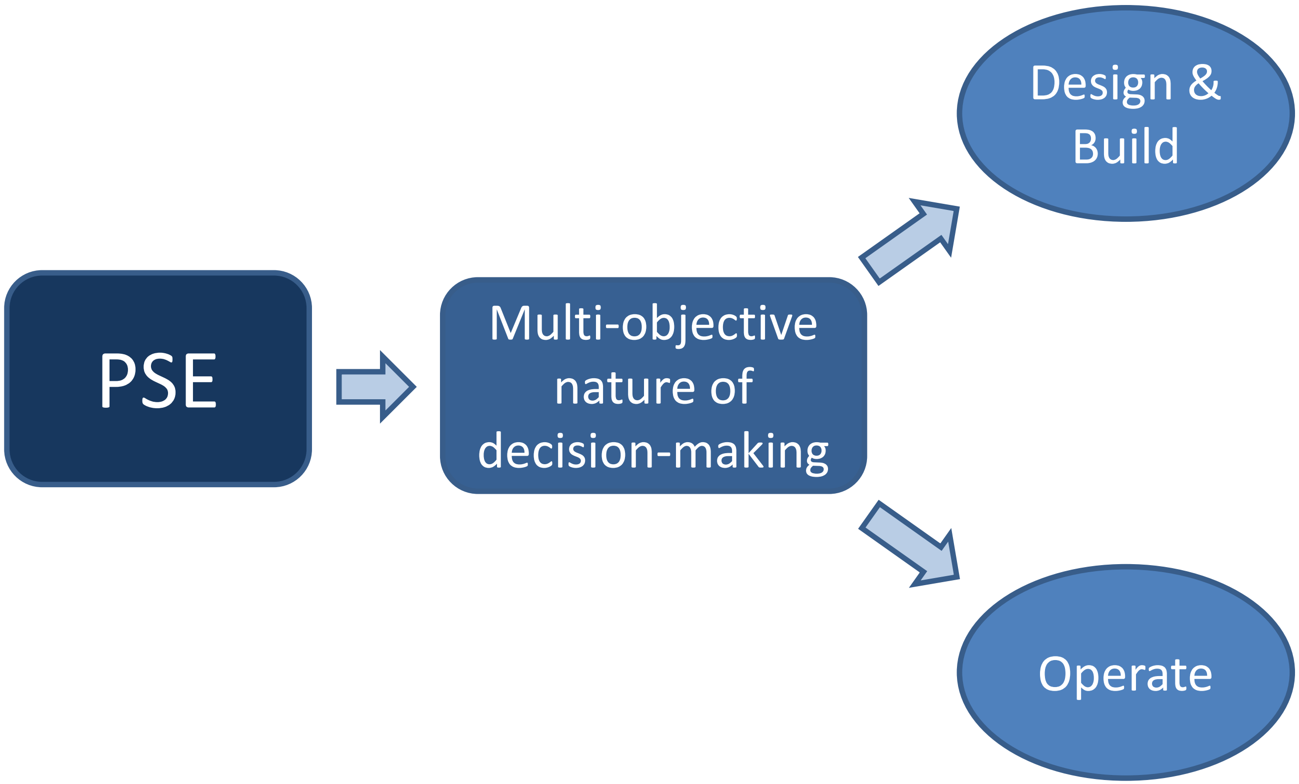
Definition of Process Systems Engineering



Definition of Process Systems Engineering



Definition of Process Systems Engineering



- Conceptual Design
- Revamping
- Retrofitting
- Process Intensification

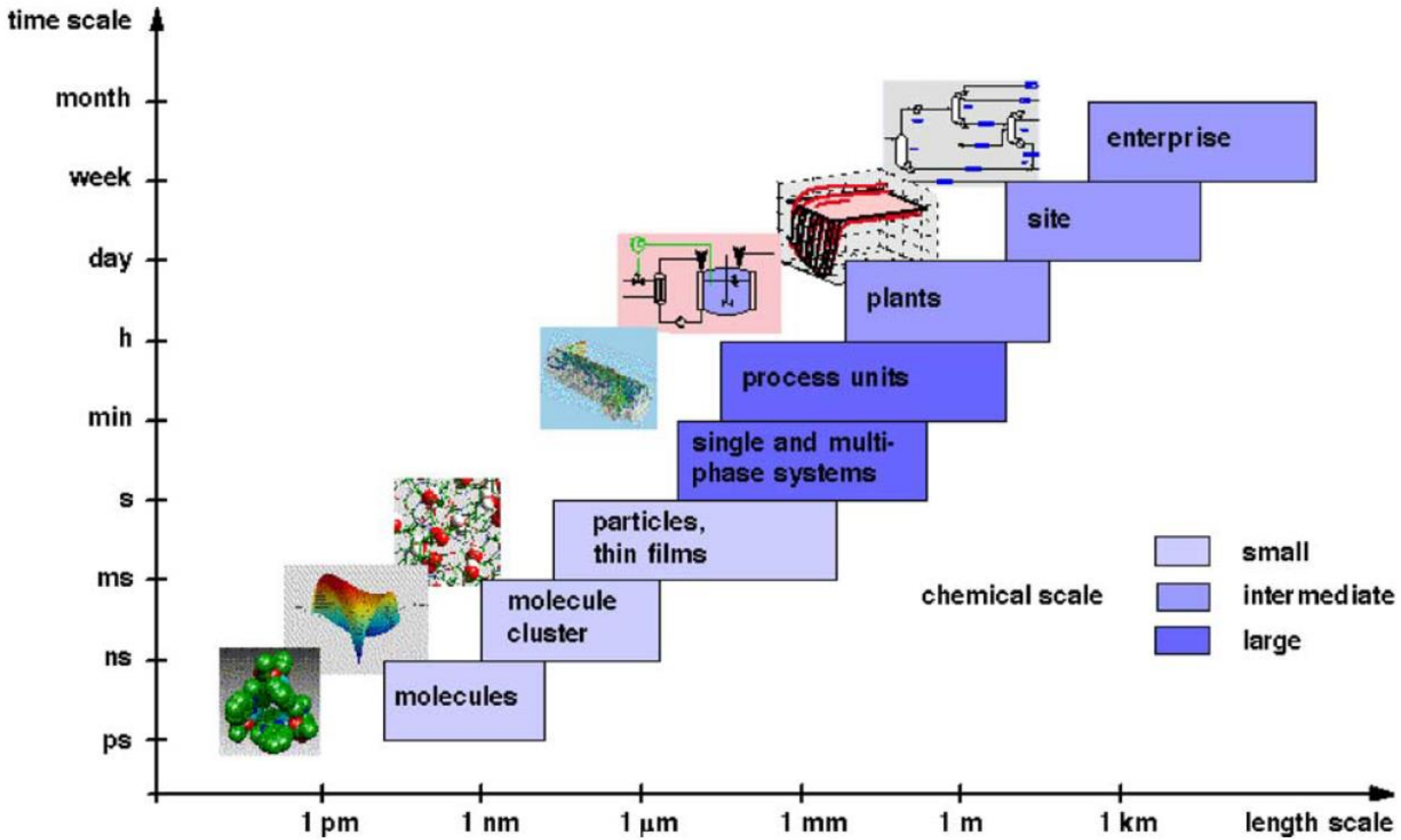
- Process control
- RTO
- Scheduling
- Planning
- Supply chain
- EWO

