RWTH

Bayer Technology Services

Perspectives for Process Systems Engineering

--

a Personal View from Academia and Industry

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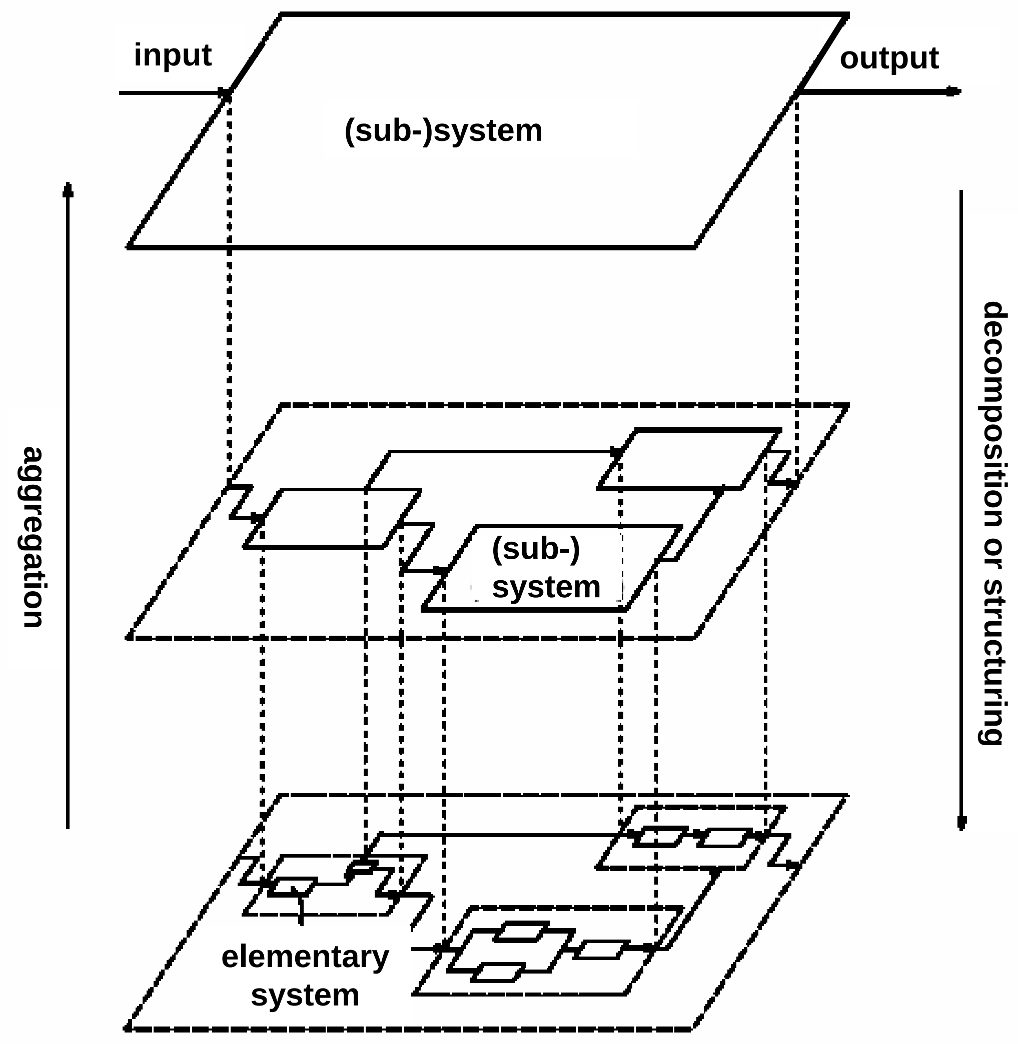
Outline

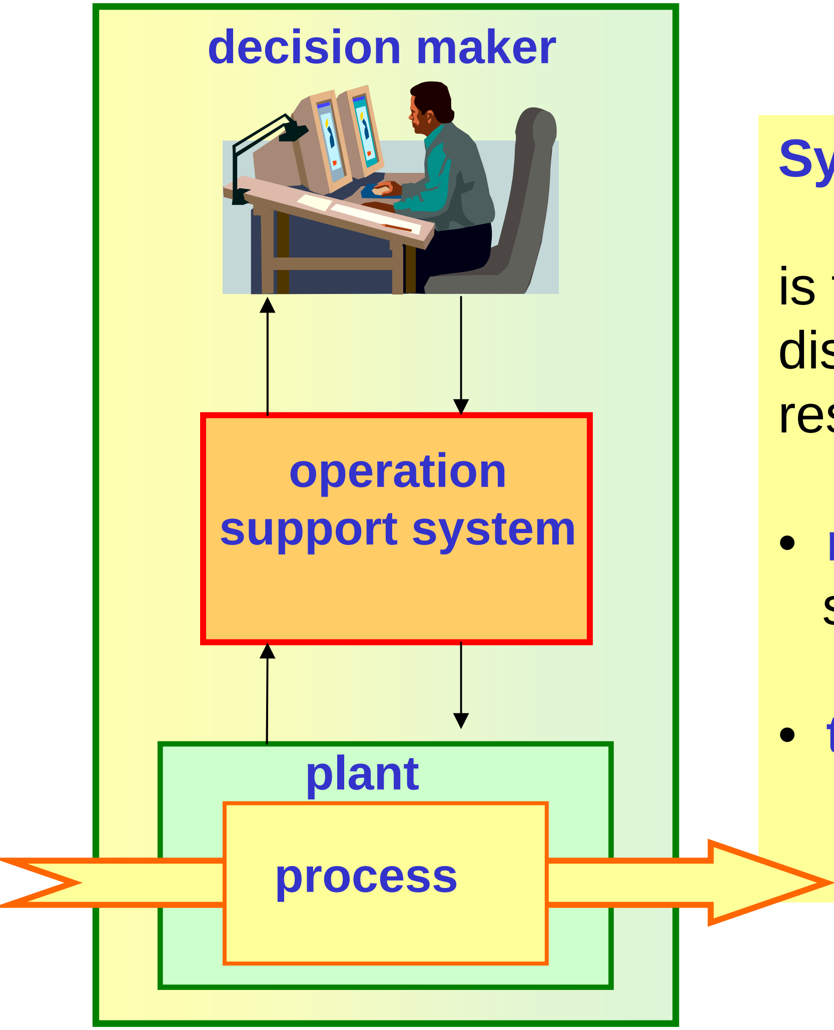
- What is the nature of **process systems engineering** ?
- Which **research topics** have been dealt with in the past 50 years ?
- What has been absorbed by **industrial practice** ?
- Which **research trends** are emerging ?
- What are the **industrial requirements** for the future ?
- What is the **future of process systems engineering** ?

General Systems Theory

(von Bertalanffy, 1930ies)

- **methodology** for analysis and synthesis of complex systems comprising interacting parts
- **analysis** – understand behavior and function of complex (natural and artificial) systems
- **synthesis** – design and implement (artificial) complex systems, which satisfy given requirements
- **representation** of systems by means of (semi-)formal and/or mathematical **models** – the basis for analysis and synthesis





Systems Engineering …

is the intellectual, academic and professional discipline the principal concern of which is the responsibility to ensure that all

- **requirements** for bioware/hardware/software system **are satisfied**
- **throughout the lifecycle** of the system

(Wymore, 1993)

1990ies –
problem solving and decision making
with **computer-support** rather than **automation !**

- If a problem statement can be formalized, an algorithmic procedure can be found for its solution.
- Every algorithmic procedure can be implemented in software and executed by a computer.
- Systems engineering problem solving can be automated by means of computers.

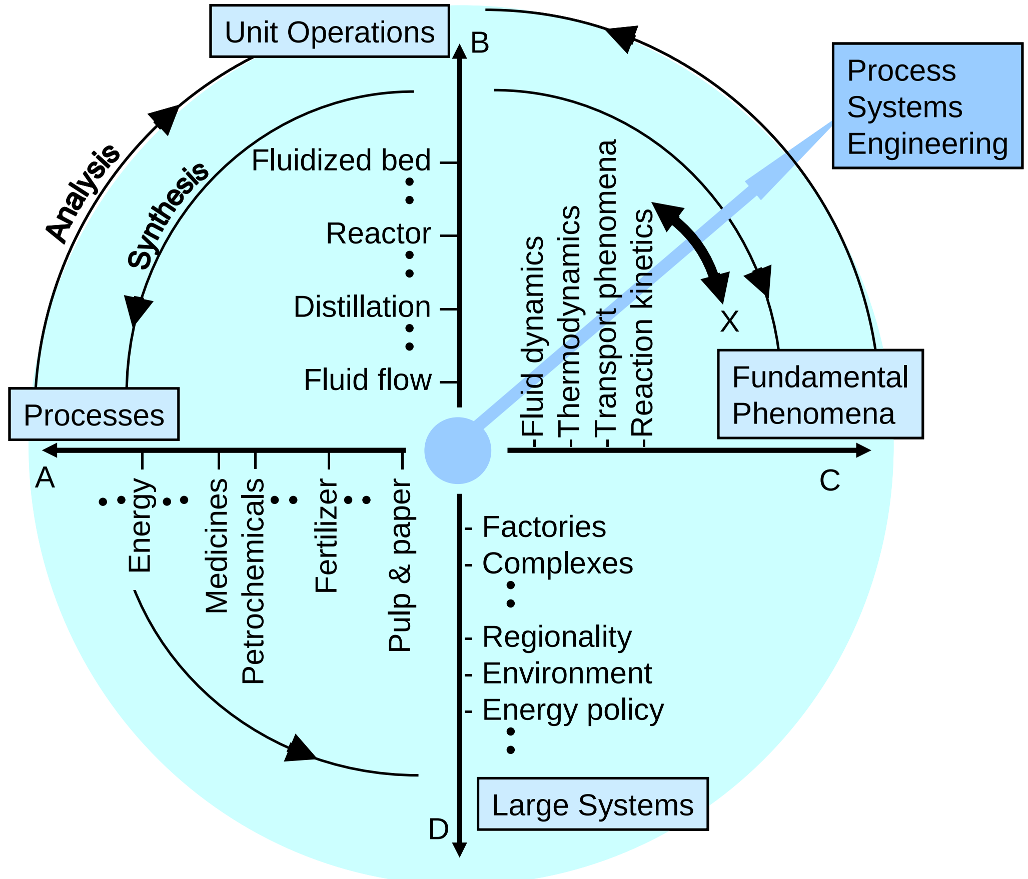
Process Systems Engineering (PSE)

„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 and chemical industries themselves.“

Takamatsu (1985)



