Applications of Artificial Intelligence in Process Systems Engineering

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"Computer Science is now reaching out to other disciplines. You see this in Engineering, Biology, Chemistry, Physics, Mathematics, Business, Psychology, and Philosophy... The symbolic processing of information is something that has interest by itself but also has something to say about the way that information is processed in all disciplines. These new contacts will be both a source of inspiration and a challenge for Computer Science..."

Nico Habermann, 1932-1993
The first Dean of the School of Computer Science
at Carnegie-Mellon University

Let us try to promote the contacts!!

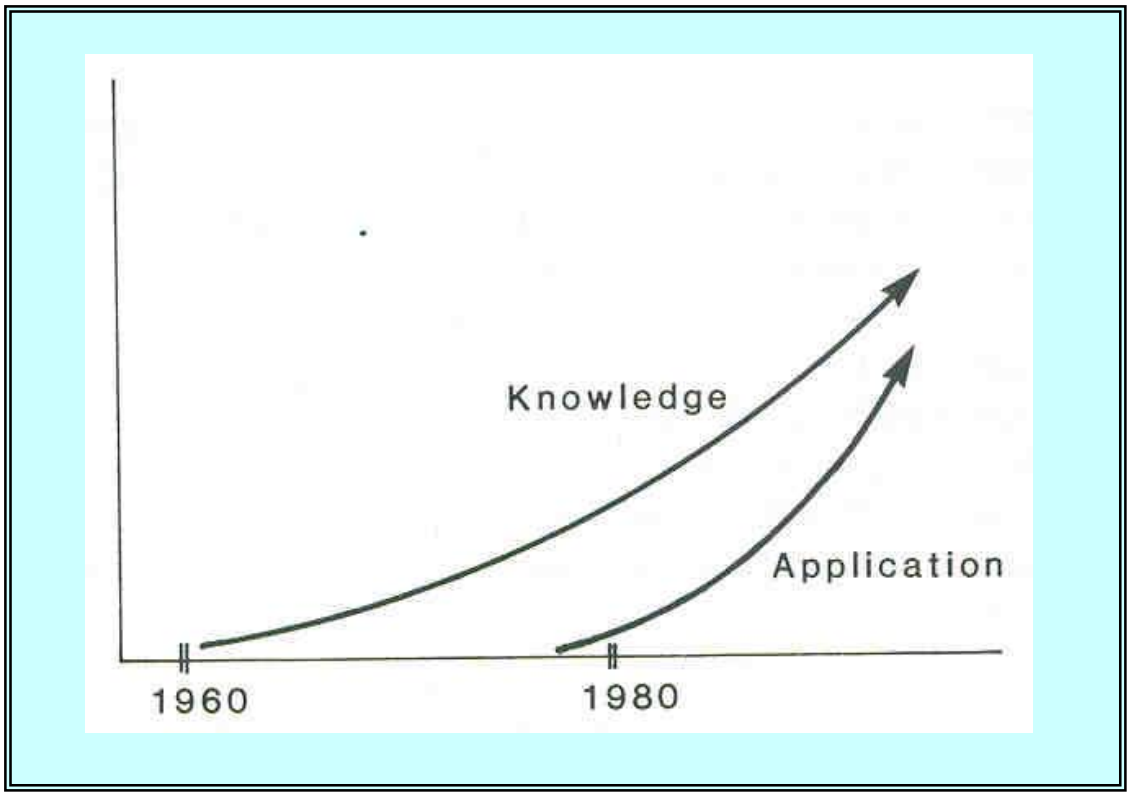
Old dreams and thoughts of the AI community

- *"To build a scientific model of intelligence, one that would capture the architecture of the human mind" - A. Newell.*
- *"At the heart of the methodology of artificial intelligence is symbolic reasoning" - P. Winston*
- *"The primary goal of artificial intelligence is to make machines smarter" - P. Winston*
- *"Basic AI components: symbolic computation, heuristic methods, human problem solving" - P. Hayes-Roth*

