# Introduction to Process Systems Engineering

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# 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 <u>systematic procedures</u> 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

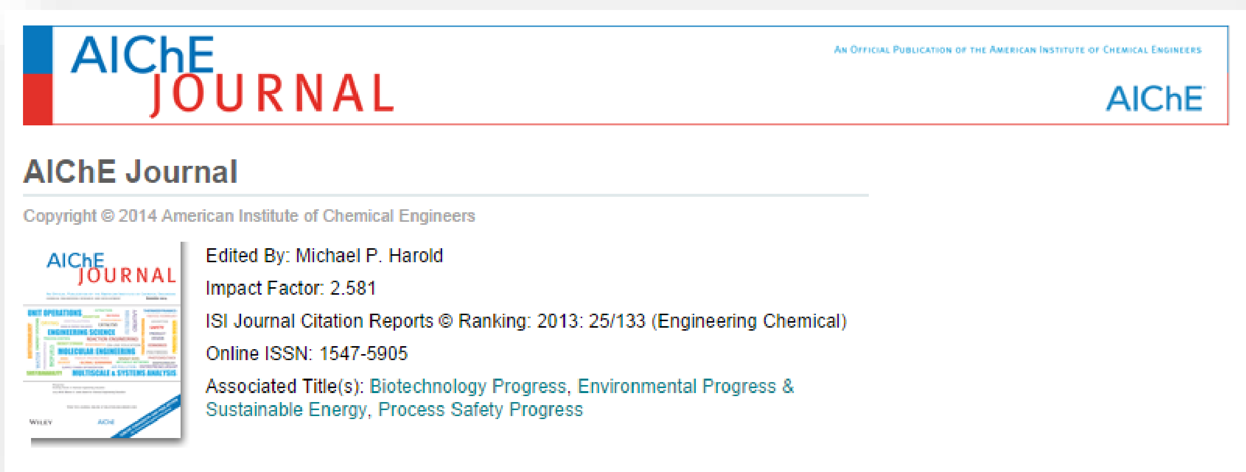
