The Use of CAPE Tools:
Why, How, for What purposes ?

What is CAPE

What are CAPE Tools

When are CAPE Tools used

Some CAPE Tools Examples

Conclusions

What is CAPE ?

Computers and Chemical Engineering

Process Modeling Simulation and Control (PMSC)

Process System Engineering

CAPE : Computer Aided Process Engineering *application of a systems approach to the study of whole processes and their control, safety environmental protection and utility systems as an integrated whole, from the viewpoints of development, design and operation*

CAPE is also a community of scientists, software providers & software users

What are CAPE Tools ?

Computer Tools Used by Process Engineers ?

- *Artificial Intelligence*
- *Biochemical Engineering, Pharmaceuticals*
- *CAD/CAM, Drafting*
- *Data Acquisition/Management*
- *Data Conversion*
- *Drying*
- *Electrical Engineering*
- *Environmental Control, Waste Management*
- *Equipment Design*
- *Fluid Dynamics, Particle Dynamics, Flow Analysis*
- *Graphics*
- *Heat Transfer*
- *Materials*
- *Mathematics, Statistics*
- *Mechanical Engineering*
- *Network Optimization*
- *Nuclear Engineering*
- *Patent and Literature Search and Retrieval*
- *Petroleum/Gas/Energy Production*
- *Physical and Chemical Properties*
- *Process Control, System Analysis, Automatic Control Process Measurement*
- *Process Design/Simulation*
- *Process Economics, Costing, Investment Analysis*
- *Programming and Software Development Tools*
- *Project and Production Management, Scheduling, Inventory, Maintenance*
- *Reaction Kinetics, Reactor Design, Catalysts*
- *Regulations*
- *Reliability, Failure Analysis, Risk Analysis*
- *Safety, Material Safety Data Sheets*
- *Scientific Word Processing*
- *Separation (Absorption, Distillation, Extraction, etc.)*
- *Software Utilities*
- *Teaching Modules*
- *Thermodynamics*

About 2 000 commercial software tools described in the Chemical Engineering Progress (CEP) Software Directory (AIChE) . . .

CAPE Tools Main Characteristics

- Software tools including <u>*models*</u> of the process
  - *Several levels of complexity depending on the objectives, generally macro-level models*
  - *Models of the process and its behavior*
  - *Models containing <u>knowledge</u> of the phenomena*
  - *“First Principle” Models*
  - *Representation of the underlying physical and chemical behavior of the materials being processed*
  - *Using others technologies: thermodynamics, thermophysical properties, chemistry, advanced IT, costing/economic evaluation or CFD (integrated or interfaced)*

- Tools providing a <u>*global view*</u> of the process
  - *Evaluation within the context of the whole process*
  - *Simultaneous consideration of several aspects: process, control, operability, safety, utility, …(concurrent engineering)*
  - *Integrated development of Products and Processes*

CAPE Tools key-words : MODELS and GLOBAL VIEW

When are CAPE Tools used ?

- Historically: mainly in process design
  - *Flowsheet simulation*
  - *Equipment design & rating*

- Today: at each stage of the Process Life Cycle
  - *Research and Development*
    - *⇒assessment of the interactions between chemistry, thermodynamics,...*
  - *Conceptual and Detailed Design*
    - *⇒development of new process structures*
    - *⇒analysis of the process structure behavior*
    - *⇒equipment design,...*
  - *Operations*
    - *⇒evaluation, tuning and optimization of process performance*
    - *⇒visualization of the plant behavior by operators and management*
    - *⇒safety and environmental impacts,...*