AI community old antagonisms

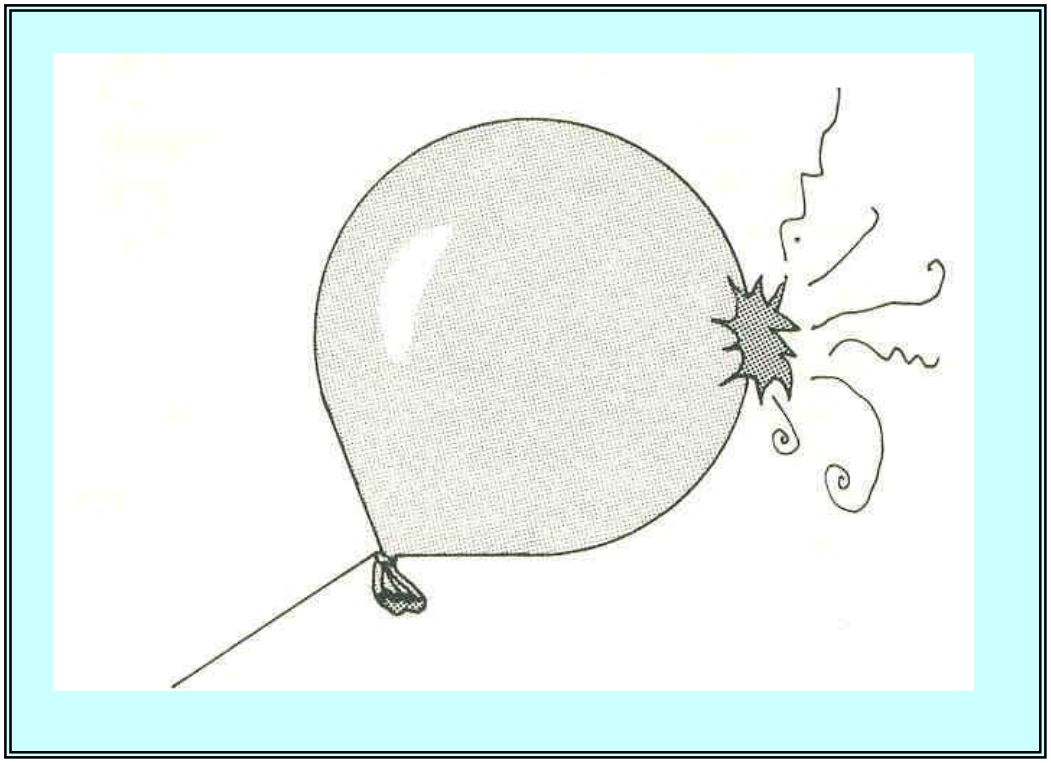
Knowing what	*Knowing how*
Logic-based representation of knowledge	*A program/implementation that implicitly uses knowledge*
Symbolic	*Numeric*
LISP	*PROLOG*
. . . . .	*. . . . . .*