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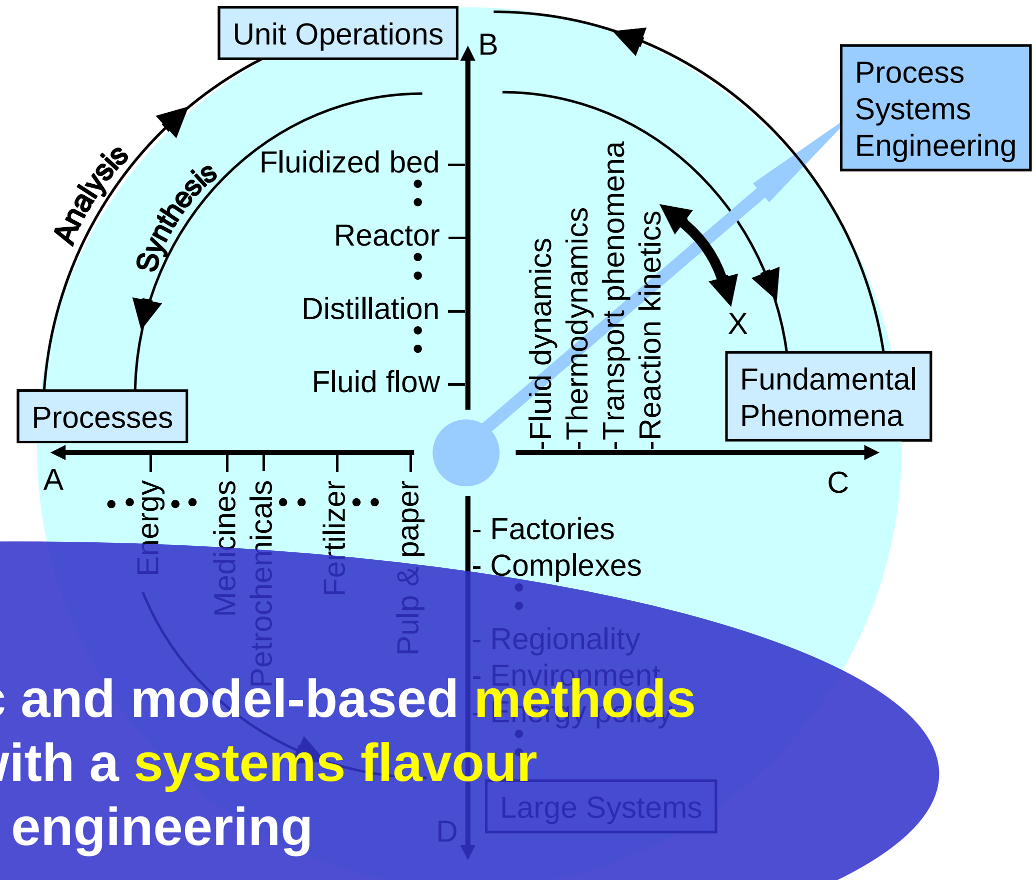
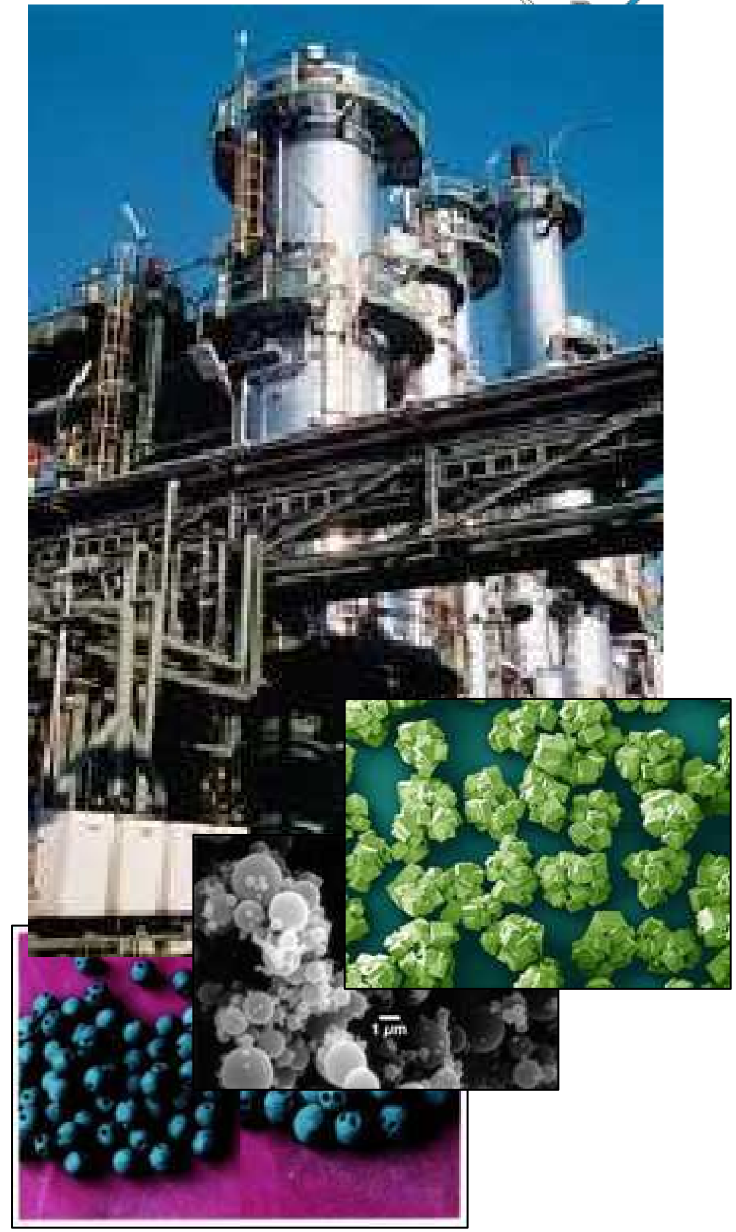


… it is all about systematic and model-based methods to solve problems with a systems flavour in chemical engineering

(Ponton, 1995)

Agreed Paradigms of PSE

- **Complexity and connectivity** in processes (and products) can be mastered on all scales by the systems approach.
- **Modelling, simulation and optimization methods** for large-scale systems is a core technology.
- Methods have to be cast into **software tools** for industrial use.
- The systematic **generation and evaluation of alternatives** is a key to success.
- **Integration across scales and lifecycle** results in better solutions.
- PSE is a **cross-sectional topic** in ChemE.
- PSE is at the **interface** of ChemE to Mathematics, Computer Science, and Economics & Management.



Relation of PSE to …

- **Chemical Engineering …**

  comprises PSE as one of its core topic areas, which aims at the development of **systems engineering methods and tools** tailored to chemical engineering applications.

- **Computer-Aided Process Engineering (CAPE) …**

  comprises all **problem-solving techniques**, which require the **use of computers** without emphasis on systems theory.

a set of skills !

- **Process Intensification …**

  aims at the systematic exploitation of kinetic phenomena on the **meso-scale** to invent **compact**, **efficient, and often multi-functional process.**

- **Product Design …**

  targets the **development of tailor-made material products** by a systematic exploitation of the molecular and morphological material properties on the microscale.

a set of objectives !

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Research Topics – The Early Days

… since the 1950ies

- mathematical modeling, simulation and optimization for the design and operation of selected process units
- exemplary use of computers to deal with model complexity

Mathematics of adsorption in beds, 1950

Solution of transient stagewise operations on an analog computer, 1953

An analysis of chemical reactor stability and control, 1958

Multicomponent distillation on a large digital computer, 1958

Studies in optimization, 1960 - 1962
1. The optimum design of adiabatic reactors with several beds

Dynamic behavior of multi-component multi-stage systems
- numerical methods for the solution , 1962

Continuous models
for polymerization, 1963

Influence of droplet size-age distribution on
rate processes in dispersed-phase systems, 1968

Evolution of Core Research Topics (1)

- **method-oriented research** at the interface to **mathematics and computer science**
  - mathematical modeling
  - numerical algorithms
  - all kinds of software tools
- extension to **systems of larger and larger scales**
  - from process units to complete processes
  - from processes to sites and supply chains
- increasing coverage of **phenomenological detail**
  - mass and energy balances, (complex) thermodynamic equilibrium
  - reaction and transport kinetics
  - (particle) population dynamics
  - fluid dynamics and complex geometries
  - from conceptual process to engineered plant

Evolution of Core Research Topics (2)

- increasing **variety of problem formulations**
  - steady-state and dynamic simulation
  - systematic process synthesis
  - monitoring and control, real-time optimization
  - production planning, supply chain management, logistics

- increasing **integration of problem formulations**
  - process design and control
  - process, environment and sustainability
  - process and product
  - process, supply chain and market

- **integration** across multiple **scales** at the interface
  - to the **natural sciences:** from flowsheet to molecule
  - to **management & economics:** from process to supply chain
  - last but not least to **mathematics:** methodologies and algorithms

What Are We Doing **Really Well** ?

- **stationary und dynamic modeling** of
  - fluid-phase unit operations and single- and multi-phase reactors
  - large-scale continuous processes, sites, supply chains

- **routine simulation of models** with
  - some 100 000 nonlinear DAEs
  - some 10 (few) nonlinear PDEs in 2D (3D)

- **(not yet routine) optimization of models** with
  - some 100 000 equality constraints, some 100 inequality constraints and some 1000 decision variables
  - some 1000 differential-algebraic constraints, some 10 inequality path or end-point constraints and 10 control variables
  - few PDE constraints in 2D with few decision variables
  - small (dynamic), moderate (nonlinear) to large (linear) mixed-integer problems

- provision of **powerful modeling tools** for industrial practice

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analysis and design support

- **(very) good process understanding for process unit modeling**
- **formulations for simulation and optimization**

Where Do We Still Face **Limitations** ?

- **modeling, simulation and optimization**
  - solids and biochemical processes
  - handling of very large and complex models
  - documentation, maintenance and reuse of models
  - model (structure) identification
- **process synthesis**
  - heat exchanger network, distillation sequences
  - integrated processes
- **monitoring and control**
  - plant-wide control structure design
  - monitoring and fault diagnosis
  - model-predictive control and real-time optimization
- **production planning & management** and **logistics**
  - batch and continuous processes
  - supply chains

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… in routine model-based solution of industrial practice problems during the product life-cycle !!

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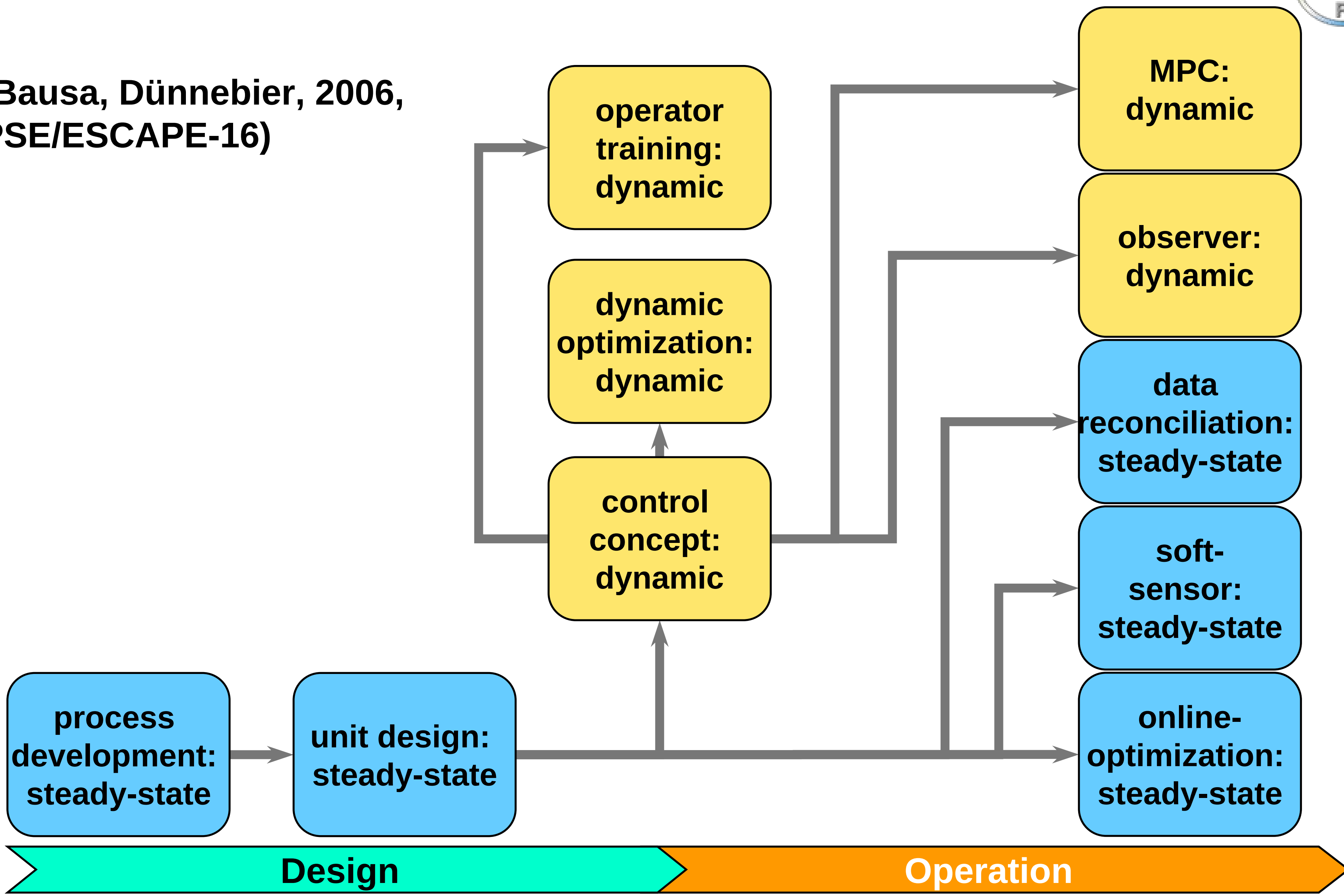
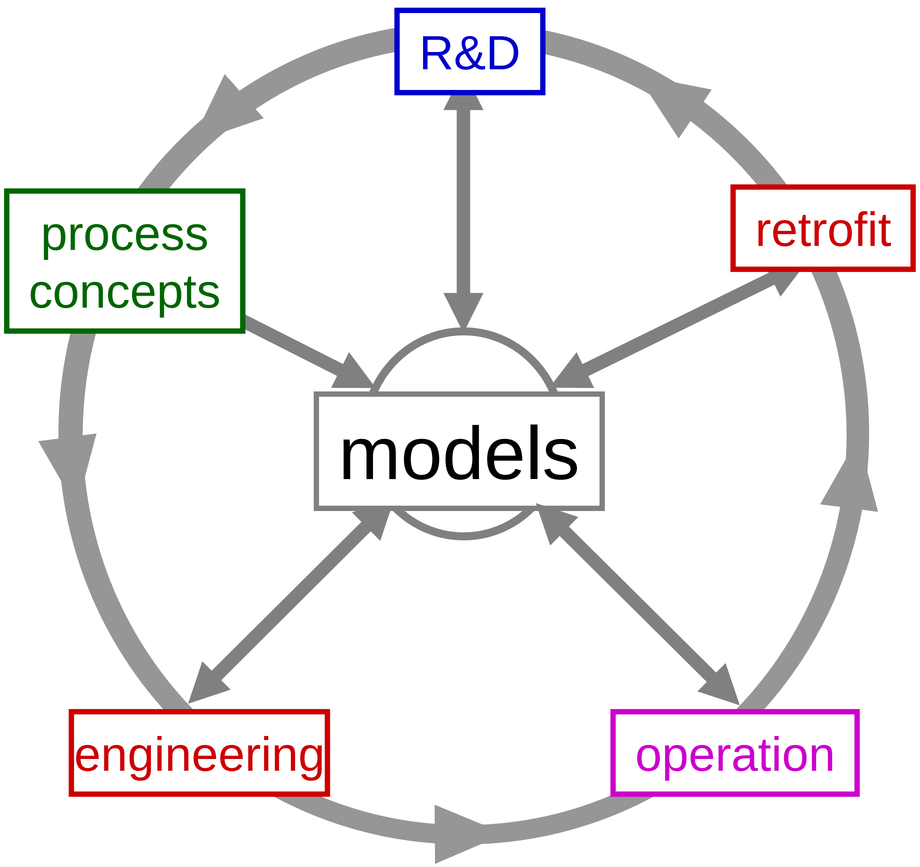
(Bausa, Dünnebier, 2006, PSE/ESCAPE-16)