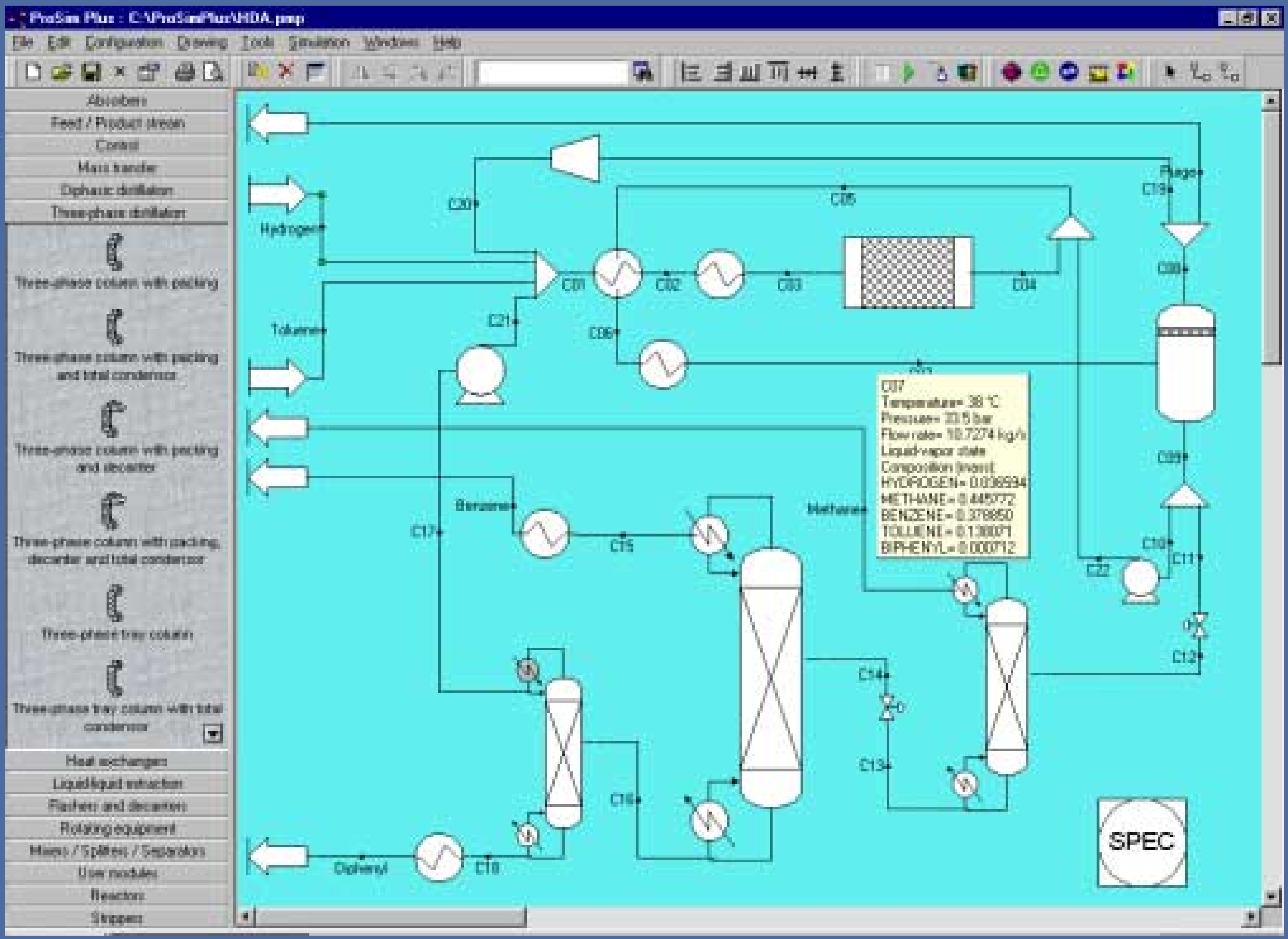
A margin of progress remains in integration, sharing and re-use of models

Main CAPE Tools

- Process simulation
  - *General-purpose steady-state flowsheet simulators*
  - *Batch operation simulators*
  - *Dynamic simulators for operators training, control system validation, operability analysis, safety…*
- Thermodynamic properties
- Process synthesis
  - *Heat Exchangers Networks, Distillation Sequences,...*
- Equipment rating and design
  - *Heat Exchangers, Distillation Columns, Chemical Reactors,…*
- Data Validation and Analysis
- Scheduling
- On-line process performance optimization

And much more...