A possible model of progress - Case 1



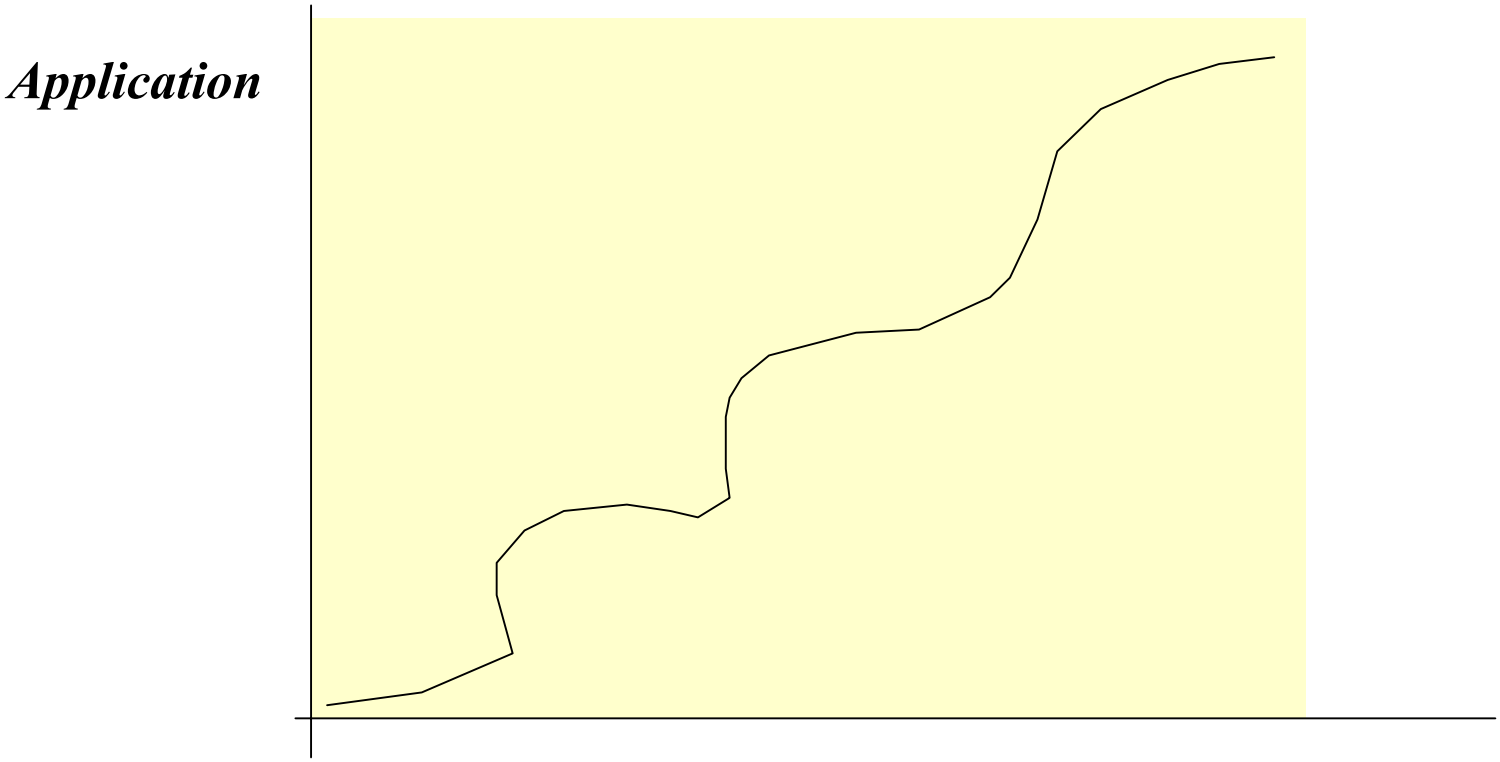
Stinction Model

A possible model of progress - Case 2



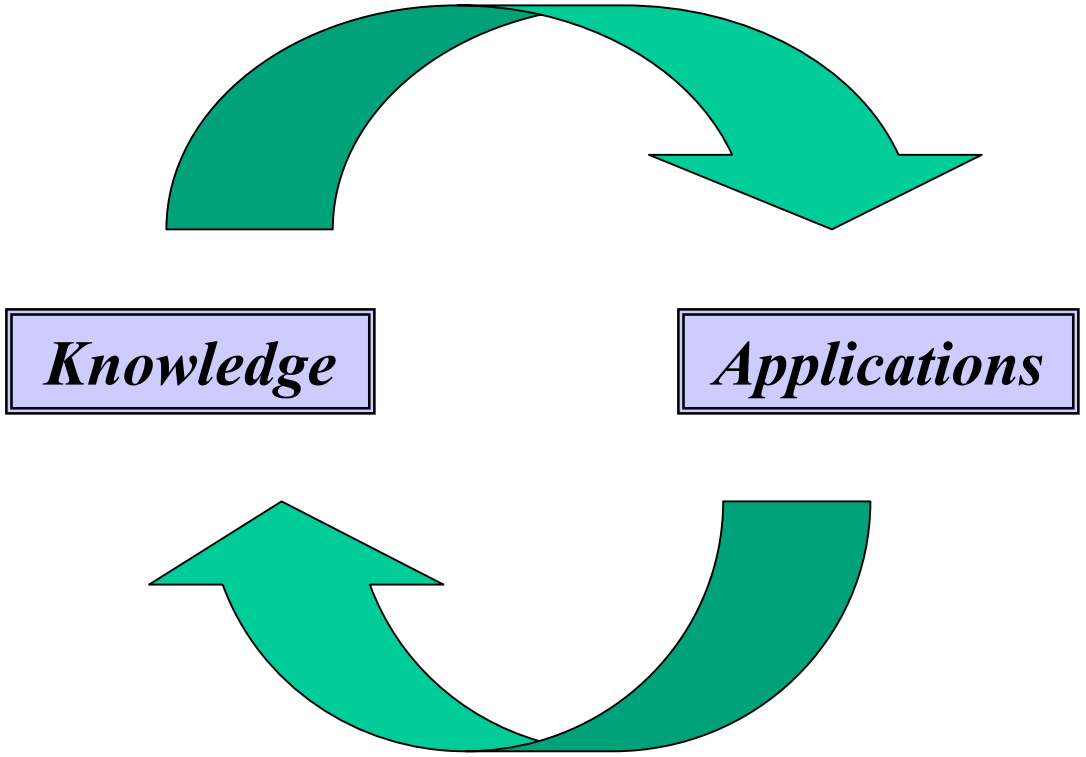
Balloon Model

A possible model of progress - Case 3



Which model applies to Process Systems Engineering and other engineering fields?

The way of progress



AI Applications in Process Systems Engineering

Product and Process Design

- *Design of molecules having desired physical properties*
- *Design of chemical and biochemical reaction pathways*
- ***Synthesis and design of processing systems***

Process Operations

- *Synthesis of operating procedures*
- *Identification and process trend analysis*
- *Fault diagnosis*
- ***Scheduling of batch processing systems***
- *Process control*
- *Supply Chain Management*

AI Applications in Process Systems Engineering

Old Perspective

- *Automate tasks → Replace experts.*
- *Select one among competitive solution methodologies.*
- *Keep AI-based systems isolated from other conventional computer systems.*