- PSE is a largely mature and well-established discipline of chemical engineering.
- The systems approach has been successfully adapted and refined to address the needs of designing, controlling and operating chemical process systems in a **holistic** manner.
- PSE has been evolving into a specialized 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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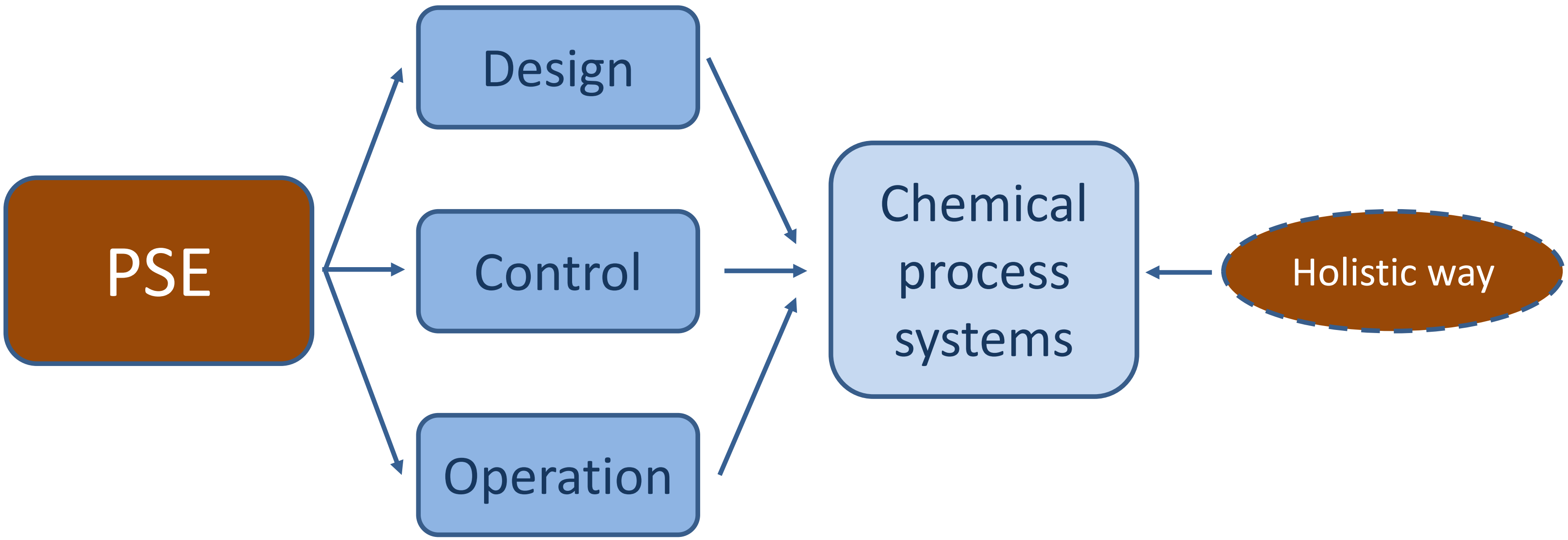
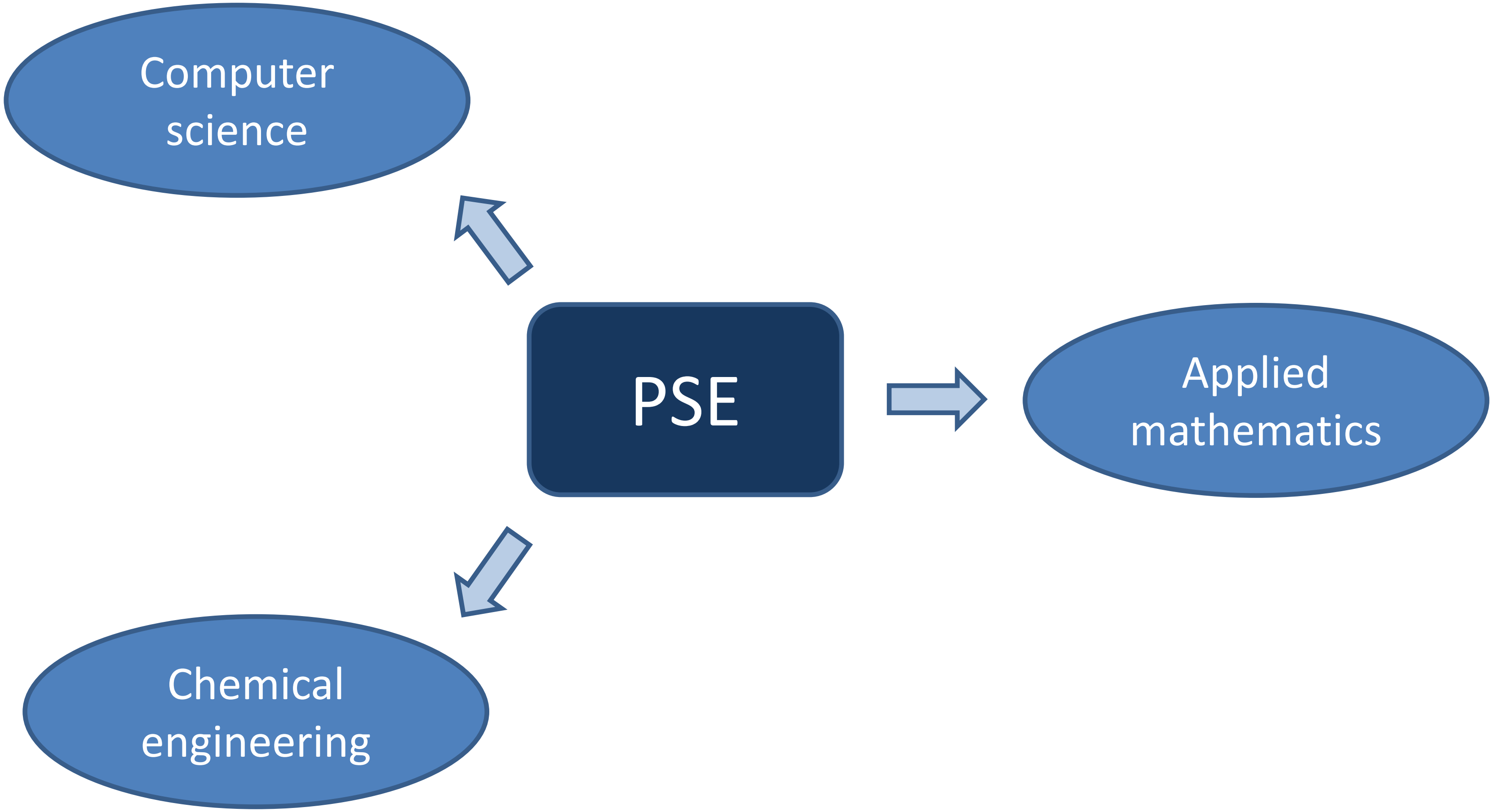
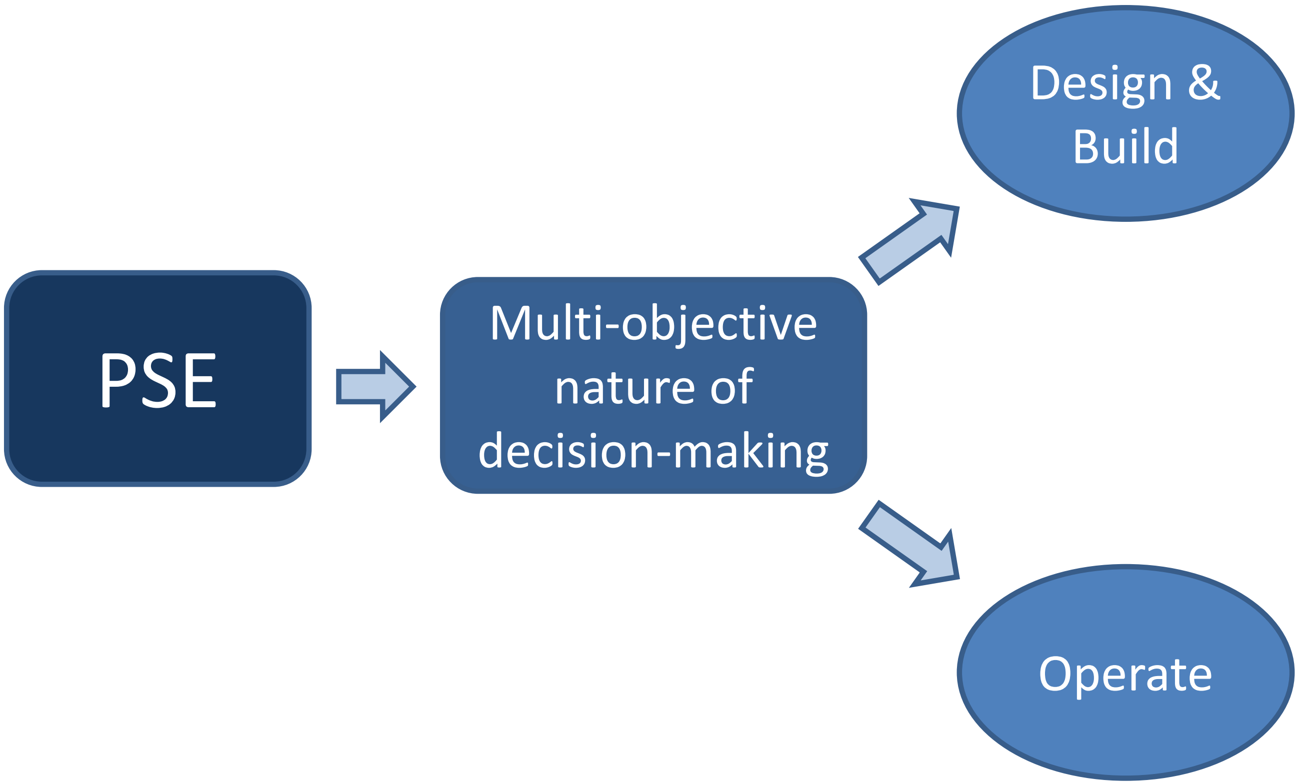
# Definition of Process Systems Engineering