The Idea of Life Cycle Modeling



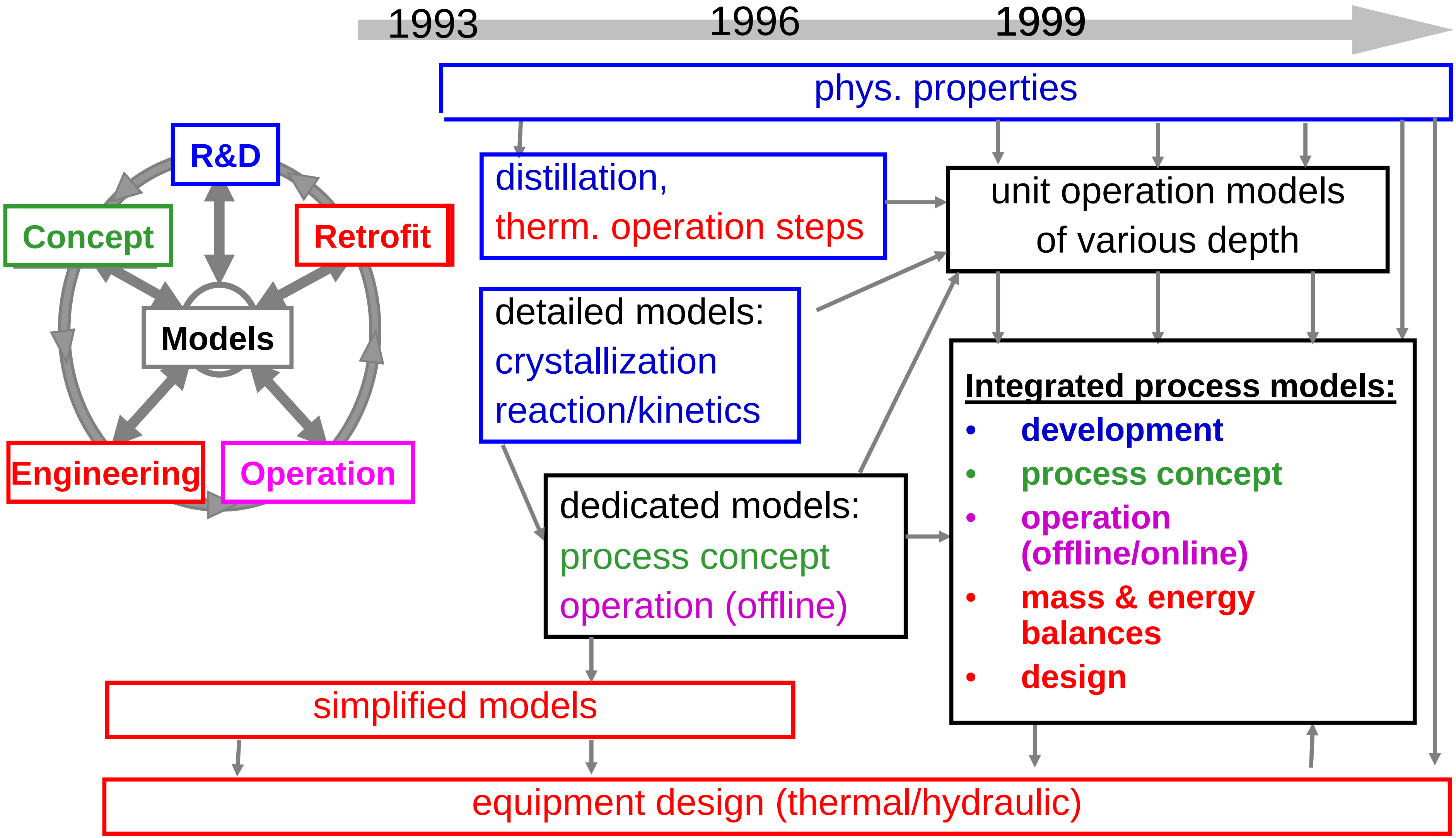
Different modeling approaches and tools are applied in different lifecycle phases.

Specific problems are associated with each of these phases.

Lifecycle Modeling:
the integration and combination
of models across lifecycle phases.

Fast and consistent process modeling,
benefits for the process

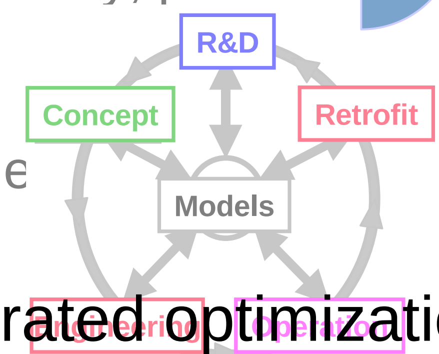
Polymer Intermediate: Towards Lifecycle Models



• Plant Capacity Expansion: + 50% by new line

model based working method:

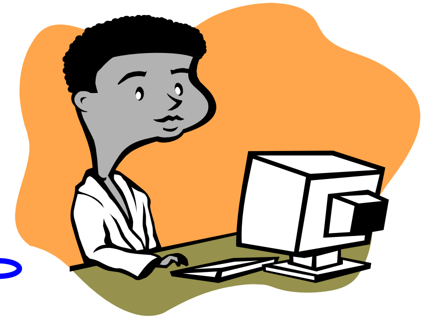
- starting point: autocalibrated model
- development of various expansion scenarios
- concept assessment (achievable quality, production and capital cost)
- consistent mass and energy balances, scale up
- detailed analysis (feasibility, potential bottlenecks)
- equipment design
- transfer into new online



Benefit: integrated optimization approach:

investment, capacity, quality, costs (engineering & operation)

Polymer Intermediate: Operation

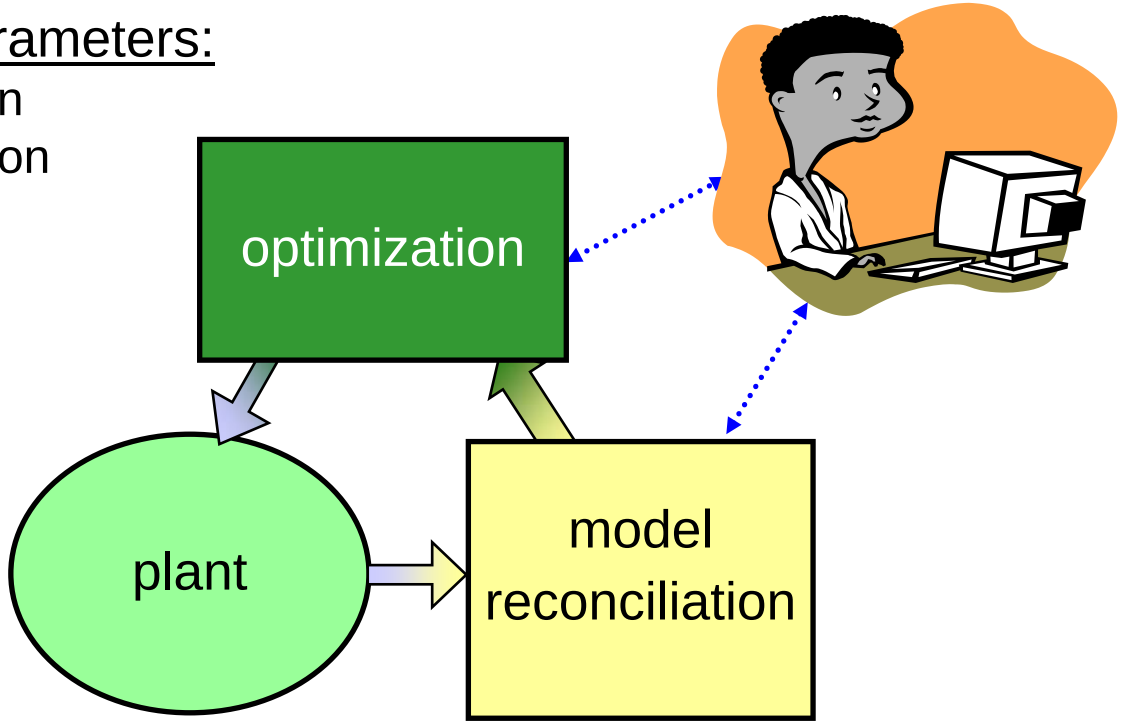


many reactors,
all different size
all different acitvities

...how should I operate
the plant to achieve in-spec
product at minimal cost?

Polymer Intermediate: Operation

<u>optimized parameters:</u>
load distribution
feed composition
temperatures



in operation
for 4 years

<u>actual plant data:</u>
load distribution,
samples,
temperatures,
...

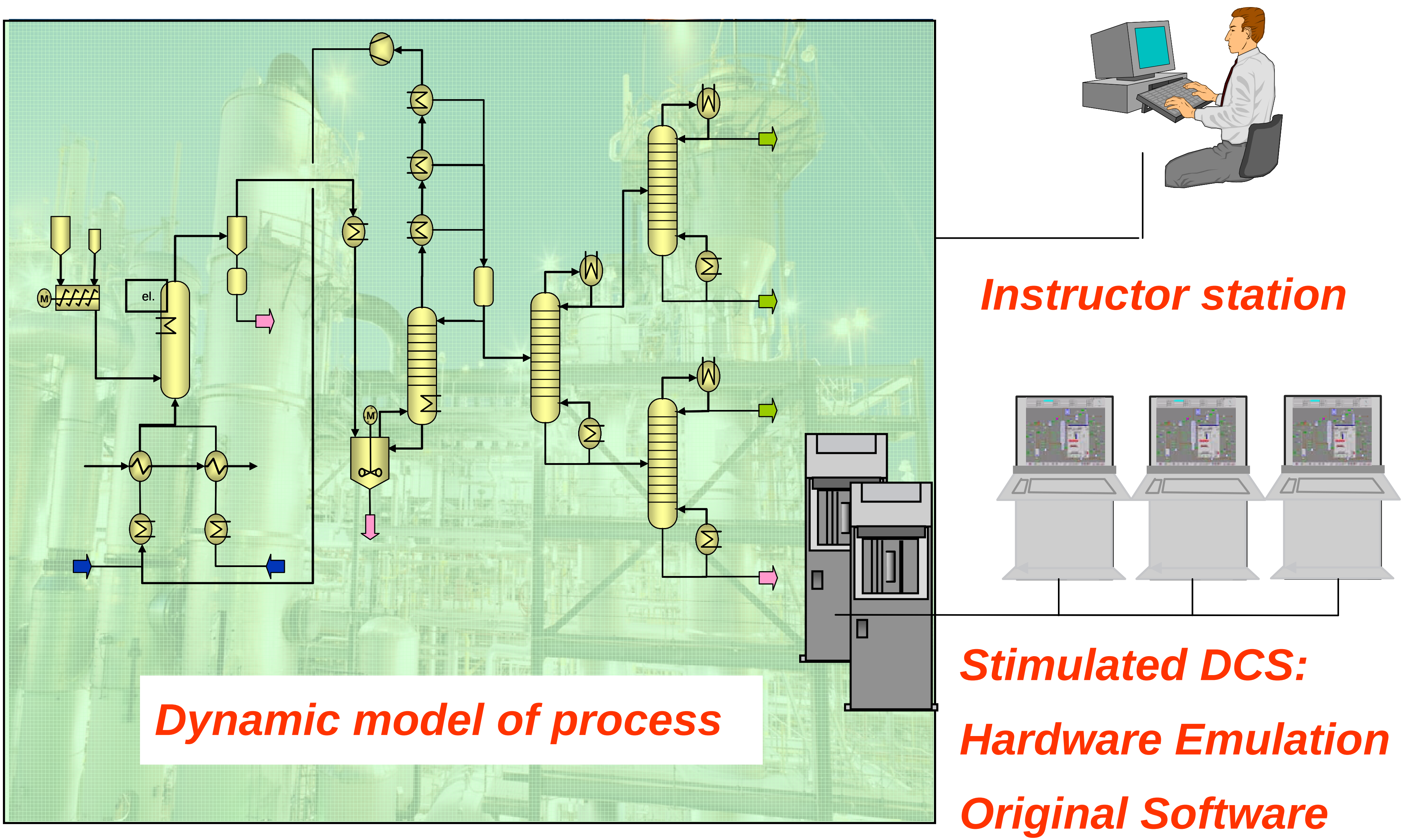
<u>model adjustment:</u>
catalyst activities

<u>autocalibrated model:</u>

improved acceptance for modeling

further applications

Operator Training Simulator (OTS)