General-Purpose Steady-State Process Simulator



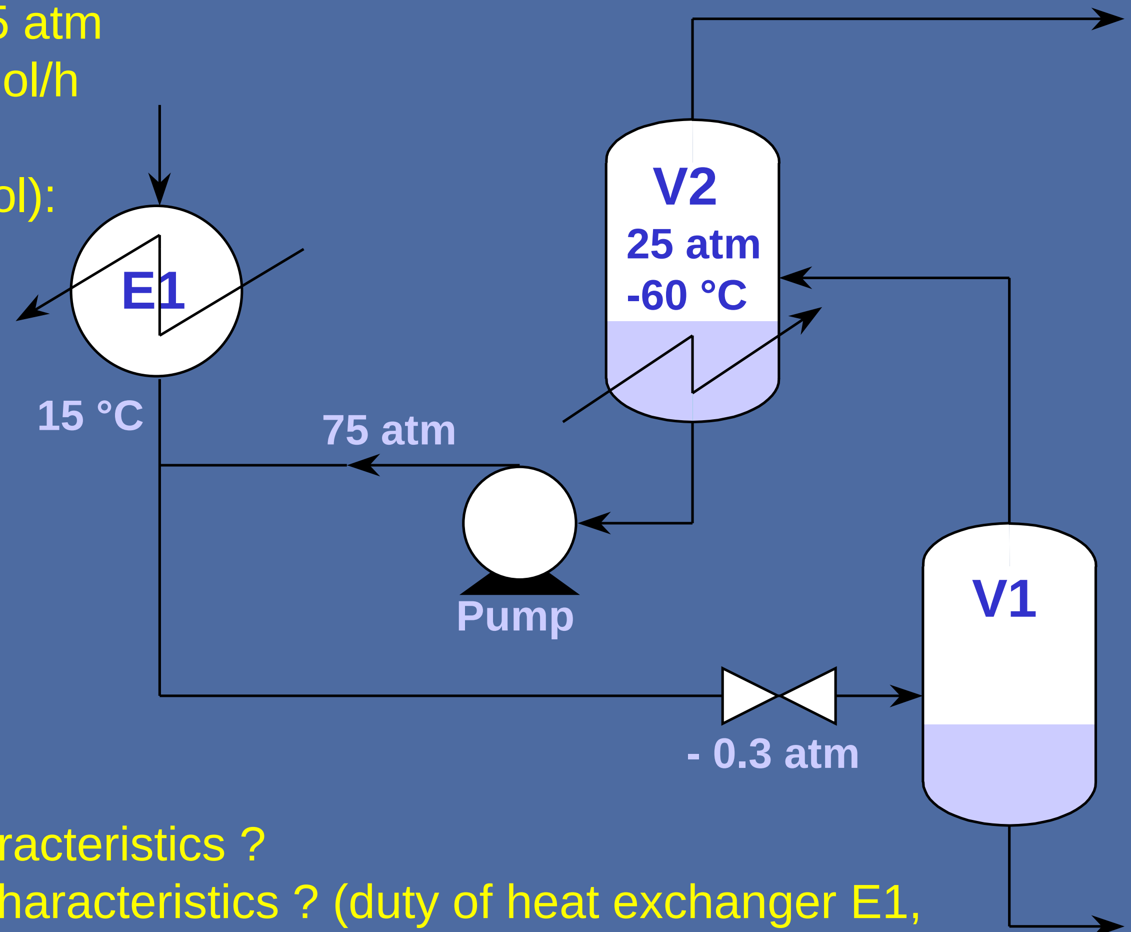
A library of unit operation models (distillation columns, heat exchangers, chemical reactors, pumps,…)

General-Purpose Steady-State Process Simulator: a simple example

Feed
T = 40 °C P = 75 atm
Flowrate = 100 Kmol/h

Composition (% mol):

Nitrogen	9.0
Methane	41.7
Ethane	11.2
Propane	6.2
Butane	5.4
Pentane	3.0
Hexane	8.1
Heptane	13.3
Octane	2.1



Other streams characteristics ?
Equipment items characteristics ? (duty of heat exchanger E1, power of pump, heat to remove from V2,...)