# 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.

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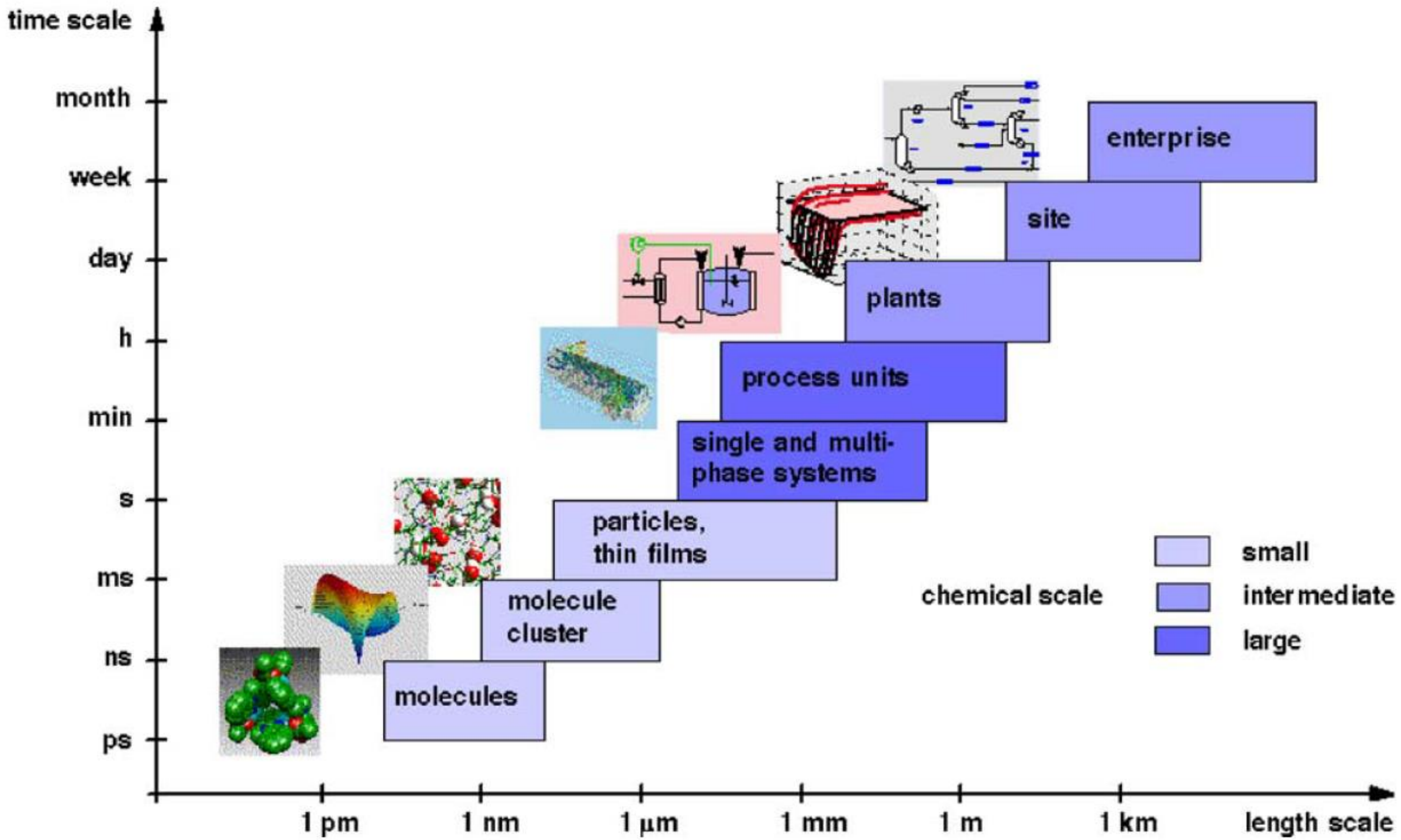
# The chemical supply chain