Process control incorporated with design phase

Operator Training Simulator (OTS) implementation

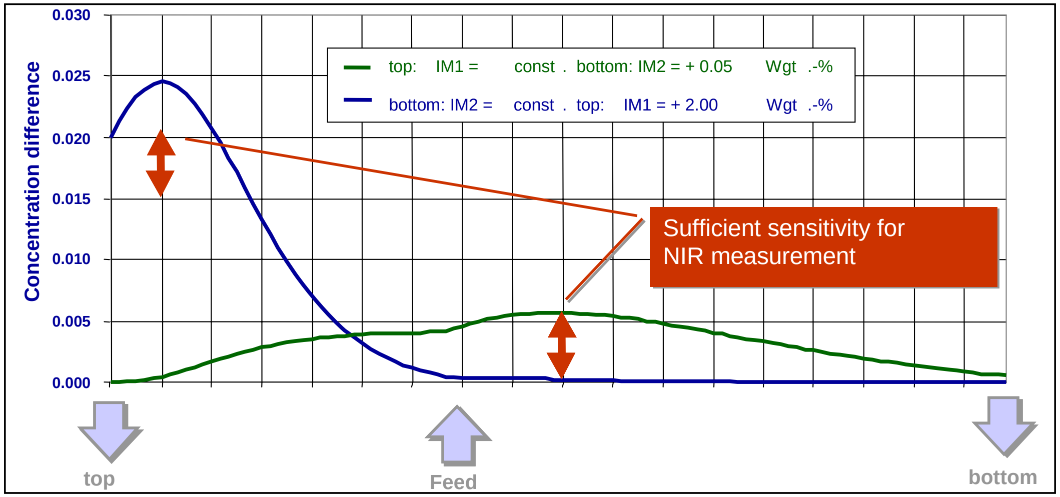
APC Project combined with OTS Project

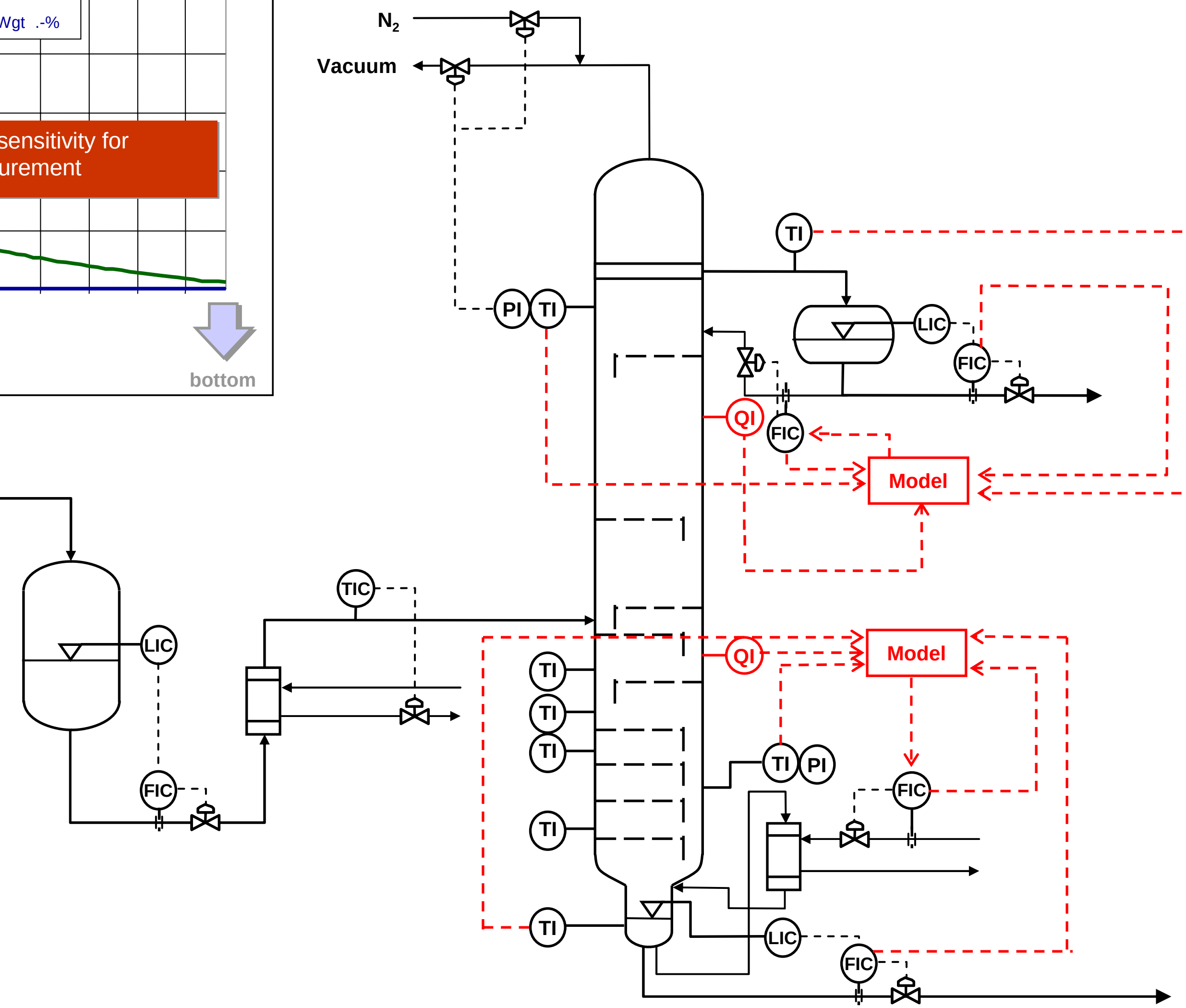
Control loops tuned on OTS before Start-up

Start-up supported by control engineer

Control loops optimally tuned directly after start-up

Model-Based Control of a Distillation Column (1)





close boiling mixture separations

- require online concentration measurement
- temperature measurement is not sufficiently sensitive

Model-Based Control of a Distillation Column (2)

Task

- capacity increase and robust automatic concentration control

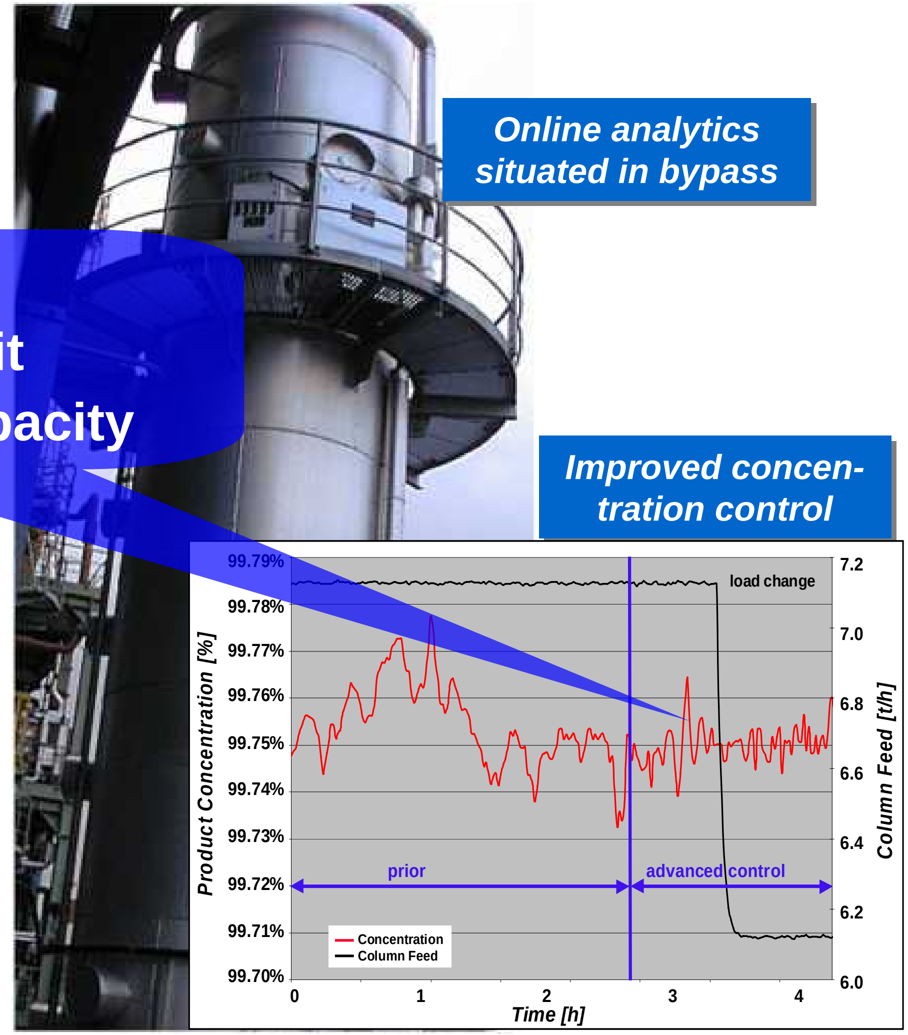
Scope

- potential assessment for combining advanced process control and NIR online analytics
- design and implemention of model-based control concept
- optimize controller performance

less variance
⇒ closer to the limit
⇒ more capacity

Benefit

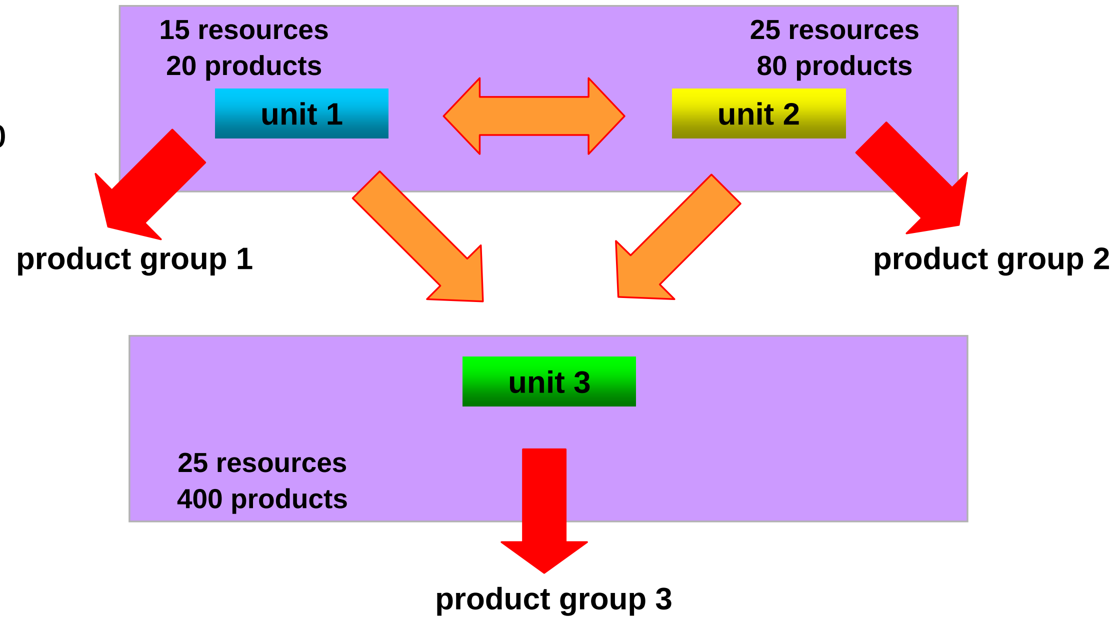
- reliable concentration control
- capacity increased by 10%



Model-Based Automated Scheduling (1)

Task

- achieve fully automated scheduling in connection with ERP/APS system
- streamline production planning to make full use of installed capacity
- reduce number of alerts (caused by infeasible production plans) by 50 %
- reduce time spent for production planning by 50 %



Solution

- integrate with existing Advanced Planning System (APS)
- perform calculation of optimal plan once per day
- use well known user interface of APS

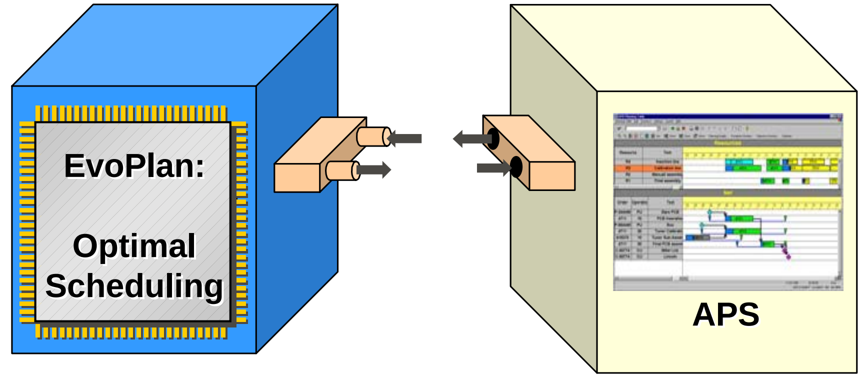
Model-Based Automated Scheduling (2)

Benefit

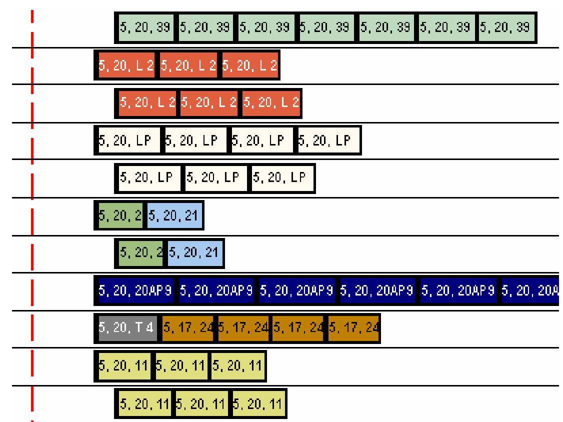
- all goals fully reached
- improved inventory planning
- number of remaining alerts reduced by 80 %
- computing time (including down-/ upload times) less than 30 min.
- excellent acceptance by planners

Process

- multi-purpose unit for production of chemical specialty products (>100 kt/a, 70 resources, 500 products)



Gantt chart



Industrial Practice – Critical Remarks (1)

- **Model-based process design, optimization, and control** are well-established in today's industrial practice, but
  - we still do not have adequate methods and tools to deal with solids,
  - the (short-term) benefit often is difficult to quantify in advance,
  - life-cycle modeling and re-use of models for different tasks do not necessarily pay-off in any case,
  - model-based solutions are often unique, costs usually cannot be cut down by quantity.
  - maintenance and sustainability are not for free.
- **Industrial process design** is mainly based on simulation studies and not on rigorous (mathematical) optimization.
- **Nonlinear model-based dynamic optimization** and control is a main focus of academic research but is on the fringes in industrial practice.