Definition of Process Systems Engineering

- Research falling under Systems Engineering has a unifying role within the discipline of Chemical Engineering. It deals with the performance of various engineering decisions/tasks through the use of mathematical tools and algorithms. For this purpose, it relies on mathematical models that capture the perceived underlying science, and adopts an optimization approach to perform the relevant tasks. In keeping with contemporary needs, most research in the PSE program employs **multi-scale** representation of the mathematical models.

www3.imperial.ac.uk/cepse

The chemical supply chain



Grossmann, 2004; Marquardt, Wedel, Bayer, 2000

Definition of Process Systems Engineering

- Systems engineering involves the following generic research themes:
  - the development of modeling frameworks and of numerical methods for the simulation and for local and global optimization
  - the development of robust strategies and methodologies for the appropriate engineering tasks
  - adoption and adaptation of computational methods to facilitate the above themes.
- A comprehensive set of the engineering tasks are:
  - product design (petrochemicals, pharmaceuticals, novel materials, commodity and specialty chemicals, etc.)
  - process synthesis
  - process control
  - planning & scheduling
- A mathematical model constitutes the center of the research focus.

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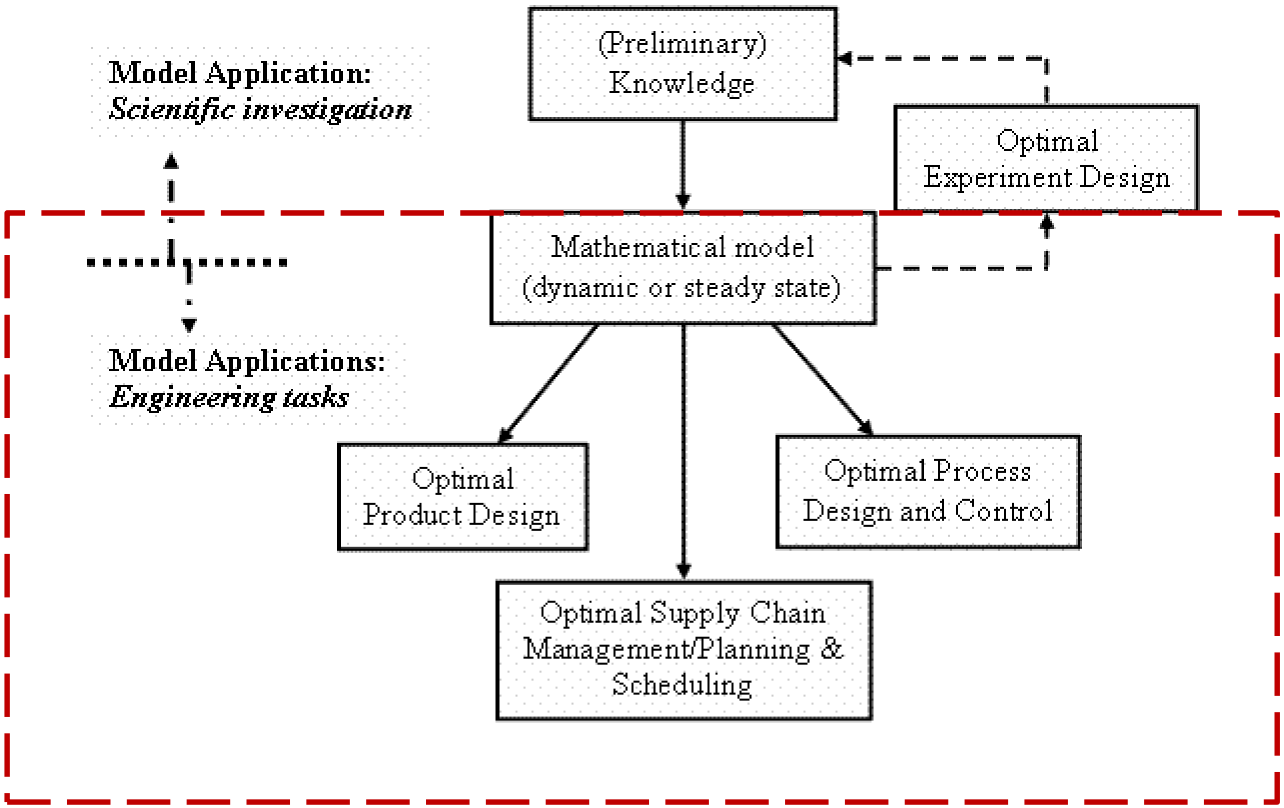
Definition of Process Systems Engineering



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Definition of Process Systems Engineering

- Clearly, the underlying science as exemplified by the model constitutes the rigorous basis for all systems engineering. However, systems engineering does not necessarily wait until a complete understanding of the process emerges from the scientific disciplines (to quote Professor John Perkins, “Roger Sargent Lecture”, Centre for Process Systems Engineering, Imperial College London, December 2005). Instead, it seeks to solve real life engineering problems by the utilization of the available knowledge through the exploitation of mathematical tools in combination with appropriate experimentation. This approach ensures a simultaneous development of both the scientific knowledge and their applications. In view of the necessity of working with limited knowledge as well as due to the plethora of constraints imposed by real life (falling under the broad classes of limitations in resources, and environmental & safety hazards), robustness assumes an ever increasing importance in systems engineering. In addition, the models would themselves serve as useful analysis tools to understand both the characteristics of the process and the model structure.