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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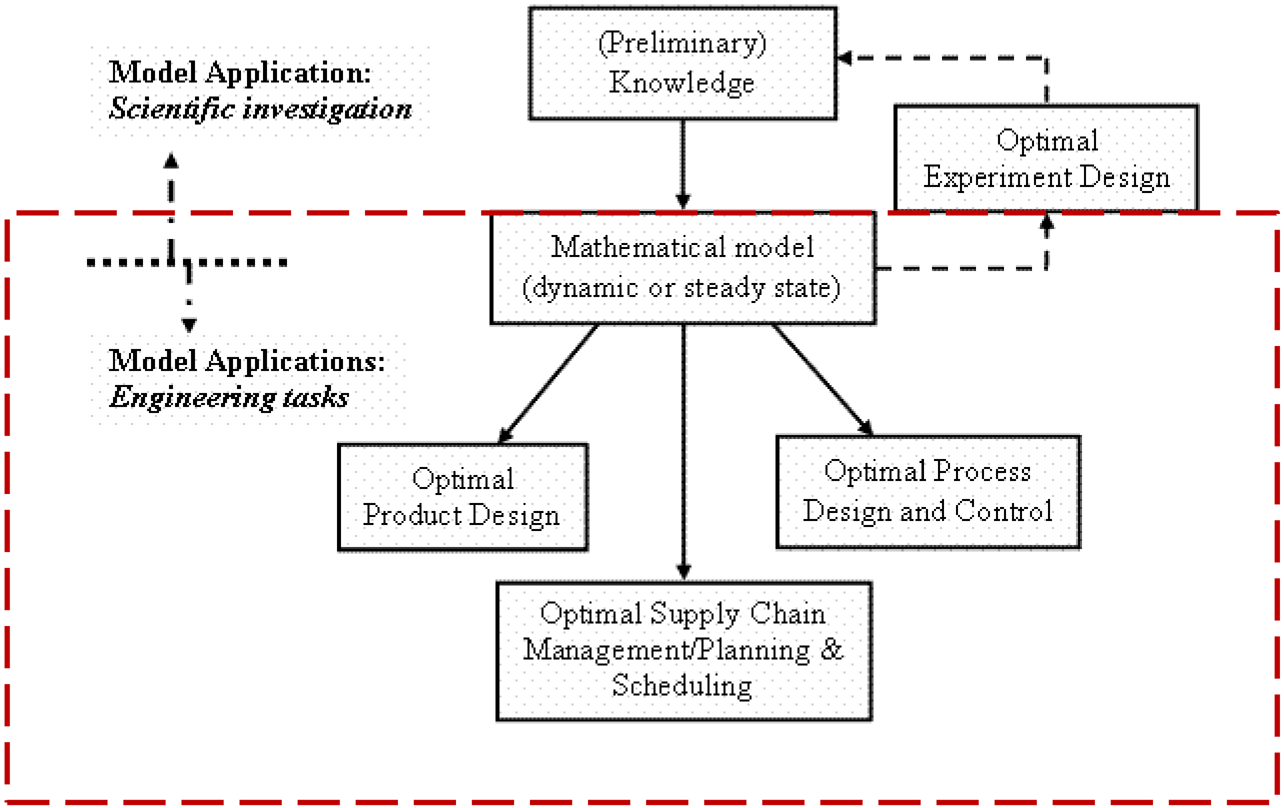
# Definition of Process Systems Engineering