Industrial Practice – Critical Remarks (2)

- **Research and development** mainly focuses on application areas with high profitability, in particular on large-scale, continuous production processes.
- **Extension to small-scale and often multi-purpose production** facilities has yet not been successfully established.
- **Long term R&D projects** are commonly difficult to establish in today's industrial practice.
- **PSE methods** and solutions often are considered to be just "nice-to-have" and not to be essential for stable and economic production.

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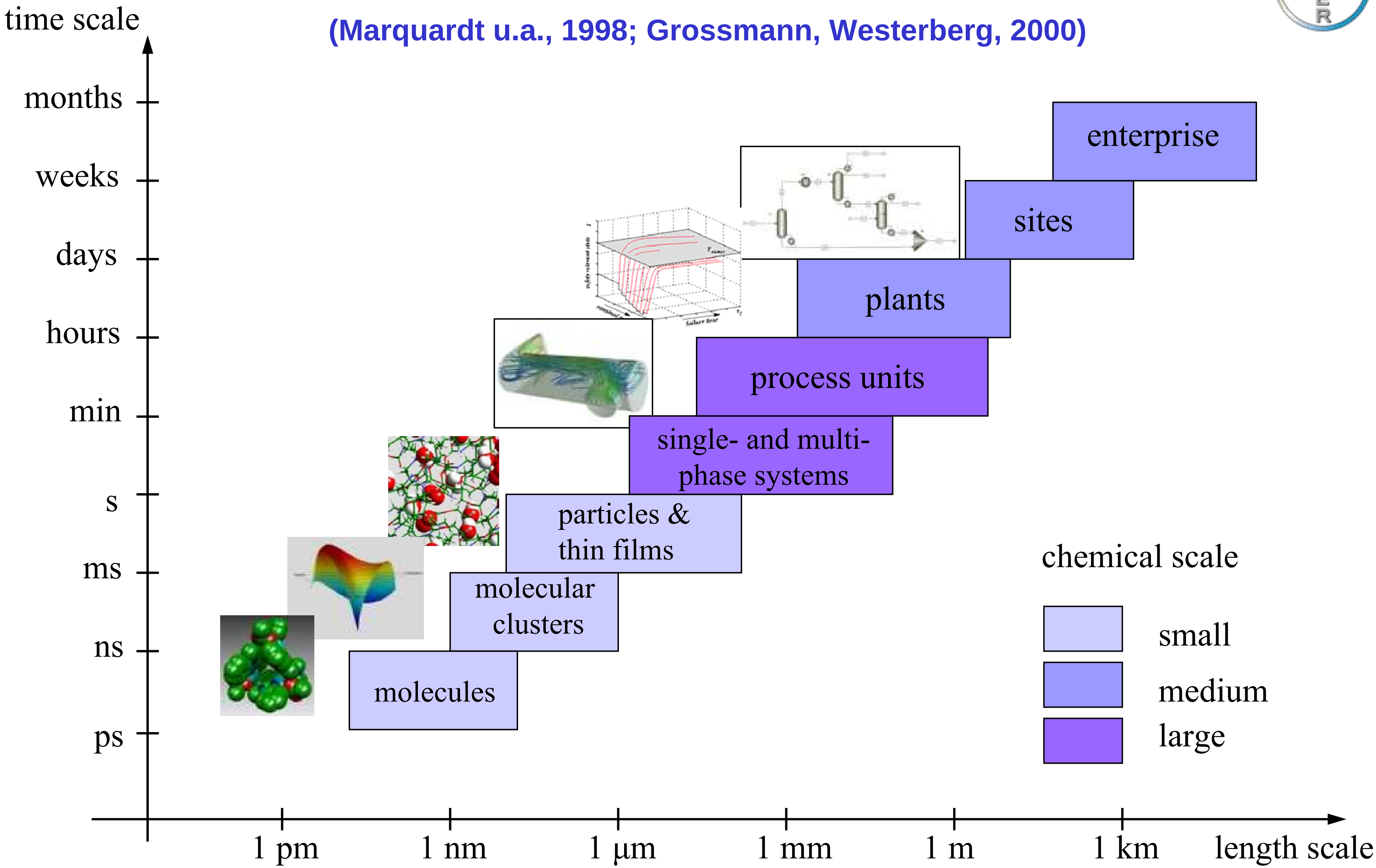
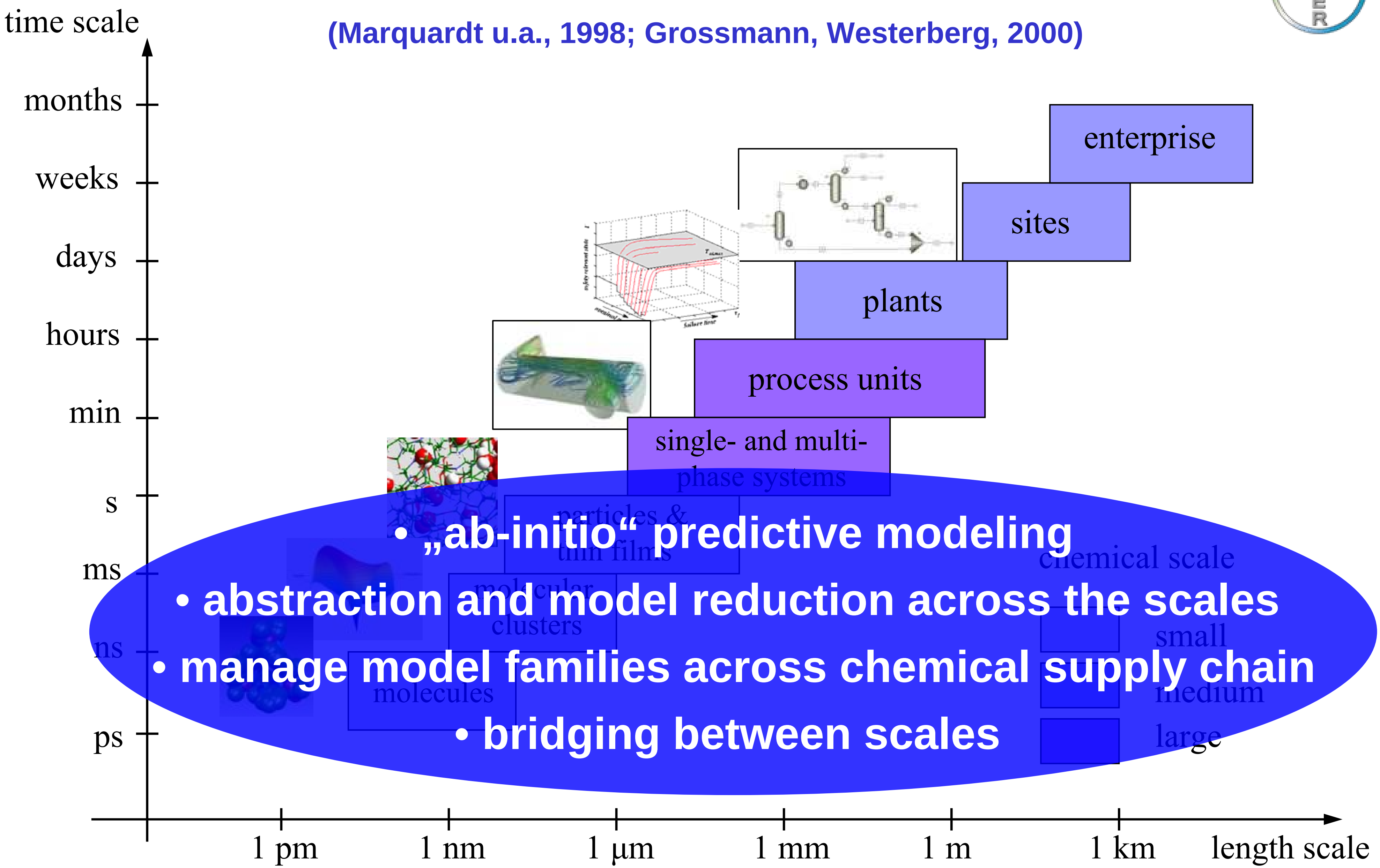
Multi-Scale Modeling in the Chemical Supply Chain

(Marquardt u.a., 1998; Grossmann, Westerberg, 2000)

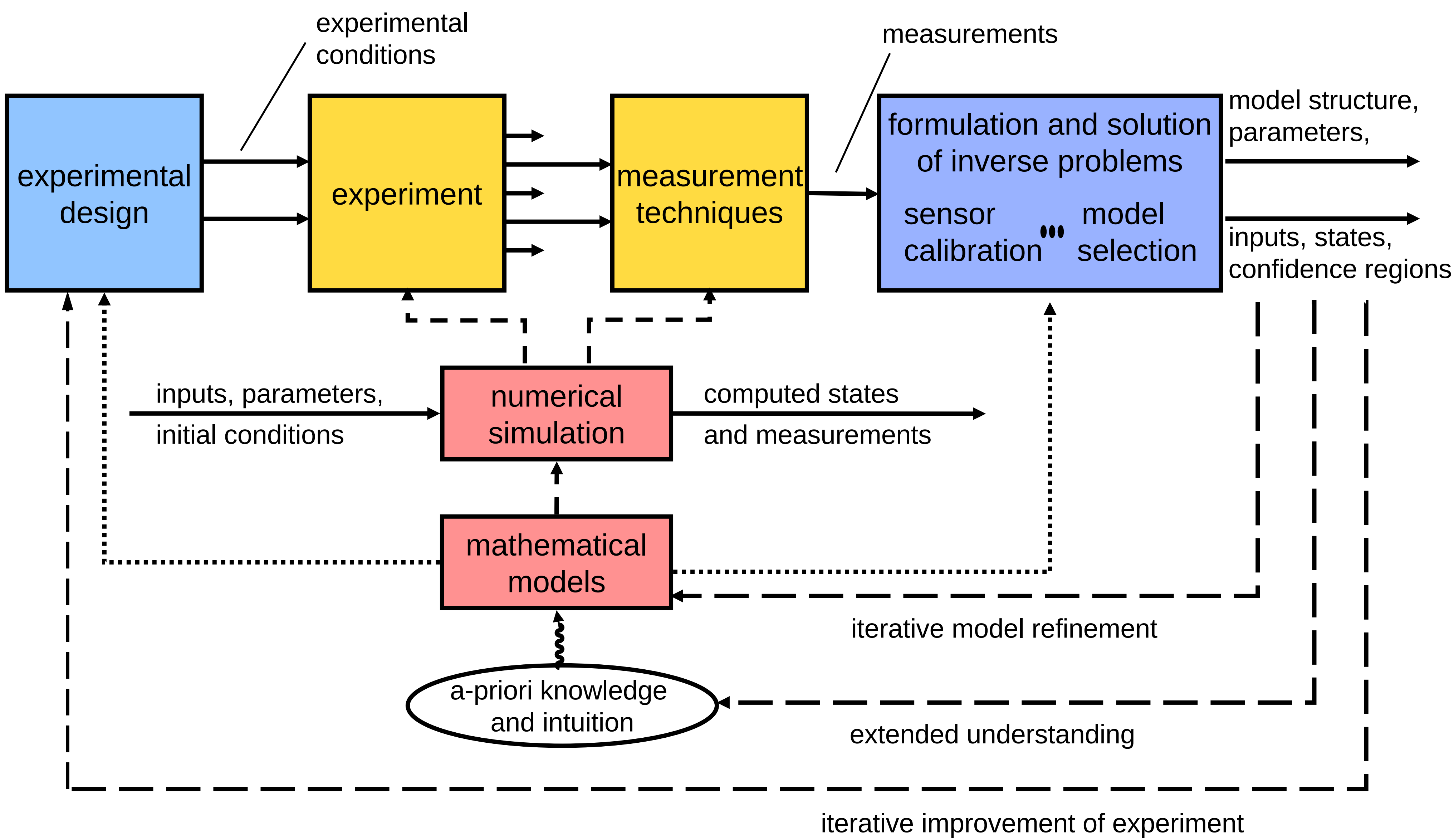


(Marquardt u.a., 1998; Grossmann, Westerberg, 2000)