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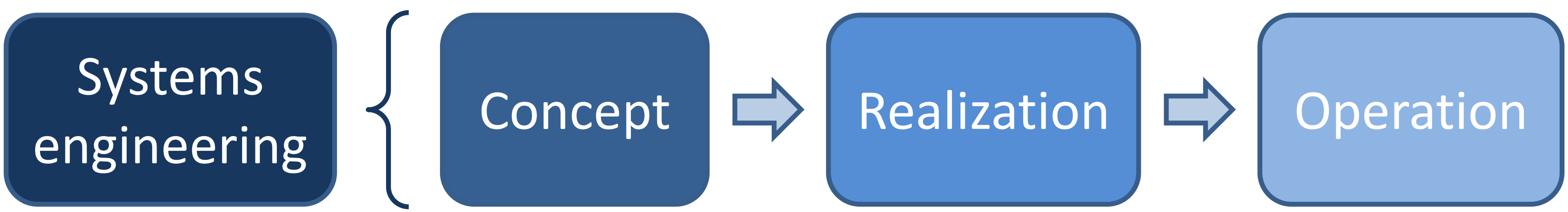
The concept of Systems engineering

- **Systems engineering** addresses all practical aspects of a multidisciplinary structured development process.

- Systems engineering proceeds from **concept** to **realization** to **operation**.



The concept of Systems engineering

- Whymore (1993) proposes the following definition of SE:

  Systems engineering *is the intellectual, academic and professional discipline, the principal concern of which is the responsibility to ensure that all requirements for a* ***bioware****,* ***hardware*** *or* ***software system*** *are satisfied throughout the life-cycle of the system*

- A technical system is composed of:
  - **Hardware** (*i.e.* the process plant and its equipment)
  - **Software** (*i.e.* the operation support system)
  - **Bioware** (*i.e.* plant operators, FOPs and CROPs, and management)

Systems engineering methodology

- **Systems engineering** is a **methodology** to solve systems design problems by means of a **systematic design process**.
- Bahill and Gissing (1998) proposed the **SIMILAR** approach to systems engineering. It consists of 7 tasks:

  1. **S**tate the problem: identify the requirements to be satisfied
  2. **I**nvestigate alternatives: define multi-criteria decision making process
  3. **M**odel the system
  4. **I**ntegrate the system with its environment
  5. **L**aunch the system: implement it, run it and produce output
  6. **A**ssess performance: measure the performance of the system
  7. **R**eevaluate: continuously monitor and improve the performance

The paradigms of PSE

- The two major paradigms in PSE are: **analysis** and **synthesis**.

- **Analysis** is a **direct problem**. It assumes that the process flowsheet, the equipment, and operating data are assigned. The **model** is used to predict the **performance indicators** of the process by **simulation studies**.

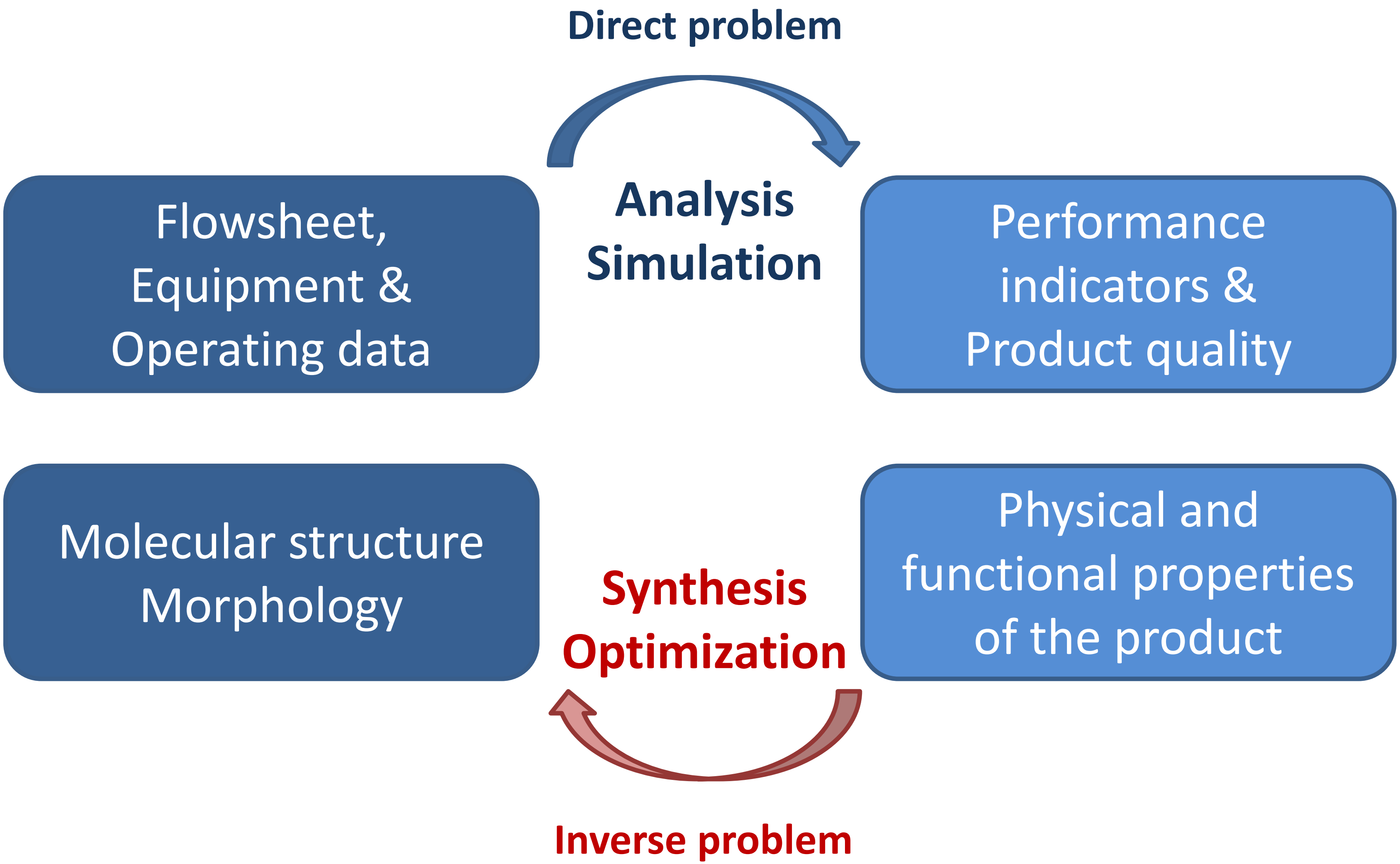
- **Synthesis** is an **inverse problem**. The process **performance indicators** are the **specifications** of the problem whose solution, by means of repetitive simulations or numerical **optimization**, allows identifying the space of the **decision variables**.