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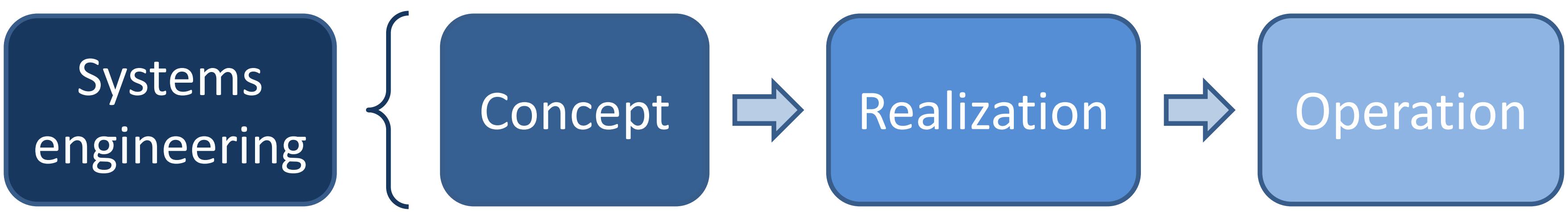
# The concept of Systems engineering

- **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

**Direct problem**

**Analysis**
**Simulation**

Flowsheet, Equipment & Operating data

Performance indicators & Product quality

Molecular structure
Morphology

Physical and functional properties of the product

**Synthesis**
**Optimization**

**Inverse problem**

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.

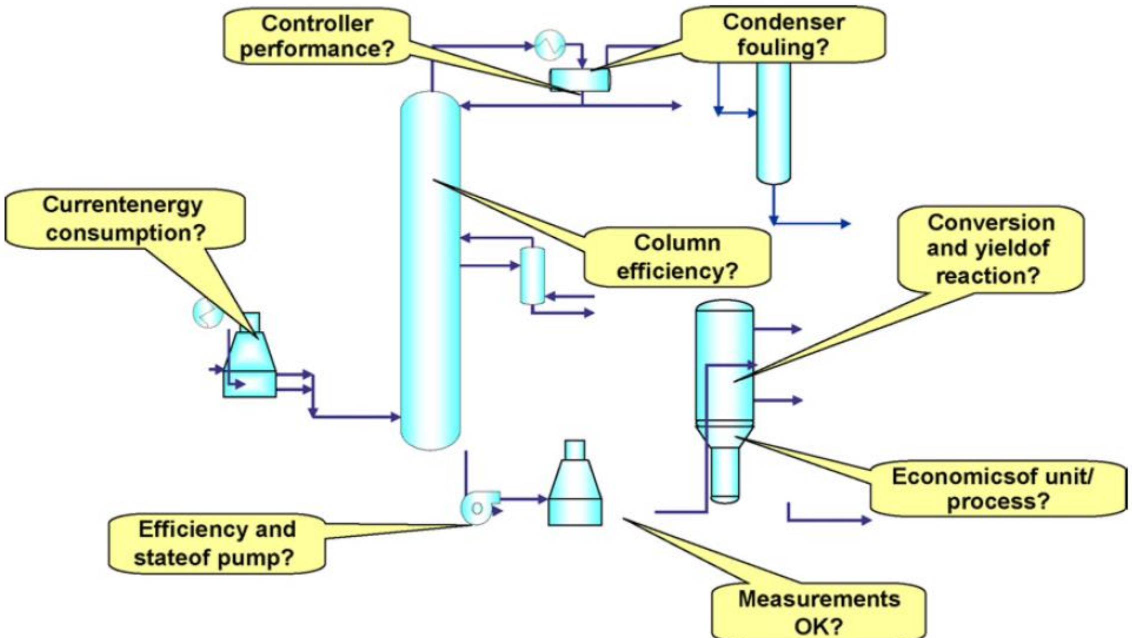
- **Process synthesis methodologies relying on rigorous optimization are rarely used in industrial practice.**

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.