- „ab-initio“ predictive modeling
- abstraction and model reduction across the scales
- manage model families across chemical supply chain
- bridging between scales

Systematic Link of Modeling and Experimentation



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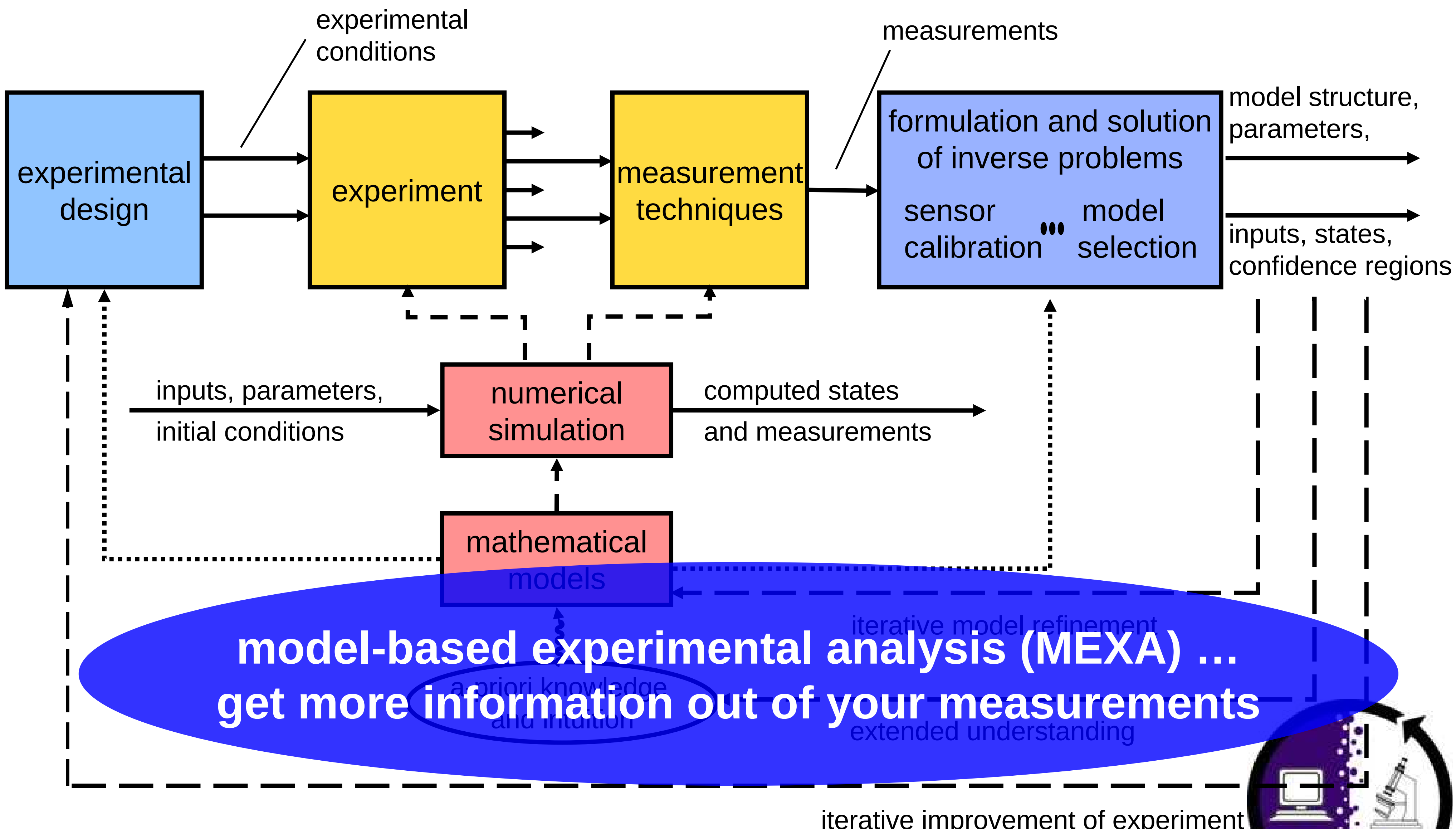


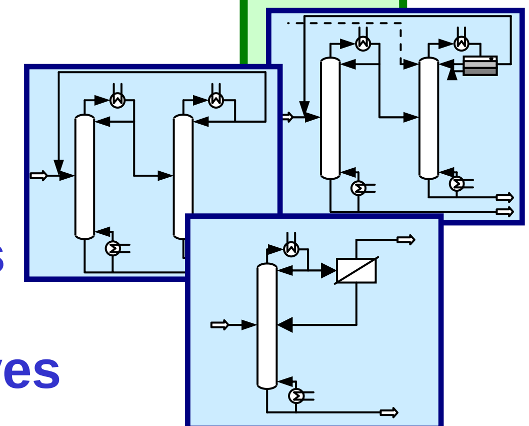
market-driven specification of desired product properties and purities

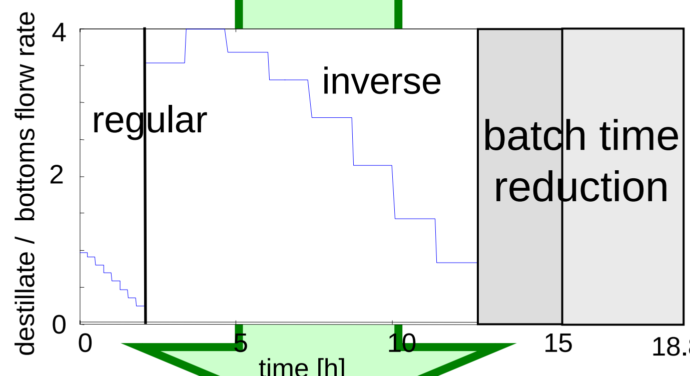
identification of favorable (catalytic) reaction pathways

invention of possible process alternatives

screening for attractive process alternatives

equipment sizing and decision on favorable operational strategies





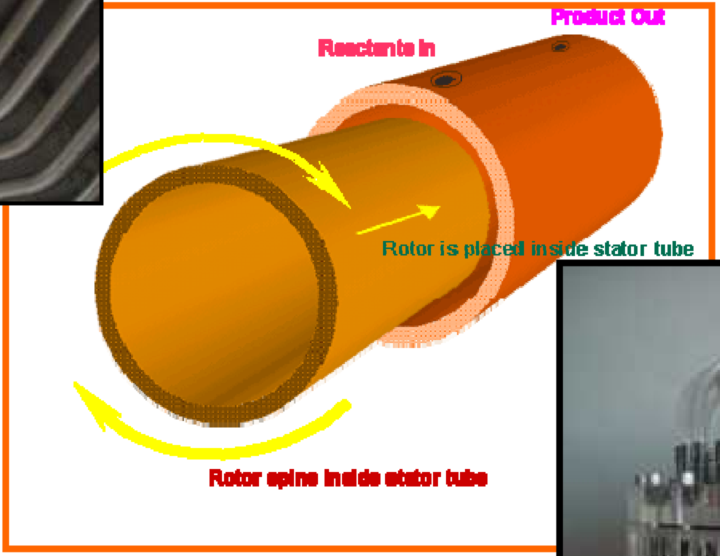
… reconciling conflicting objectives
… managing uncertainty and risk
with systematic & integrative methods

product leadership

Exploit the Mesoscale – Equipment Synthesis

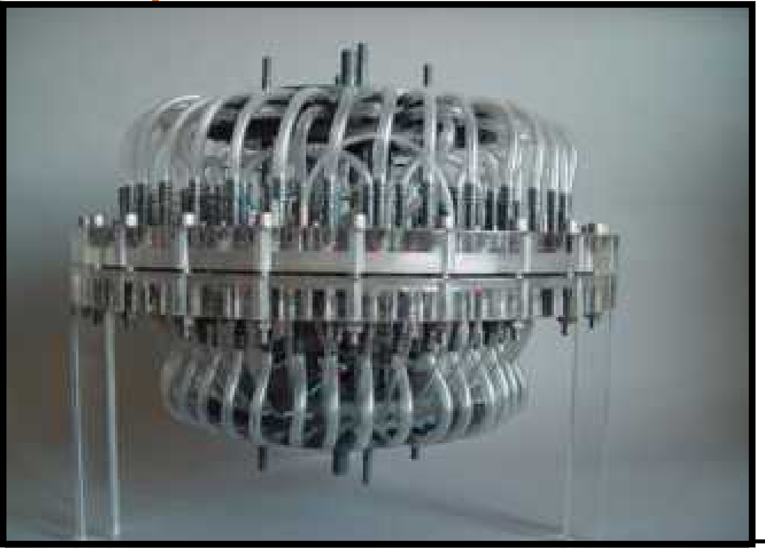
… for process intensification employing PSE methods and tools

absorption tower tray with integrated heat exchanger to control strongly exothermal process



Generate Kolomogoroff-vortices in a shear flow for shorter reaction times

Holl Technologies Inc.



From analytics to preparative separation, electrophoresis for protein purification

Melin and co-workers, RWTH Aachen

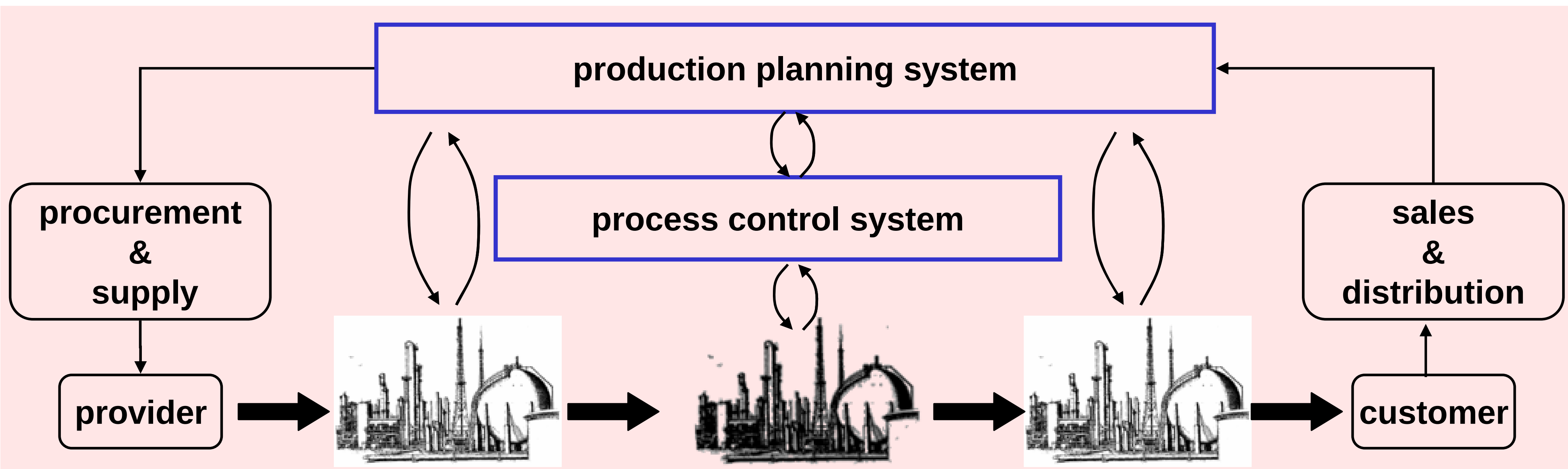
Supply Chain Conscious Process Operations

today

- an isolated view of the plant
- separation of automation tasks
- „stationary“ operation offers limited flexibility
- largely autonomous production management of plant
- heuristic methods

tomorrow

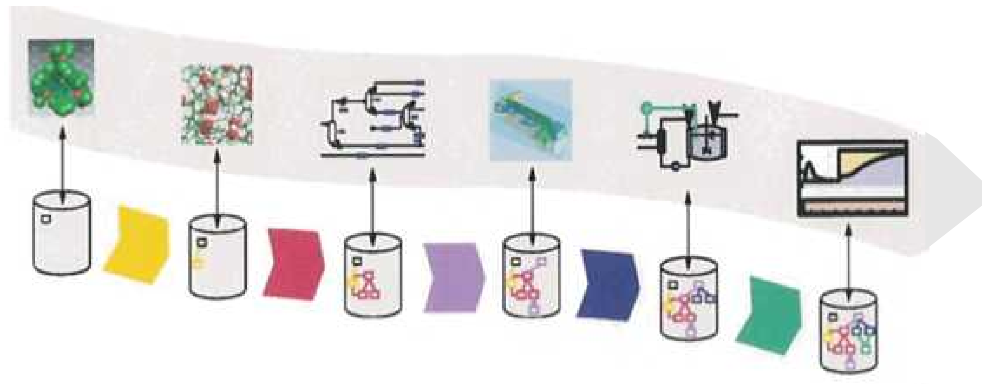
- integration along supply chain
- integration of automation tasks
- „agile“ operation of supply chain in a dynamic business environment
- reconciled objectives of stake holders for maximum profit
- model-based methods