The paradigms of PSE

- **Analysis** is the process of breaking a complex topic or substance into smaller parts to gain a better understanding of it. The word is from the ancient Greek ἀνάλυσις (“a breaking up”, from ἀνά “up, throughout” and λυσις “a loosening”).

- **Synthesis** refers to a combination of two or more entities that together form something new. Alternately, it refers to creating something by artificial means. The word is from the ancient Greek σύνθεσις (σύν “with” and θέσις “placing”).

The paradigms of PSE



From Klatt & Marquardt, 2009

The paradigms of PSE

- **Since World War II, engineering education has moved strongly towards analysis**, with courses dealing with individual process operations and phenomena. **Transport Phenomena**, **Unit Operations**, **Process Control**, **Reaction Engineering**, and other engineering science courses greatly strengthened engineering education by showing how things are and how they work. **Unfortunately, there was not a parallel development of courses dealing with synthesis**…. This deficiency has been recognized for years, but the remedy awaited the development of sufficiently general principles of synthesis about which to organize educational material.
- **The tension between analysis and synthesis is key to the health of any engineering discipline**, and the existence of the complementary views of chemical engineering in analysis (the culture of chemical engineering science) and synthesis (the re-emergent culture of process engineering; which from the 60s is referred to as Process Systems Engineering) helped ensure the vigorous international development of academic chemical engineering in the 1960s and beyond.

From Rudd, Powers & Siirola, 1973

The paradigms of PSE

- In addition to **the impact that the synthesis culture of PSE had on educational curricula**, its contributions to the advancement of industrial practice have been nothing less than spectacular. Starting in late '60s, academic research develops **systematic Process Synthesis** ideas, which in turn allow process engineers to begin with given chemistries and end up with quite **inventive process flowsheets**. Douglas' hierarchical approach to the conceptual design of process flowsheets offers an unparalleled systematization for the "invention" of processing schemes. Subsequent coupling of Douglas' approach with formal optimization formulations proposed by Grossmann and other researchers provided the missing quantification and thus the objective "optimality" of the resulting processing schemes. Finally, after nearly 100 years **the core activity of PSE**, *i.e.* **process development**, can be put into a rational and systematic framework. The impact of this development on the industrial practice cannot be overestimated. **Now engineers have a systematic way of "inventing" new processing systems, not simply analyzing existing ones**.

From Stephanopoulos & Reklaitis, 2011

On the adoption of the PSE techniques

- While the direct model-based solution of the (inverse) process design problem, by means of optimization methods, is more rigorous and exact from a systems engineering point of view, **today's industrial practice mainly features a pragmatic solution** of the design problem by **educated guesses**, supported by an **iterative solution** of the process simulation and an experience-based analysis of the respective simulation results.

- **Process synthesis methodologies relying on rigorous optimization are rarely used in industrial practice.**

From Klatt & Marquardt, 2009

- **N.B.**: this course is aimed at closing the gap between the Academia and the Industry. It provides the necessary notions to improve the design capabilities of industrial engineers.

Going deeper

Deepening the definition of PSE

- According to Stephanopoulos & Reklaitis (2011), PSE is the field that encompasses the activities involved in the engineering of systems involving physical, chemical, and/or biological processing operations.
- These systems, whose variety and purpose are very broad, include, but are not limited to, the following:
  - **Processing plants**, producing intermediate chemicals and materials that societal needs require
  - **Manufacturing systems** for the production of a very broad variety of consumer goods (foods, clothing, materials and devices that enhance quality of life at home and workplace)
  - **Diagnostic and therapeutic products** and processes to treat human diseases
  - **Energy production**, distribution, and consumption systems
  - Systems which ensure the **quality of the environment** in which humans, plants and animals live.

Deepening the definition of PSE

- Within the scope of any of the above classes of processing systems, one may identify other types of processing systems, such as:
  - **Networks of chemical reactions** (catalytic or not)
  - **Networks of biological processes** in living cells
  - Structured systems of **monitoring signals and actuating control actions**, which are at the core of any diagnostic and control system
  - **Structured interactions among molecules** (*e.g.* free or guided self-assembly), leading to the emergence of supra-molecular constructs, or among molecular fragments, determining the physical properties of the molecules they make up
  - **Networks of interacting processing equipment and humans** (*e.g.* operators, maintenance personnel, process engineers, managers) who are at the heart of any process' safe, reliable and optimal operation.

Deepening the definition of PSE

- The activities involved in the engineering of such systems include:
  - Process design
  - Optimal scheduling and planning of systems' operations
  - Monitoring, diagnosis, control, optimization of systems' operations
  - Identification of the underlying structured network of processing operations
  - Mathematical modeling and simulation of systems' behavior

Deepening the definition of PSE

- There is even a broader scope for modern PSE:
  - Process design involves the cycle of ***synthesis*** (invention, conceptualization) and ***analysis*** tasks, which leads to a processing system that satisfies certain objective(s).
  - The design of a processing system may require the study and resolution of engineering questions regarding the reliability, operability, safety, flexibility, and robustness of the operating system.