# 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.



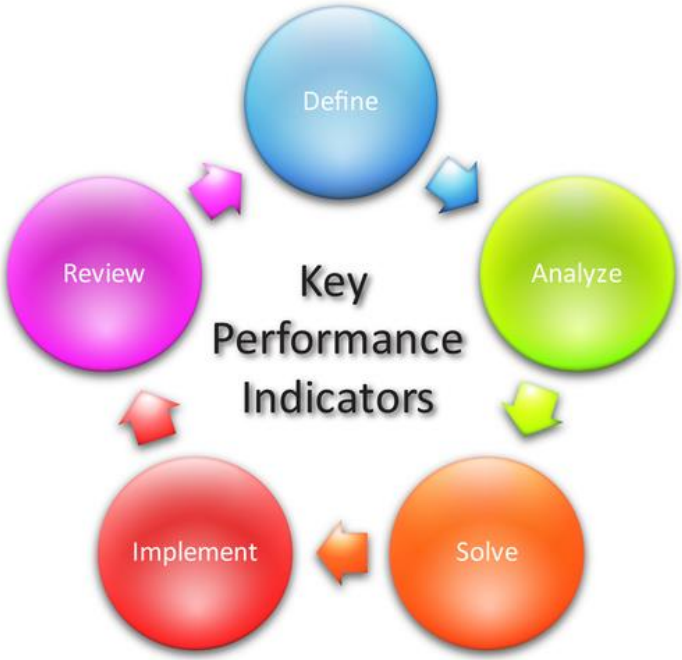

From Klatt & Marquardt, 2009

# 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).

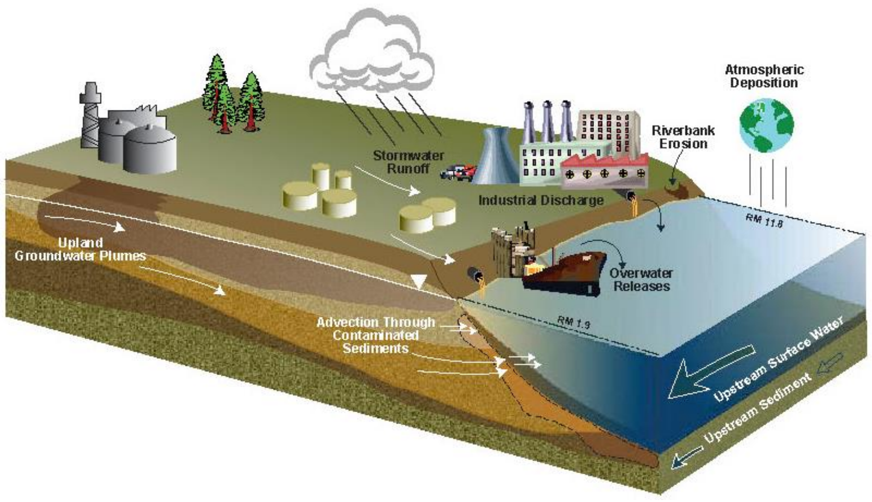
# Tools for PSE

- **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.



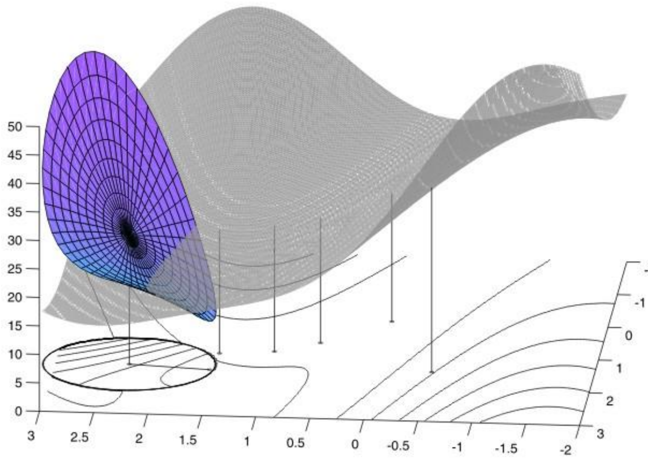
# Tools for PSE

- 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; <u>he invented new types of equipment</u> for <u>integrating these operations</u> and carrying them out <u>continuously</u> on a <u>large scale</u>. He himself dealt with all aspects of an <u>integrated chemical processing system</u>: the chemistry, the materials handling, and the engineering of an integrated processing system, such as <u>operating conditions</u> and the <u>design of specific equipment</u>.*
- *The <u>Solvay process</u> may be seen as the model process in which <u>all aspects of PSE</u> are explicitly delineated and directly addressed, in a fairly <u>systematic</u> and more importantly, <u>system-wide basis</u>.*