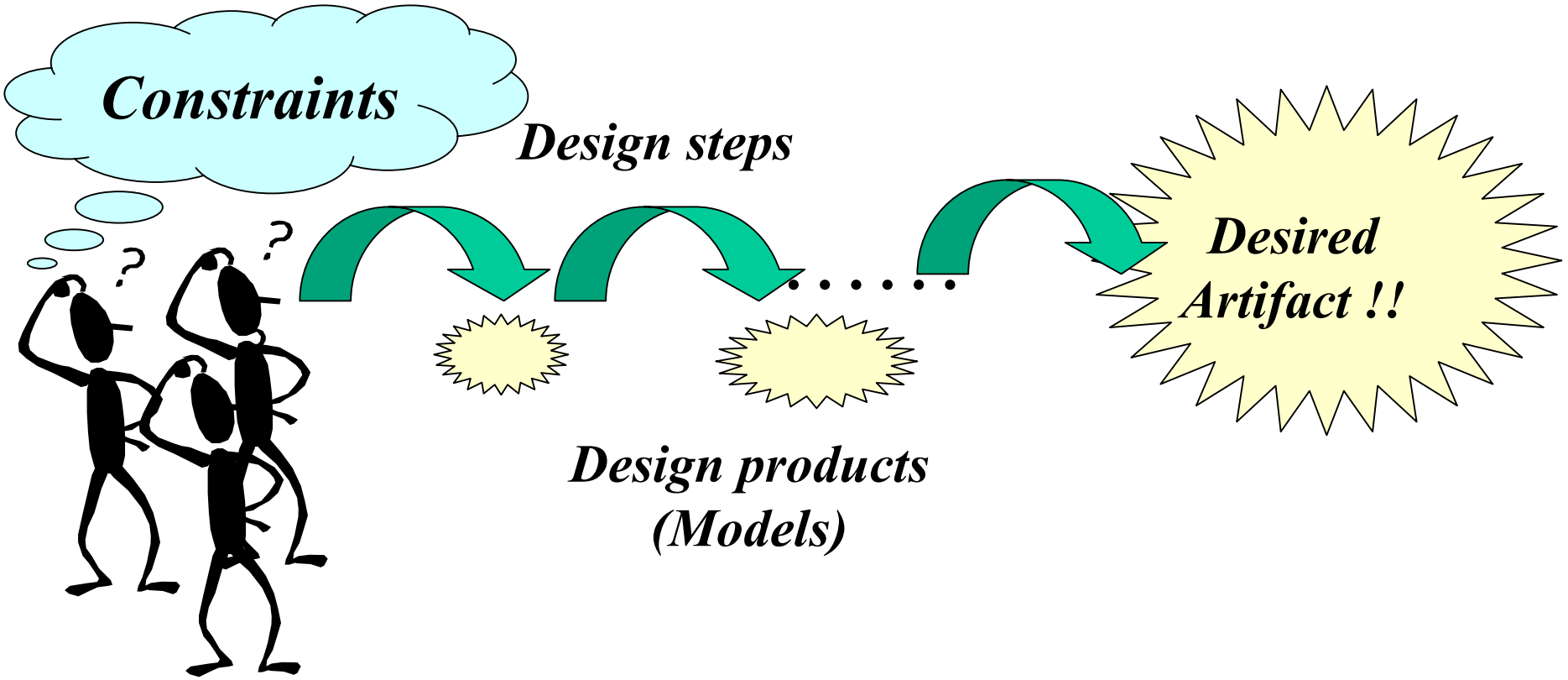
New Perspective

- *Provide computer support to the human user, enhancing his/her capabilities.*
- *Integrate different solution approaches.*
- *Integrate AI-based systems with conventional ones.*