- Finally, the identification of the underlying structures in poorly known systems may involve subsidiary tasks such as:
  - experimental design
  - evolutionary learning
  - model generation
  - complexity analysis

Drivers of PSE

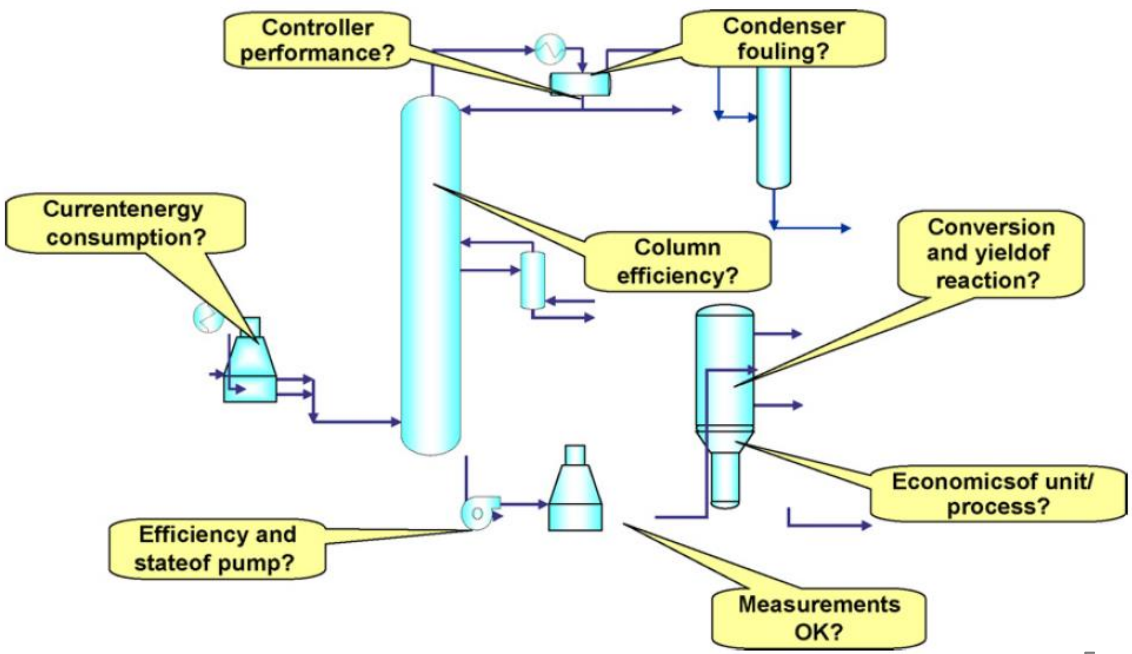
- PSE is driven by two considerations:
  - **The interest is in the ''behavior'' of the system as a whole**
  - The emphasis is on studying how the **components of the system and their interactions** contribute to the overall ''behavior'' of the system.
- PSE is the integrative complement of all subareas of chemical engineering and the one that determines the significance and criticality, or absence thereof, of ''local'' engineering questions.
- For example:
  - the **operational and economic ''behavior'' of a chemical process** is the integrated effect of all its unit operations, whose criticality in determining the behavior of the process can be systematically analyzed.
  - **A drug** is not just its active component, but a system with three interacting elements: **medically active ingredient, formulation additives, and delivery vehicle**. The efficacy of a drug deteriorates precipitously if the highly active ingredient cannot be delivered to the cells effectively, or its dissolution into the blood stream is hampered by poorly selected excipients.

Drivers of PSE

- Similar interactions can be easily recognized in the following examples:
  - the components of a product and associated fabrication lines such as:
    - digital processors
    - memory chips
    - LCD or OLED displays
    - batteries
    - fuel cells
  - the components of global production and transportation of energy systems;
  - The constituents of energy and the environment policy-making systems
- No manufacturing process or product reaches the market without the integrative scrutiny of systems engineering.

Tools for PSE

- **KPIs** are the **Key Performance Indicators** that allow measuring and assessing the operation of a process unit, of a plant, of a production site, of a company.



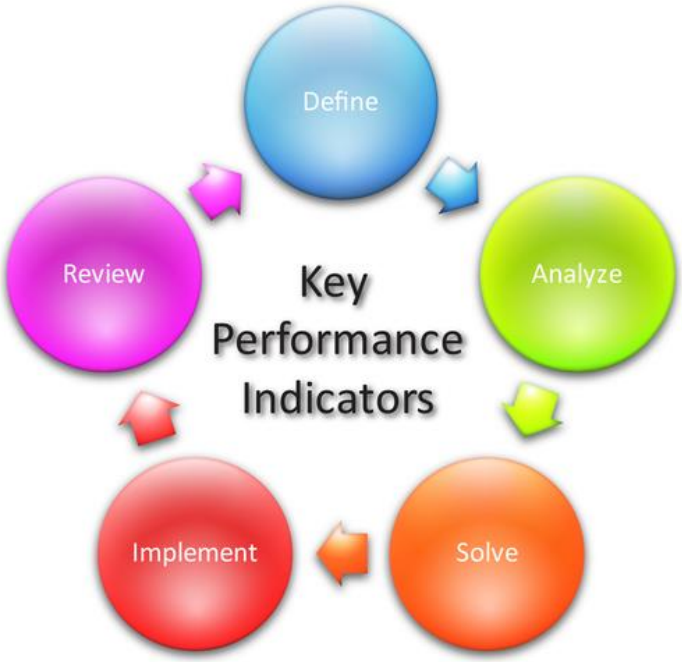
From Klatt & Marquardt, 2009

Tools for PSE

- KPIs are evaluated by taking into account one or more of the following terms:
  - **on-line process data**,
  - **inferred measures and quantities**
  - **results produced by available numerical models of the process/plant**
  - **engineering experience and knowledge**
- Specifically developed “monitoring tools” allow evaluating the KPIs by using either detailed models or data driven tools (and even a mix of the two).

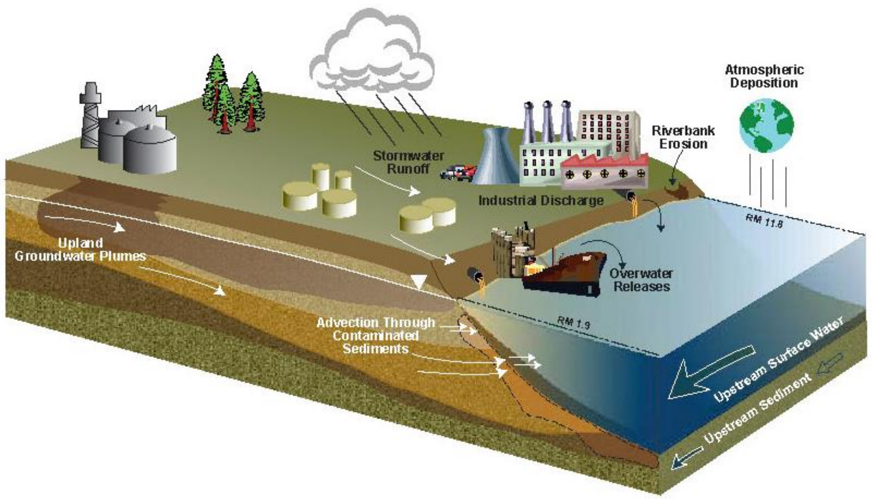
Tools for PSE

- Process simulators (either steady-state or dynamic) allow performing the process/plant computations required to determine the KPIs (as far as detailed models are concerned). Moreover, the KPIs assessment may also be supported by mixing the information produced by such simulators to the data measured or inferred on-line.