General-Purpose Steady-State Process Simulator

- Performs complete and rigorous calculations of heat and mass balances equations for all the operating units and a whole process
  - *Calculation of all process streams characteristics (flow-rate, temperature, pressure, composition, physical properties,...)*
  - *Calculation of process data required for equipment sizing*

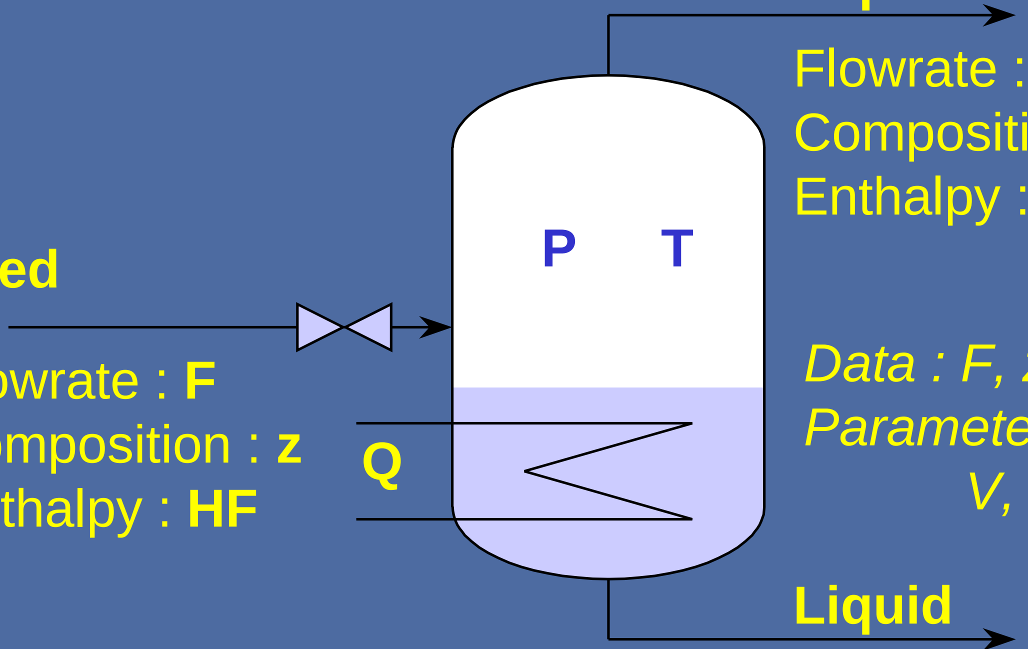
- Typical application in process design
  - *Process flow-sheet design*
  - *Choice of unit operations and of their arrangement*
  - *Sensitivity analysis to operating conditions*
  - *Process evaluation according to several criteria: cost, risk,….*

- Typical application in plant operations
  - *Optimization of operating conditions*
  - *Revamping studies to face new regulations (safety, pollution, ...)*
  - *Debottlenecking of units*
  - *Analysis of operation with new feeds or products quality changes*

General-Purpose Steady-State Process Simulator: example of a flash unit

Feed

Flowrate : **F**
Composition : **z**
Enthalpy : **HF**



Vapor

Flowrate : **V**
Composition : **y**
Enthalpy : **H**

Data : F, z, HF
Parameters : P, T, Q, V, L, y, x, H, h

Liquid

Flowrate : **L**
Composition : **x**
Enthalpy : **h**

General-Purpose Steady-State Process Simulator: example of a flash unit

Mathematical model

(flash without chemical reaction)

- Global mass balance : $L + V - F = 0$
- Partial mass balances : $L \cdot x_i + V \cdot y_i - F \cdot z_i = 0$
- Enthalpy balance :

  $$L \cdot h(T,P,x) + V \cdot H(T,P,y) - F \cdot HF(T,P,z) - Q = 0$$

- Thermodynamic equilibrium relations :

  $$f_i^V(T,P,y) = f_i^L(T,P,x) \quad \text{or} \quad y_i = K_i(T,P,x,y) \cdot x_i$$