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

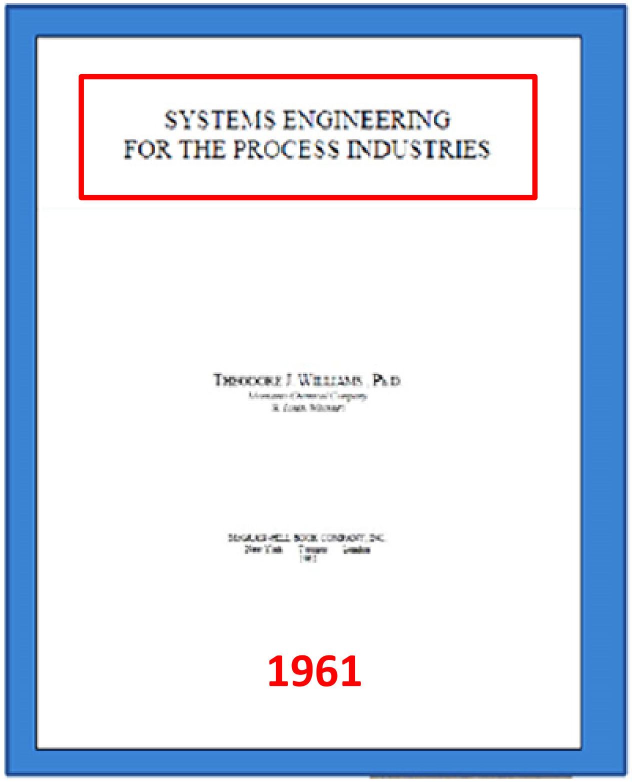
# Historical background

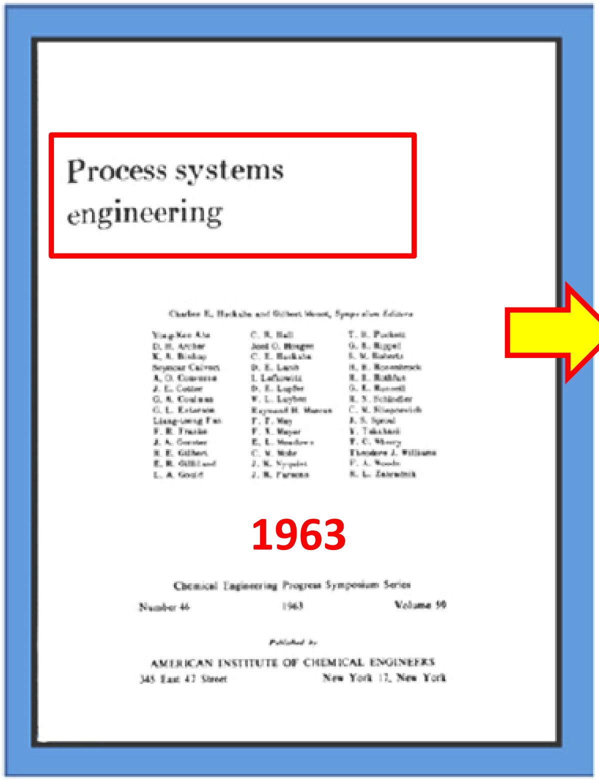
- The **1960s to 2020 period** is a **computer-driven period** of explosive expansion and growth.
- By early 1960s three factors are aligned to cause the onset of an explosive growth period for PSE:
    1. Chemical industry has been growing rapidly, worldwide, for more than 10 years, exerting significant 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

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