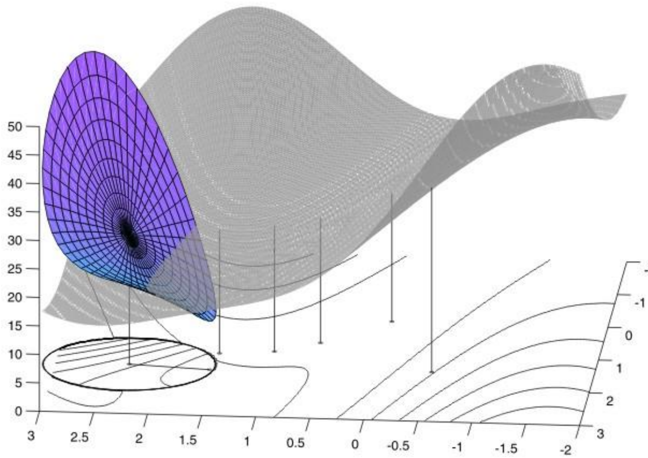
Tools for PSE

- The availability of **numerical models** describing the features of the plant/process paves the way to the following consolidated activities:
  - Conceptual design
  - Model based control
  - Data reconciliation
  - Process optimization
  - Operator training simulation
  - Planning & scheduling
  - Supply chain management
  - Enterprise wide optimization
  - …



Tools for PSE

- The necessity to solve problems by means of specific methodologies and by applying suitable methods calls for the implementation of **numerical algorithms**, such as:
  - Linear and non-linear algebraic equation solvers
  - Ordinary, partial differential and differential-algebraic eq. systems solvers
  - Linear and non-linear (mixed integer) (constrained) optimization techniques
  - Finite difference equation solvers
  - Integro-differential equations
  - Stochastic algorithms
  - …



Historical background

Historical background

- The first approach in history to PSE is the Solvay Process, patented by the Belgian Ernest Solvay in 1861. **Solvay may be seen as the first Process Systems Engineer**. His 1872 ammonia-based soda production process was a break-through. He synthesized the process by *integrating distinct operations of gas–liquid contacting, reaction with cooling, and separations; he invented new types of equipment for integrating these operations and carrying them out continuously on a large scale. He himself dealt with all aspects of an integrated chemical processing system: the chemistry, the materials handling, and the engineering of an integrated processing system, such as operating conditions and the design of specific equipment.*
- *The Solvay process may be seen as the model process in which all aspects of PSE are explicitly delineated and directly addressed, in a fairly systematic and more importantly, system-wide basis.*

Ernest Solvay (1838- 1922)

Historical background

- **Solvay went beyond the parts to the whole**, as the essence of the manufacturing system. The result was: a continuous process with careful integration of chemical and physical operations; use of recycles for improved yields and reduction of wasted raw materials; reduction of environmental pollution; and significant cost efficiency.
- In the course of the following 50 years, Solvay's essential guidelines for process development and the philosophy that one should take a process-wide, systemic approach to process development were adapted by many in England, Germany and the United States.

From Stephanopoulos & Reklaitis, 2011

Historical background

- By the late **1910s early 1920s**, the process development experience of the previous 50 years had set the **general scope of the PSE core**. *A chemical process is a system and its overall behavior is the coordinated effect of basic ‘‘Unit Operations’’*; a concept introduced by George Davis in his Manchester Lectures in **1888**, and a term coined by Arthur D. Little in **1915** in his report to the President of MIT.

- The **1920s to 1950s period** may be referred to as the “**waiting period**”. During this period the focus is on the components of a process, *i.e.* **Unit Operations**, not the overall process as an integrated system.