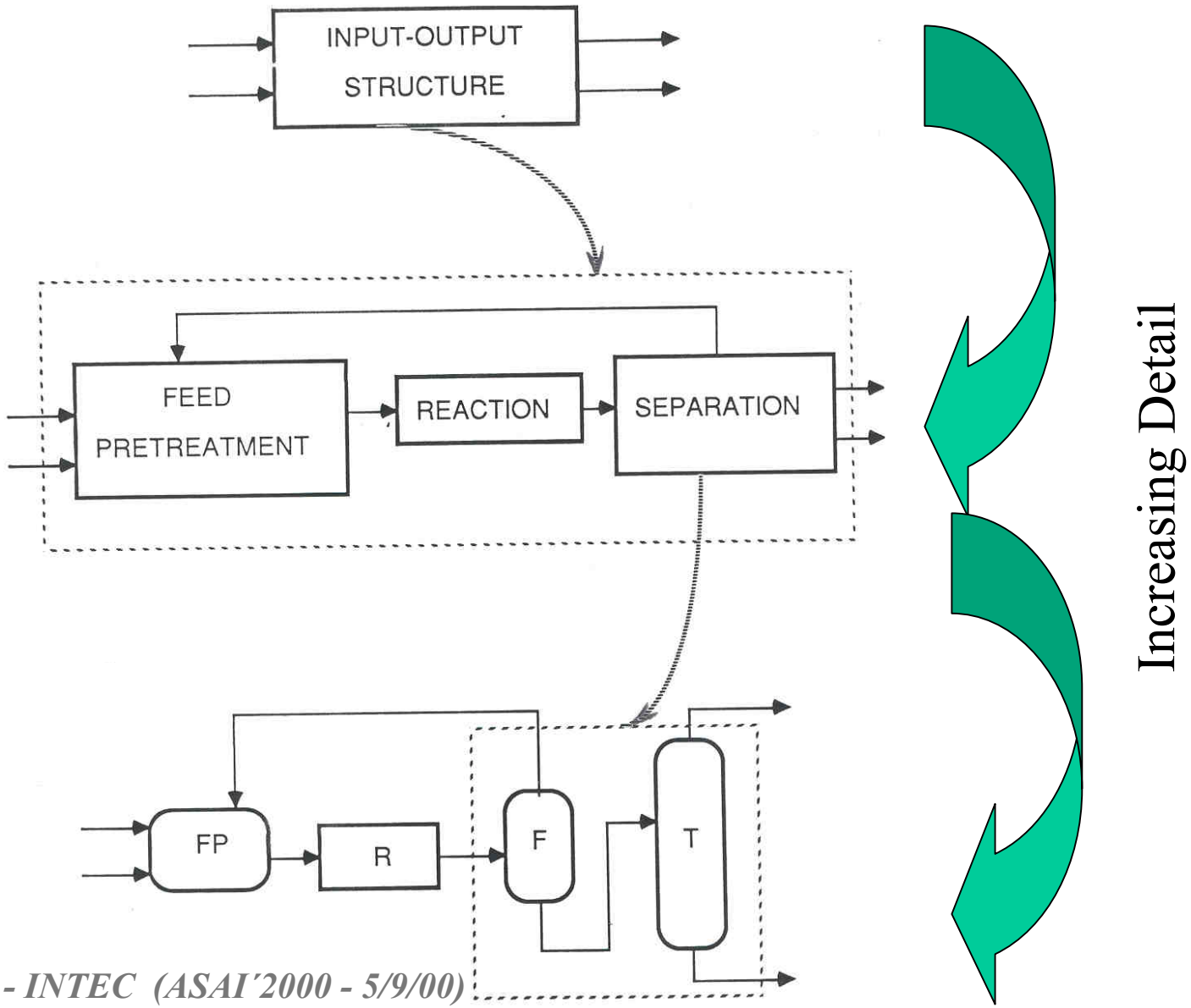
Design of Molecules having Desired Physical Properties

- *Atoms → Functional Groups → Molecules with distinct behaviour: pesticides, refrigerants, solvents, etc.*
- *Requires to efficiently search in a space of combinatorial alternatives in order to identify the molecules which satisfy the desired constraints on a set of physical properties.*
- *A combination of chemistry, engineering, AI and discrete mathematics allows the generation and screening of new molecular structures in a man-machine friendly interaction environment.*
- *Cranium: A commercial package.*

The Process Design Process



The Evolutionary Process Design Process



The challenge of supporting process design activities

Challenges of the design problem:

- Design is characterized as a creative, ill-defined and very complex task, which is poorly understood.
- Activities of model creation, model solution, results' analysis and decision-making continuously interplay at several levels of abstraction.
- The design process generally proceeds in a top-down fashion. However, the evolution is not always linear.
- Several designers participate in a design project.
- Need to: Explore alternative solutions.
  Consider several objectives.
  Combine symbolic and numeric knowledge.
  Trace the solution process!!

How to support the synthesis and design of processing systems?

- ***Development of high-level modeling languages able to automatically generate the mathematical model of processing artifacts.***
  - ***Use of phenomena -based natural languages.***
  - ***Use of graphical environments.***
  - ***Incorporation of symbolic processing capabilities.***
- ***Modeling the design process itself. It involves:***
  - ***Modeling the structure of design tasks.***
  - ***Representing design decisions associated to each task (assumptions, simplifications, etc.).***
  - ***Modeling the state of the evolving design.***

Characteristics of a modeling language

Reactor X is a two liquid phase jacketed CSTR

Interpreted as

- ***Reactor X is composed of two sub-systems: jacket and continuous stirred-tank.***
- ***The reacting mixture in the stirred tank is made up of two liquid phases.***
- ***There is mass transfer between the two liquid phases.***
- ***There is heat transfer between the reacting mixture and the jacket.***
- ***Materials enter and leave the reactor through convective flows.***
- ***Enthalpy enters and leaves the reactor through convective flows.***