Take a Broader View – Knowledge Management

knowledge about product & process design and manufacturing

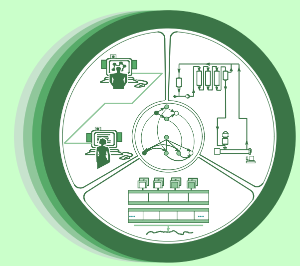
- capture
- structure and rectify
- store and reuse



the asset of any enterprise

- innovation capability
- business process optimization
- sustainability of differentiating know how

- it is a modeling problem and we are good in it !
- mathematical models seemlessly integrate with ontologies
- basis for modern software systems like advanced modeling, synthesis, process and supply chain management tools



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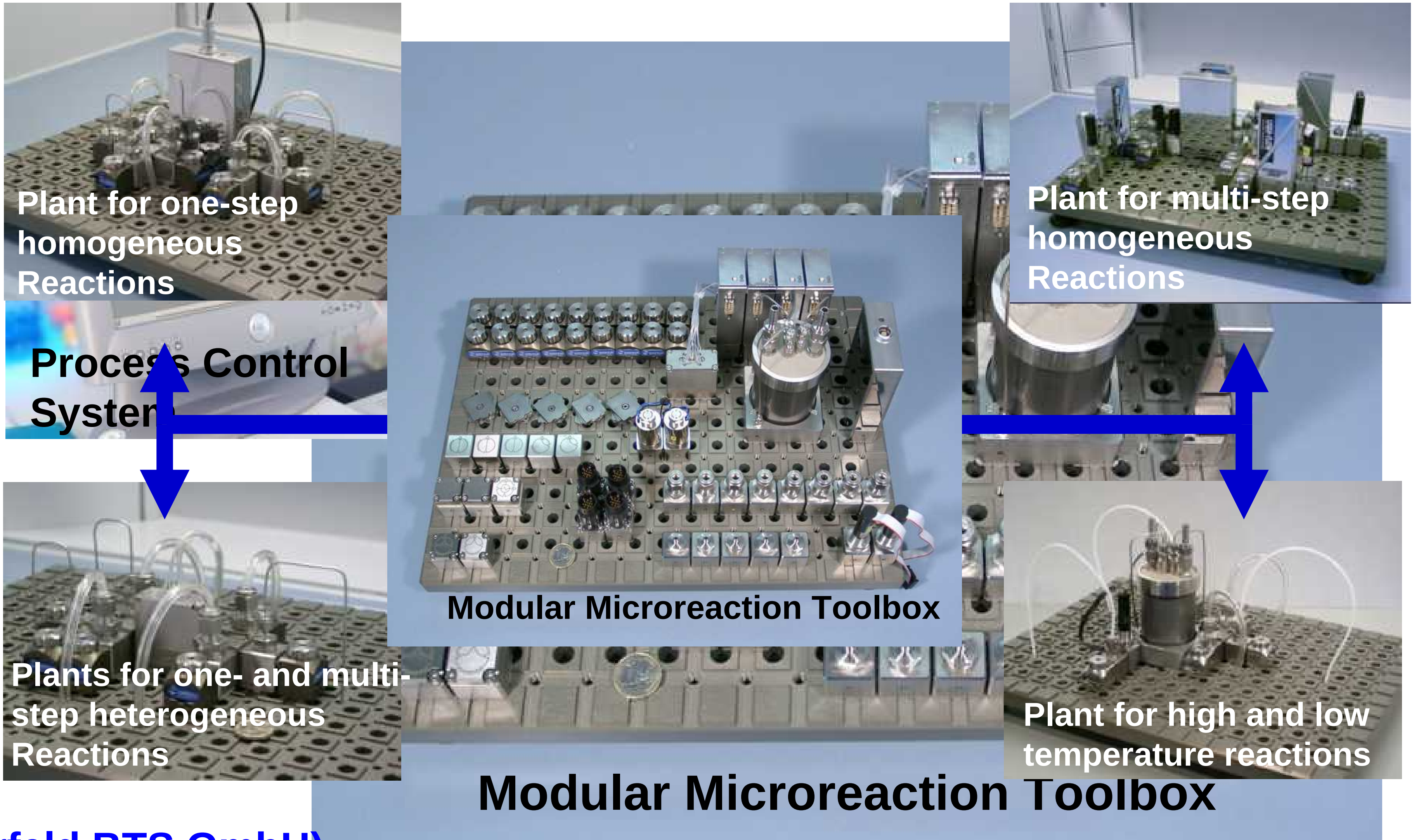
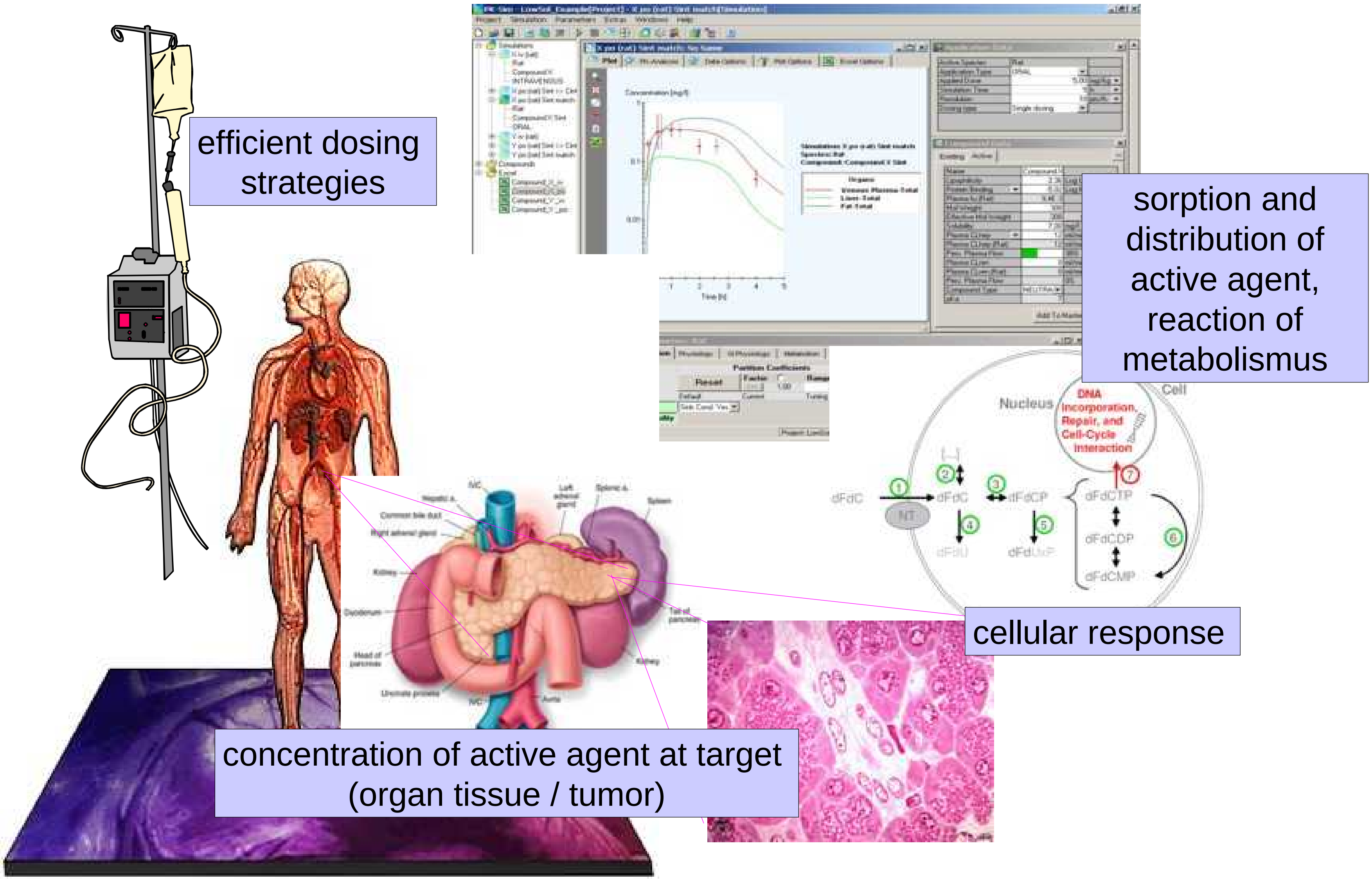
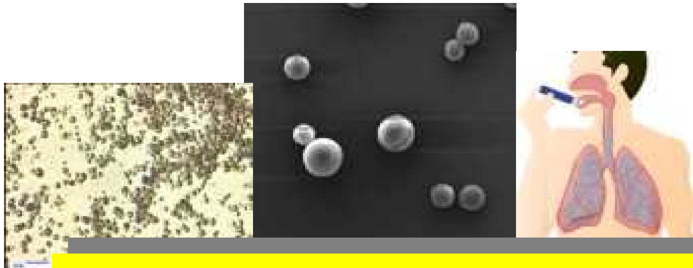


(Ehrfeld BTS GmbH)

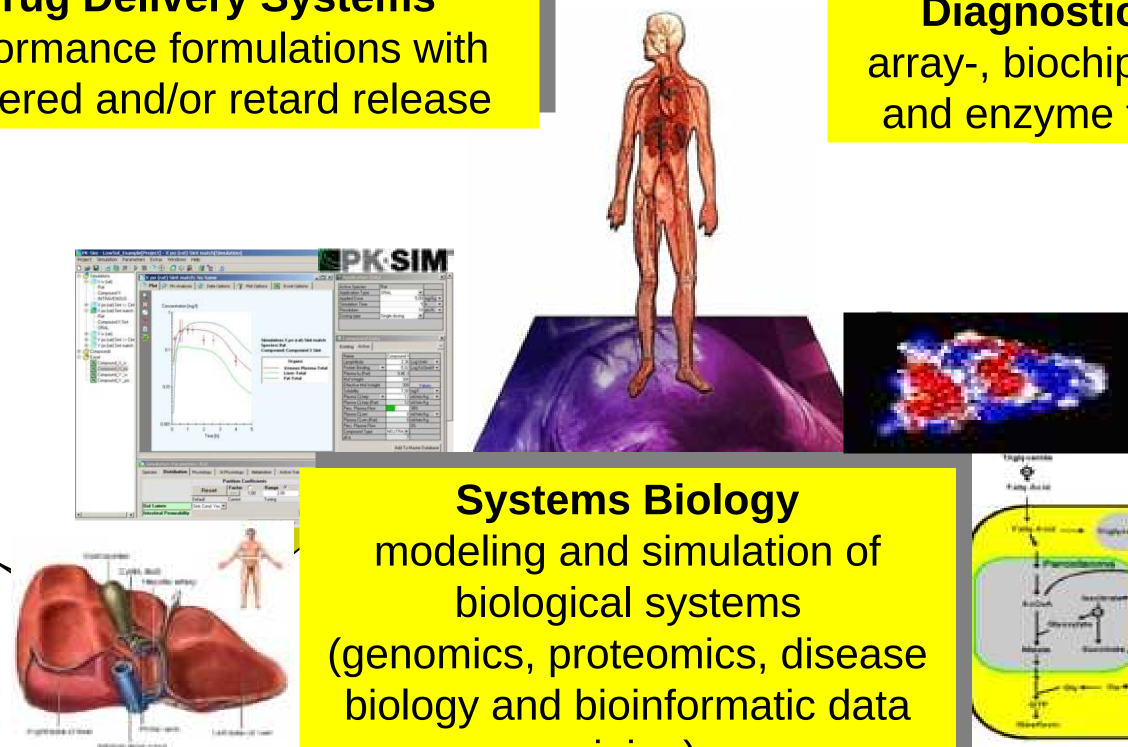
Systematic Design of Structured Products


efficient dosing strategies
sorption and distribution of active agent, reaction of metabolismus
Nucleus
Cell
DNA Incorporation, Repair, and Cell-Cycle Interaction
dFdC
dFdCP
dFdCTP
dFdCDP
dFdCMP
NT
cellular response
concentration of active agent at target (organ tissue / tumor)



Drug Delivery Systems
performance formulations with triggered and/or retard release

Diagnostic Systems
array-, biochip-, biomarker- and enzyme technologies



Systems Biology
modeling and simulation of biological systems (genomics, proteomics, disease biology and bioinformatic data mining)

… and Many More Exciting Challenges !

- **shift from petroleum to renewable feedstocks**
  - reinvent chemicals and fuel supply chains
- **infrastructure systems**
  - energy, water, waste, and transportation networks
- **small-scale production**
  - market-driven, evolutionary design during production
- **disposable process-units**
  - in life-science applications
- **etc. etc. etc.**

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Industrial Requirements – R & D (1)

- **Industrial end user's common opinion**
  - topics in scientific publications > 80% the same than 20 years ago
  - too much incremental improvement of with no or little economic impact.

  Even if this may not really apply, it is alarming that this impression occurs!

- Any new method has to be **benchmarked** against state-of-the art best practice both from an economic and technical point of view.

- We need more modern, **computer-based short-cut methods** to pick the low hanging fruits.
  - Most plant managers are only willing to support longer lasting projects if they get at least some benefit rather quickly.

- More attention has to be paid to the integration of design and control.
  - acutally no formal method which is suitable for application in industrial practice.