From Stephanopoulos & Reklaitis, 2011

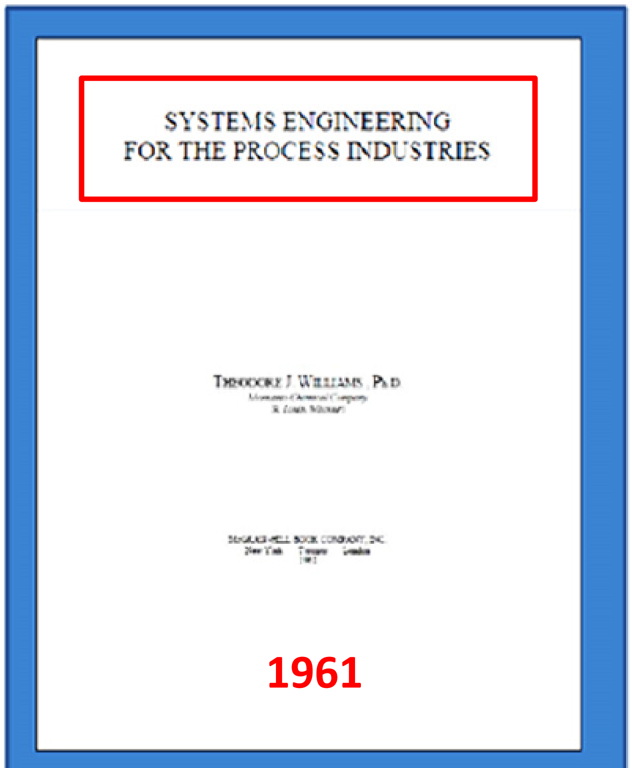
Historical background

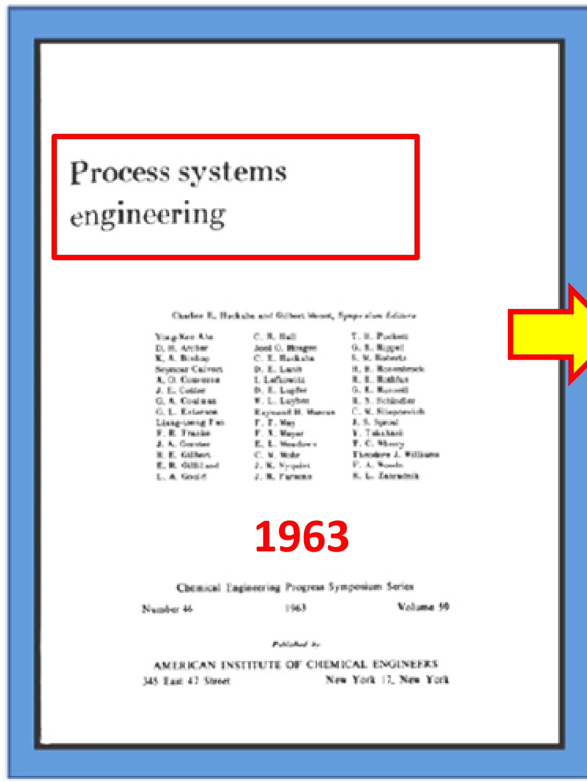
- The **1960s to 2000 period** is a **computer-driven period** of explosive expansion and growth.
- By early 1960s three factors are aligned to cause the onset of an explosive growth period for PSE:
    1. Chemical industry had been growing rapidly, worldwide, for more than 10 years, exerting significant pressure for less costly and safer processes.
    2. A science-based description of the basic physico-chemical phenomena in unit operations is vigorously pursued, producing more reliable quantitative descriptions of processing operations.
    3. The computer is entering industrial life in a very rapid and determined way and affects all aspects of process engineering.
- The large jumps in energy and petrochemical raw materials, 10 years later, would further accentuate the need for better processes. From the **1960s** to the end of the century we witness a remarkable growth in the quality and number of PSE activities and practitioners, worldwide. **The term, Process Systems Engineering, is introduced during this period**.

From Stephanopoulos & Reklaitis, 2011

Historical background

- The term, **Process Systems Engineering**, is introduced in the 1960s.
- Its closest forerunner was coined by T.J. Williams, of Monsanto and Purdue University, in his Schoch Lectures at the University of Texas in 1959, with the title ''**Systems Engineering for the Process Industries**''.





Chemical engineers are primarily interested in process systems in which the systems approach is employed in the design and operation of chemical processing plants.

From Stephanopoulos & Reklaitis, 2011

Historical background

- The historical evolution of PSE is very closely related to:
  - the evolving needs of the chemical, materials and biological industries
  - the advances in chemical engineering science
  - the academic developments in a variety of supporting disciplines, such as:
    - applied mathematics
    - operations research
    - control and identification theory
    - risk analysis
    - management

Significant accomplishments in PSE in the past four decades

Process Design	Process Operations
Synthesis of energy recovery networks	Scheduling of process networks
Synthesis of distillation systems (azeotropic)	Multiperiod planning and optimization
Synthesis of reactor networks	Data reconciliation
Hierarchical decomposition flowsheets	Real-time optimization
Superstructure optimization	Flexibility measures
Design multiproduct batch plants	Fault diagnosis
Process Control	**Supporting Tools**
Model predictive control	Sequential modular simulation
Controllability measures	Equation based process simulation
Robust control	AI/Expert systems
Nonlinear control	Large-scale nonlinear programming (NLP)
Statistical Process Control	Optimization of differential algebraic equations (DAEs)
Process monitoring	Mixed-integer nonlinear programming (MINLP)
Thermodynamics-based control	Global optimization

From Grossmann & Westerberg, 2000

PSE perspective

PSE in the 21^{st} century

- At the beginning of **21^{st} century** **PSE is fully embedded in all engineering activities** surrounding large commodity chemicals processes such as:
  - Refineries
  - Petrochemicals
  - Organic and inorganic intermediates

- Its main activities are:
  - early stage of synthesizing the conceptual processing scheme
  - strategy of plantwide process control
  - detailed process design
  - engineering and construction
  - start-up, operation, optimization, and supply-chain management
  - subsequent process revamps and capacity expansions
  - continuous improvement for process safety and quality control
  - final decommissioning

PSE in the 21st century

- According to Stephanopoulos and Reklaitis (2011), in the first decade of 21st century and as far as **large commodity chemical plants** are concerned, PSE focused mainly on:
  - Process intensification
  - Multi-plant integration
  - Dynamic optimization of operations

- At the same time there have been also research and development activities in the **manufacturing of pharmaceutical and specialty chemicals** with reference to:
  - Single process dedicated plant
  - Multiproduct plant
  - Multipurpose plant

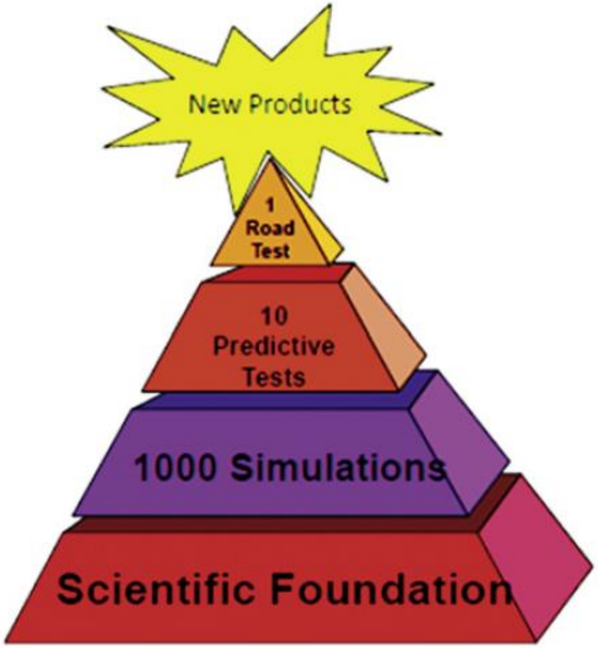
- Nonetheless, there has been very little work in the area of conceptual design and process synthesis for batch processes.