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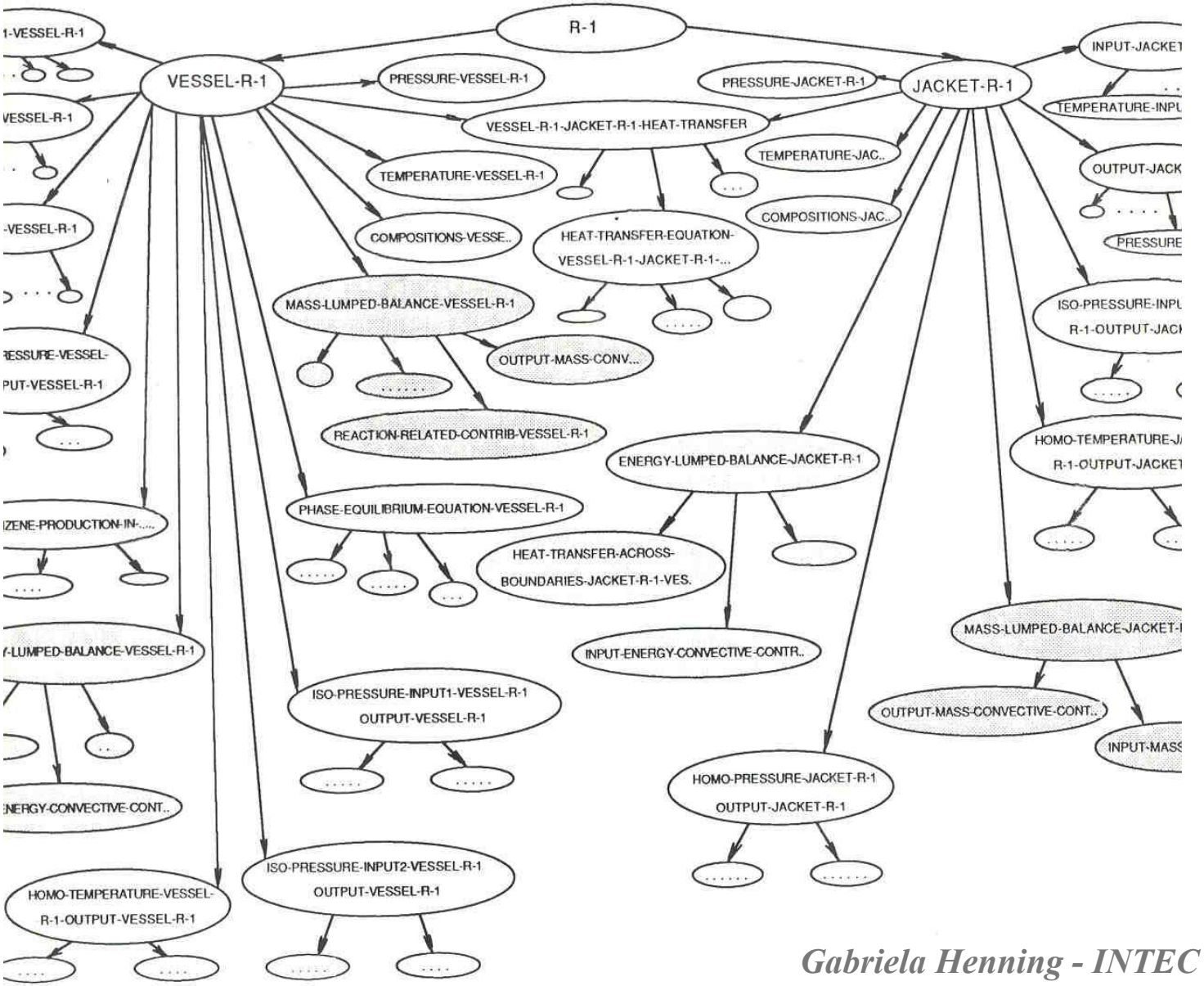
Translated into

Heat and Mass Balance Equations that are automatically created and can be symbolically manipulated

Obtained Object -Oriented Model



Desired features of a system for computer-aided design

- ***Knows** the basic design methodology and its rationale.*
- ***Can carry out automatically***
  - *– Design reasoning*
  - *– Design computations*

  for routine tasks.
- ***Knows** how a design was carried out and why.*
- ***Interacts with humans at a high level in cooperative design environments.***
- ***Interacts with other conventional systems.***

Capturing engineering design rationale

- *Engineering design entails the generation, evaluation and selection of alternatives. Then, the design rationale is of vital importance to the documentation, analysis, verification, auditability and reusability of the decision process and the resulting design (models of the processing systems).*
- *DRAMA - Design RAtionale MAnagement, is a software package that allows engineering design rationale capture by using an extended form of IBIS to record:*
- *WHAT decisions are made*
- *WHEN they are made*
- *WHO made the decision*
- *and WHY*

Scheduling is another challenging problem !!