Industrial Requirements – R & D (2)

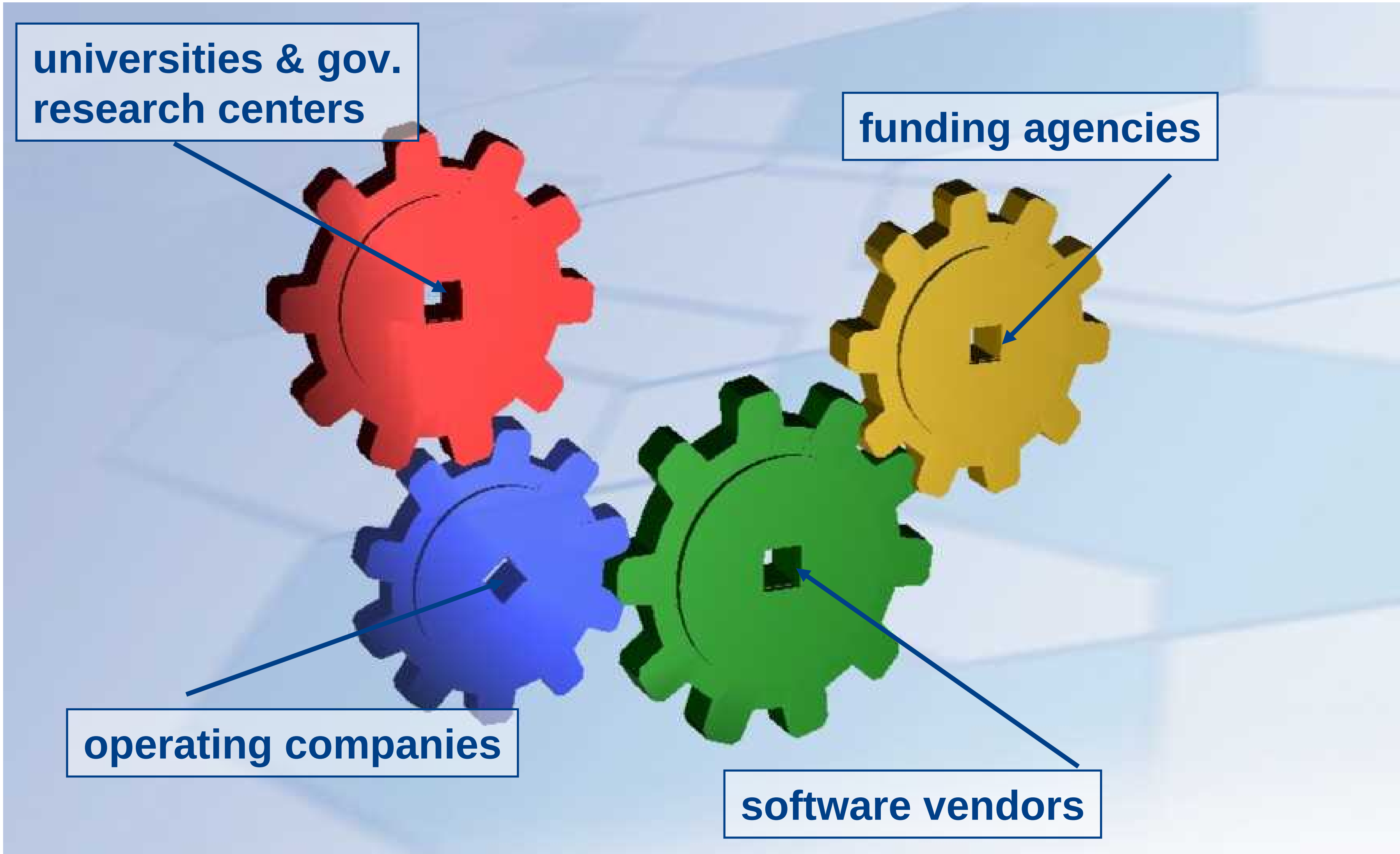
- Process Systems Engineering has to **increasingly address the new challenges** arising e.g. from nanotechnology, systems biology, functional products, …..

- **New fields of application** require (at least in parts) a fundamental adaptation of methods and tools:
  - no simple transfer of the methods and tools established in the area of large-scale continuous production of bulk chemicals to the life science area,
  - customized solutions for batch processes, small scale productions and multipurpose plants which result in reasonable payback times

… but keep it smart and simple !

- The **model-based methods** both have to be enhanced further and made available to a larger number of users.

Cooperation – the Key to Progress



RWTH

Cooperation – the Industrial Perspective

BAYER

- The main reason for the commonly addressed **gap between industrial practice and academic research** seems to be the different scope:
  - industry: economic profit
  - academia: scientific progress

  Note: The mere existence of a technical solution doesn‘t guarantee it‘s profitability in routine industrial problem solving.

- It is a challenging task not to let this gap grow but to benefit from this complement.

- We need consistent co-operations between academia and industry. This is challenging, especially in times of budget shortage.

- To guarantee a sustainable success of PSE in industrial practice, a closer co-operation between academia and industry is necessary … … and also in engineering education.

Outline

- What is the nature of **process systems engineering** ?
- Which **research topics** have been dealt with in the past 50 years ?
- What has been absorbed by **industrial practice** ?
- Which **research trends** are emerging ?
- What are the **industrial requirements** for the future ?
- What is the **future of process systems engineering** ?

Strengthen Classical Fields of Activity …

… even if does not look like a trendy hot topic

the classics …

- modeling, numerical methods and software tools
- product and process design
- control, operations and production management

… but benchmarking with established methods

back to the roots …

- focus on methods development
- emphasize systems approach, the use of computers is not sufficient
- horizontal and vertical extension of system boundaries

task integration along development lifecycle

- product and process design
- process control and operations
- …

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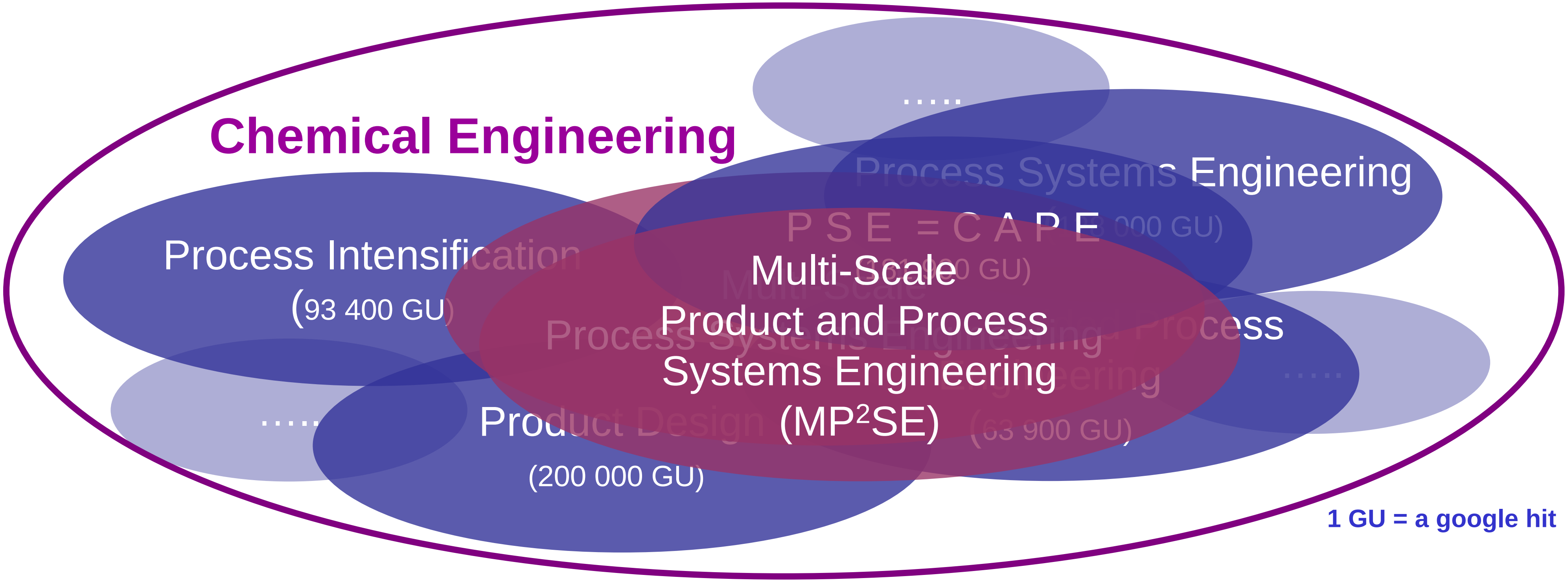
… but reach out at the same time

integrate available methods in PSE toolbox and

adapt PSE toolbox to related systems problems

Desirable Mergers to Strengthen our Field

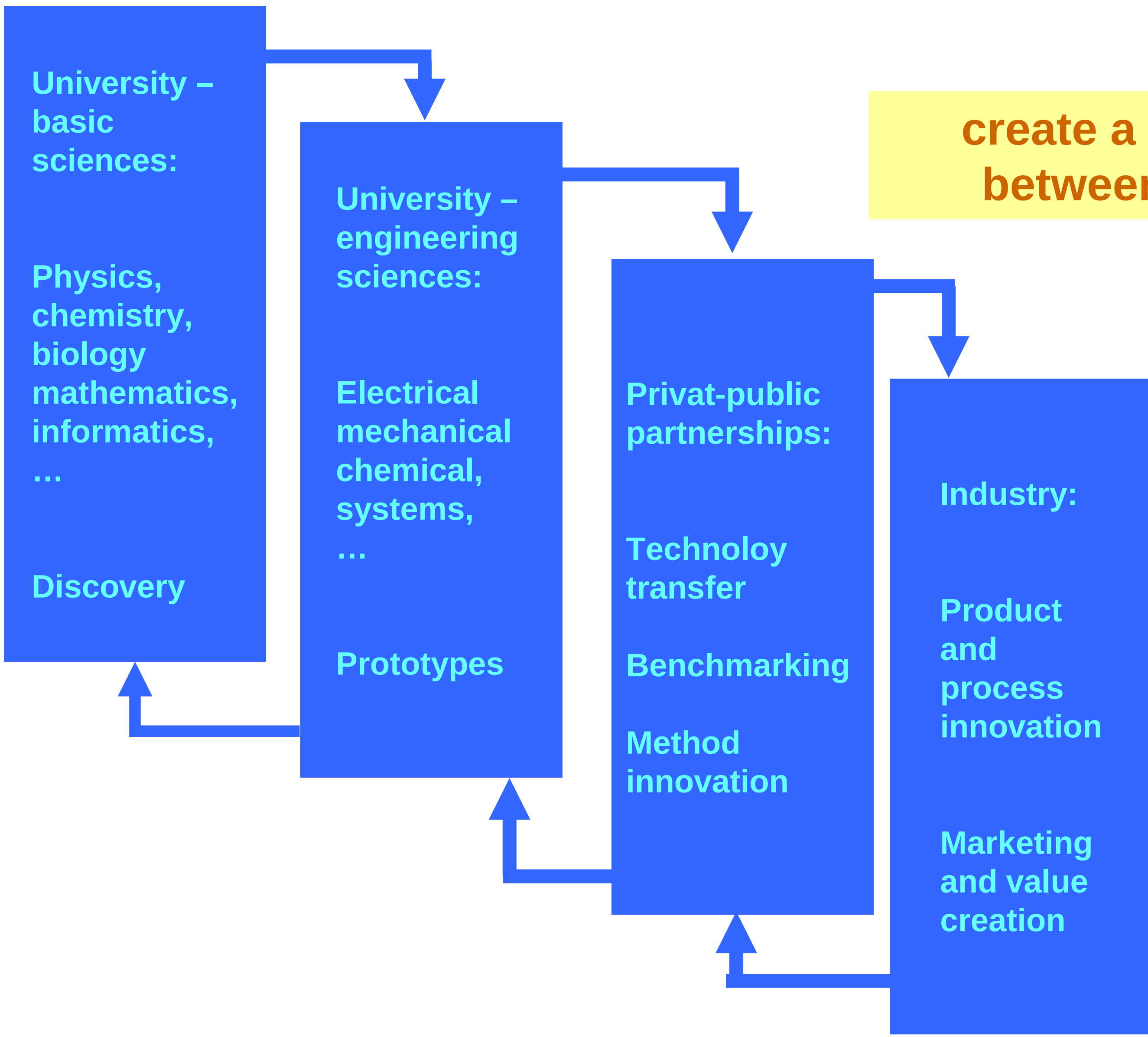


As the scope of process systems engineering has widened, so it has become more diffuse, and it is more and more difficult to define its boundaries or identify an essential core or expertise. … an area which cannot be adequately defined risks loosing its appeal.

R.W.H. Sargent, 2004

Build Value Driven Innovation Networks

create a push-pull situation between all stake holders



Five Summarizing Theses

1. **PSE** has significantly contributed to **scientific progress and industrial practice** in the last 50 years, in particular in modeling, simulation and optimization methods and tools.
2. **PSE principles** form a core element of chemical engineering education and practice.
3. **Research in PSE** should
   - focus on methodological basis with a long-term perspective
   - provide its expertise to solve "non-traditional" systems problems
   - contribute to and drive progress in "non-ChemE" application domains.
4. **PSE** has to strengthen its position as a scientific discipline through collaboration within and outside ChemE.
5. **PSE methods and tools** have to further penetrate industrial practice through a balanced push-pull collaboration effort.

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… a bright future, if WE actively shape it !