PSE in the 21st century

- Another research thread has been devoted to the **integrated management of process operations** with special attention to:
  - Control and optimization
    - Regulatory control
    - Dynamic optimization (short horizon scheduling of process operations)
    - Static optimization (longer horizon scheduling of operations)
  - Diagnosis and adaptation
    - Diagnosis of faults in the sensors, actuators, control laws
    - Diagnose the onset of process faults or process model deterioration
    - Assessment of production plans and identification of potential faults in their implementation
- **Supply-chain management** deals with decision making structured into:
  - Geographically distributed facilities and organizations
  - Hierarchical levels of decision-making: strategic, tactical, organizational
  - Business functionalities (operations, marketing, finance, R&D, management)

PSE in the 21st century

- **Computer-aided modeling languages and simulation**: from sequential modular to equation oriented simulators
- **From process-centered to product-centered**



From Stephanopoulos & Reklaitis, 2011

PSE in the 21st century

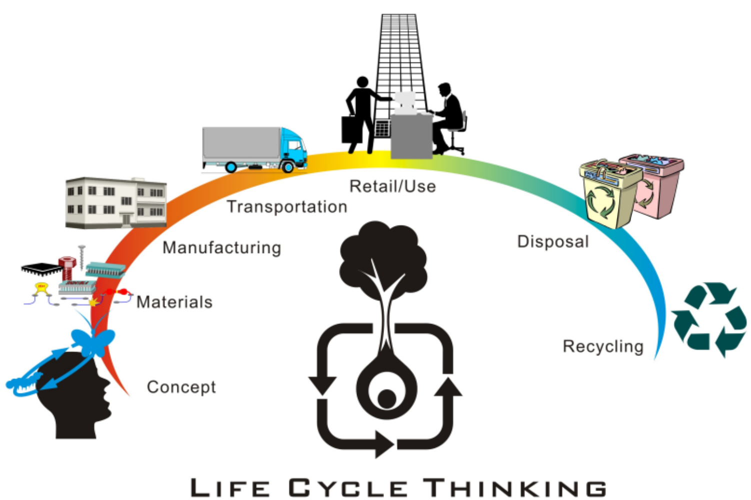
- **Risk management and process safety**: while traditional reliability engineering techniques are often effective in increasing reliability, they do not necessarily increase safety. In fact, their use under some conditions may actually reduce safety. **Process Systems Safety** adopts a system-wide view of the process and the development of potential hazards is seen as an emergent property that arises at the system level through the interaction of the various process components, *e.g.* processing units, control systems, safety instrumentation systems, design weaknesses and errors, and human actions. This allows achieving and implementing:
  - **Inherently Safer Process Designs**
  - Advanced Monitoring, Diagnostic, and Hazards Mitigating Systems
  - Process Safety Management through Continuous Improvements

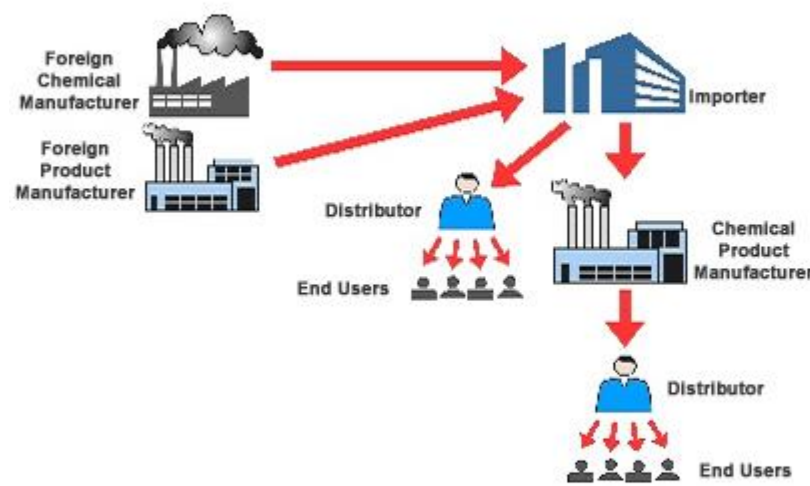
Broadening the scope of PSE

- According to Grossmann and Westerberg (2000) the PSE activity area should be broadened:
  - *Process Systems Engineering is concerned with the improvement of **decision-making processes** for the creation and operation of the **chemical supply chain**. It deals with the discovery, design, manufacture, and distribution of chemical products in the context of many conflicting goals.*
- This definition, which relies on the concept of the chemical supply chain, ties fundamental scientific discoveries at the molecular or microscopic level with strategies and logistics for manufacturing and production planning.
- This definition directly ties to industrial needs from R&D to product distribution. The major goal is to improve all these activities by systematic decision-making, which has both practical and theoretical implications.

Broadening the scope of PSE

- The enlarged definition proposed by Grossmann and Westerberg (2000) focuses on the **chemical supply chain** and is aimed at providing knowledge and tools to support the industries both in the:
  - "value preservation" (*e.g.*, large-scale commodity chemicals)
  - "value growth" (*e.g.*, specialty chemicals, biotechnology, and pharmaceutical products)
- The goal is to ensure that both types of industries remain competitive and economically viable.





References

- Bahill, A. T., & Gissing, B. (1998). Re-evaluating systems engineering concepts using systems thinking. IEEE Trans. Systems, Man and Cybernetics-Part C: Applications and Reviews, 516–527.
- Grossmann, I. E. (2004). Challenges in the new millennium: Product discovery and design, enterprise and supply chain optimization, global life cycle assessment. *Comput. Chem. Engg.*, *29*(1), 29–39.
- Grossmann, I. E., & Biegler, L. T. (2004). Future perspective on optimization. *Comput. Chem. Engg.*, *28*(8), 1193–1218.
- Grossmann, I. E., &Westerberg, A.W. (2000). Research challenges in process systems engineering. *AIChE J.*, 46, 1700–1703.
- Marquardt, W., von Wedel, L., & Bayer, B. (2000). Perspectives on lifecycle process modeling. In M. F. Malone & J. A. Trainham (Eds.), *Proceedings of the 5th international conference foundations of computer-aided process design, FOCAPD 1999, AIChE Symp. Ser. No. 323, Vol. 26* (pp. 192–214).
- Klatt, K.U., Marquardt, W. (2009). Perspectives for process systems engineering—Personal views from academia and industry, *Comput. Chem. Engg.*, 33, 536–550.
- Rudd, D.F., Powers, G., Siirola, J.J., 1973. Process Synthesis. Prentice Hall.
- Sargent, R.W.H. (1991). What is chemical engineering? CAST Newsletter, 14(1), 9–11.
- Takamatsu, T. (1983). The nature and role or process systems engineering. *Comput. Chem. Engg.*, 7, 203–218.

- http://www3.imperial.ac.uk/cepse/
- http://pselab.chem.polimi.it/