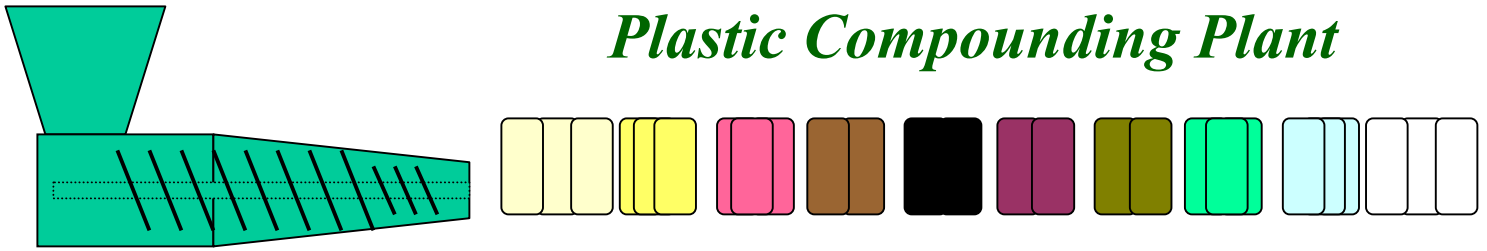
- *Scheduling is also an ill-defined problem.*
- *The solution methodology needs to address the characteristics of the processing system (flow-shop, job-shop, etc.), the customer orders' attributes, the required set of resources, and the pursued objectives.*
- *Many techniques and methodologies originated from AI have been proposed: expert rules, genetic algorithms, neural-networks, constraint-satisfaction techniques, etc.*
- *Scheduling is a dynamic problem: Once a schedule has been adopted, there are unexpected circumstances that may force its revision, leading to the reactive scheduling activities.*

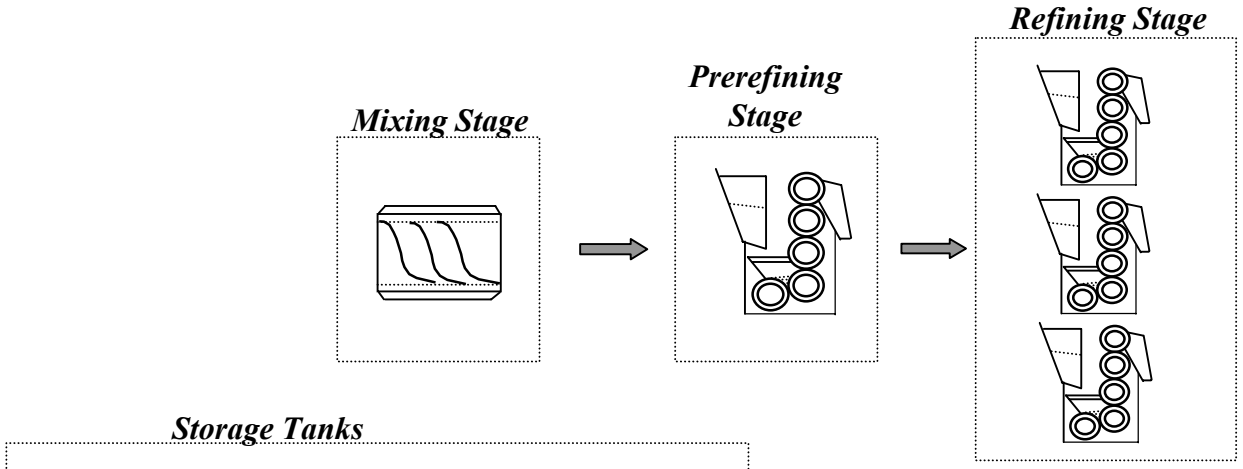
Knowledge-based approach to the solution of real world industrial scheduling problems

- *Three real industrial scheduling problems were addressed by building knowledge-based support systems.*
  - *A Plastics' Compounding Plant*
  - *A Candy Facility*
  - *A Chocolate Paste Production Plant*
- *The systems where built using a hierarchical decomposition of the problem and a task-based approach. An explicit object-oriented representation of the domain has been adopted.*
- *Two of the systems are used with daily frequency.*

Scheduling Problems - Schematic Lay-outs

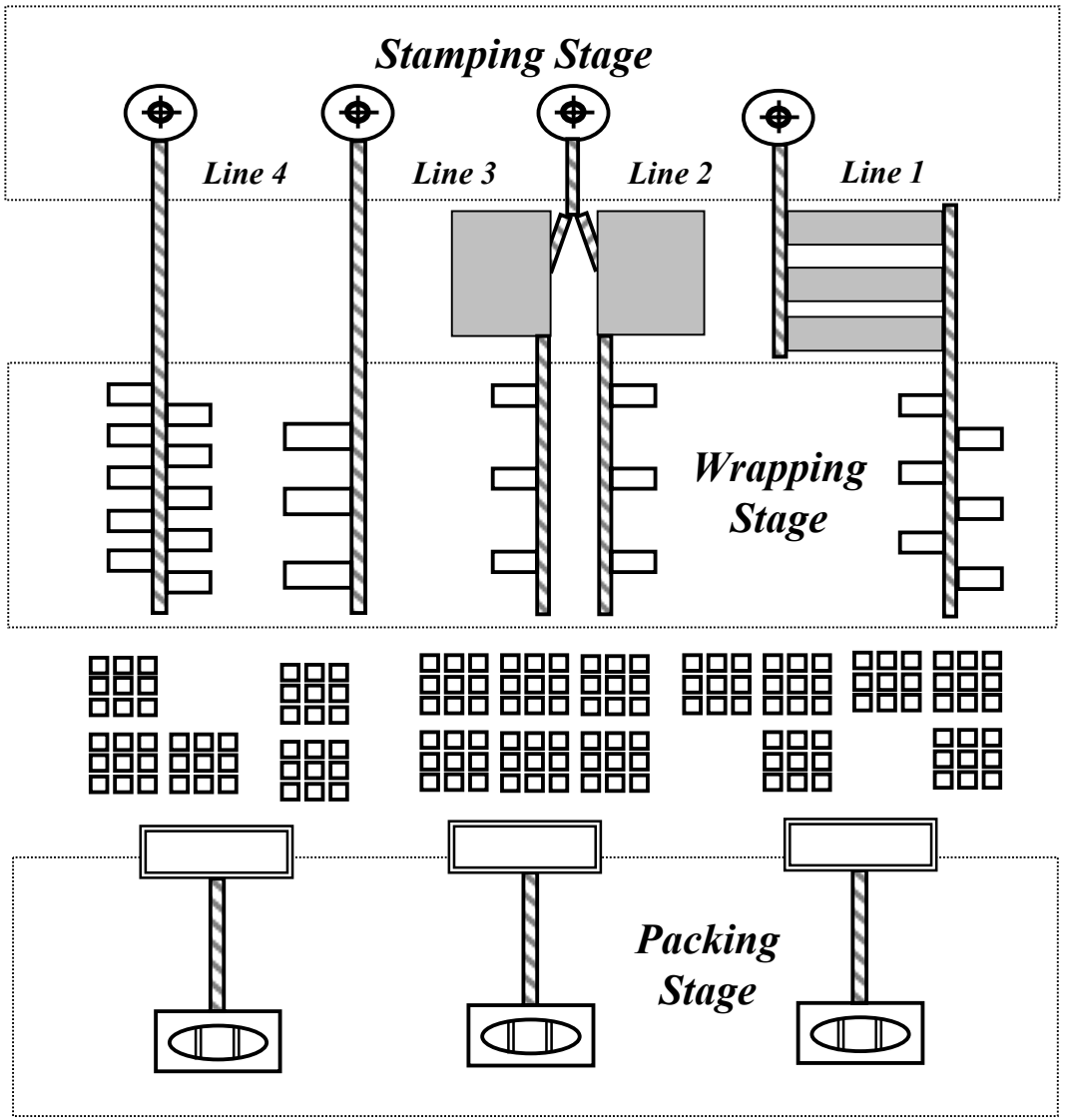
Plastic Compounding Plant





Chocolate Paste Production Plant

Candy Production Facility - Schematic Lay-out



Knowledge-based approach to the solution of real world industrial scheduling problems

- ***Lessons that were learned***
  - ***Scheduling problems are inherently ill-defined and dynamic.***
  - ***Scheduling tools should be integrated with other support tools.***
  - ***Scheduling methodologies should handle resources (renewable and non-renewable)***
  - ***The scheduler wants to play an important role in the solution process → Need for interactive tools.***
  - ***Discovery of new problems.***
- ***Results***
  - ***Design of a knowledge-based environment for the development of scheduling systems for multi-product plants.***

Desired features of a Scheduling Support System

- *Enhance the problem-solving capabilities of a human domain expert without replacing him/her.*
- *Capture intricate product models.*
- *Explicitly represent the complex structure of processing networks and their associated operating policies.*
- *Explicitly represent scheduling knowledge, allowing flexible reuse and adaptation of scheduling algorithms as well as expert's compiled knowledge.*
- *Combine different knowledge-based components.*
- *Envision the scheduling function as a knowledge management activity.*

Conclusions

- ***Real-world applications are the best field to test new theoretical developments.***
- ***Besides providing new case-studies they supply new challenges.***
- ***Design and scheduling are challenging fields.***
- ***In many applications, the user should play an active role during the solution process.***
- ***The combination of different solution approaches should be stressed.***
- ***Some real applications are quite different from the ones envisioned by the AI pioneers!!***