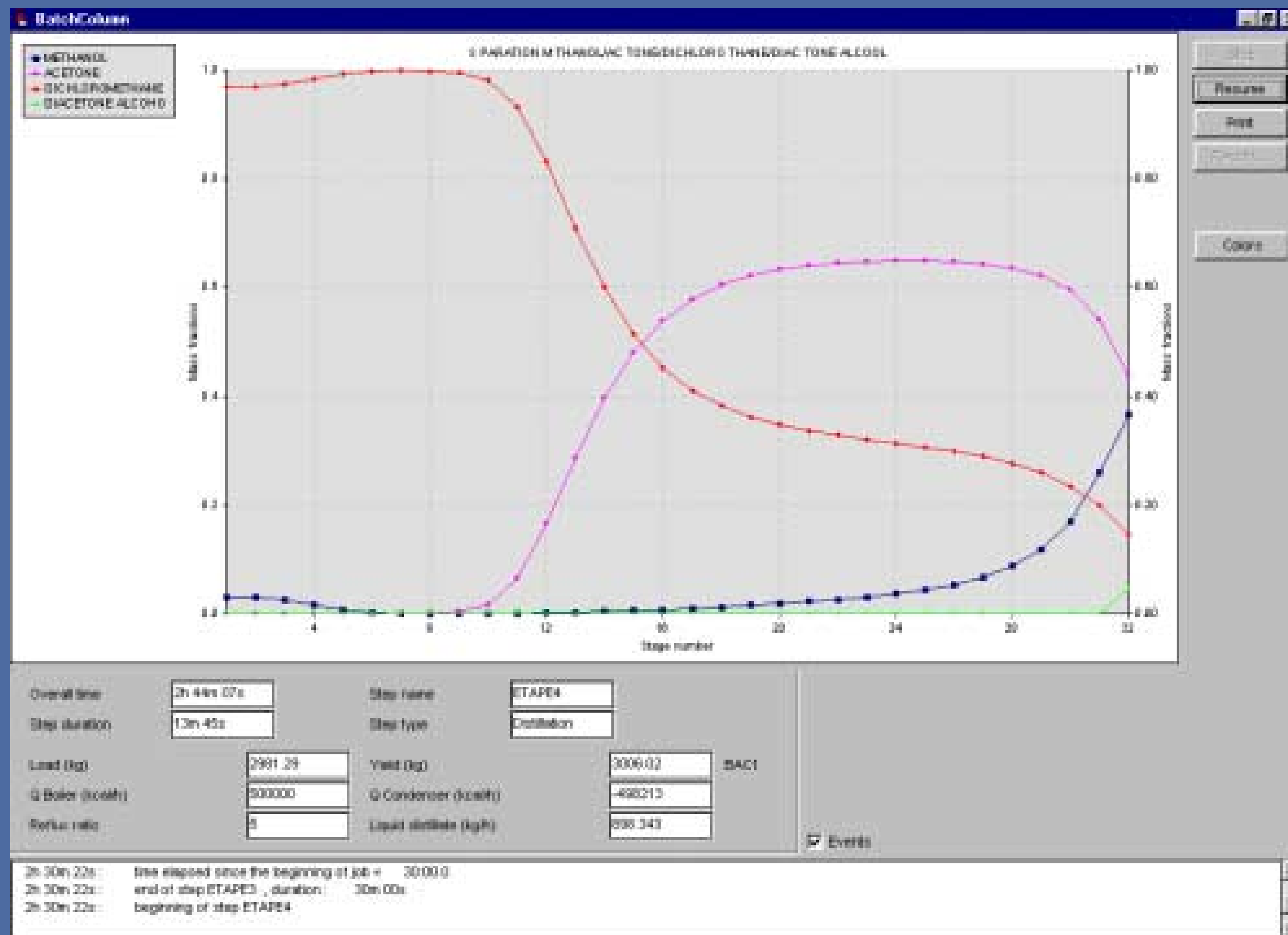
- Constraints : $S\, x_i = 1$ $\quad S\, y_i = 1$ $\quad S\, z_i = 1$

⇨ Thermodynamic models

⇨ Numerical methods

Here a very simple model, but for a whole process including complex unit operations, the number of equations to be solved increase dramatically

Batch distillation columns simulator

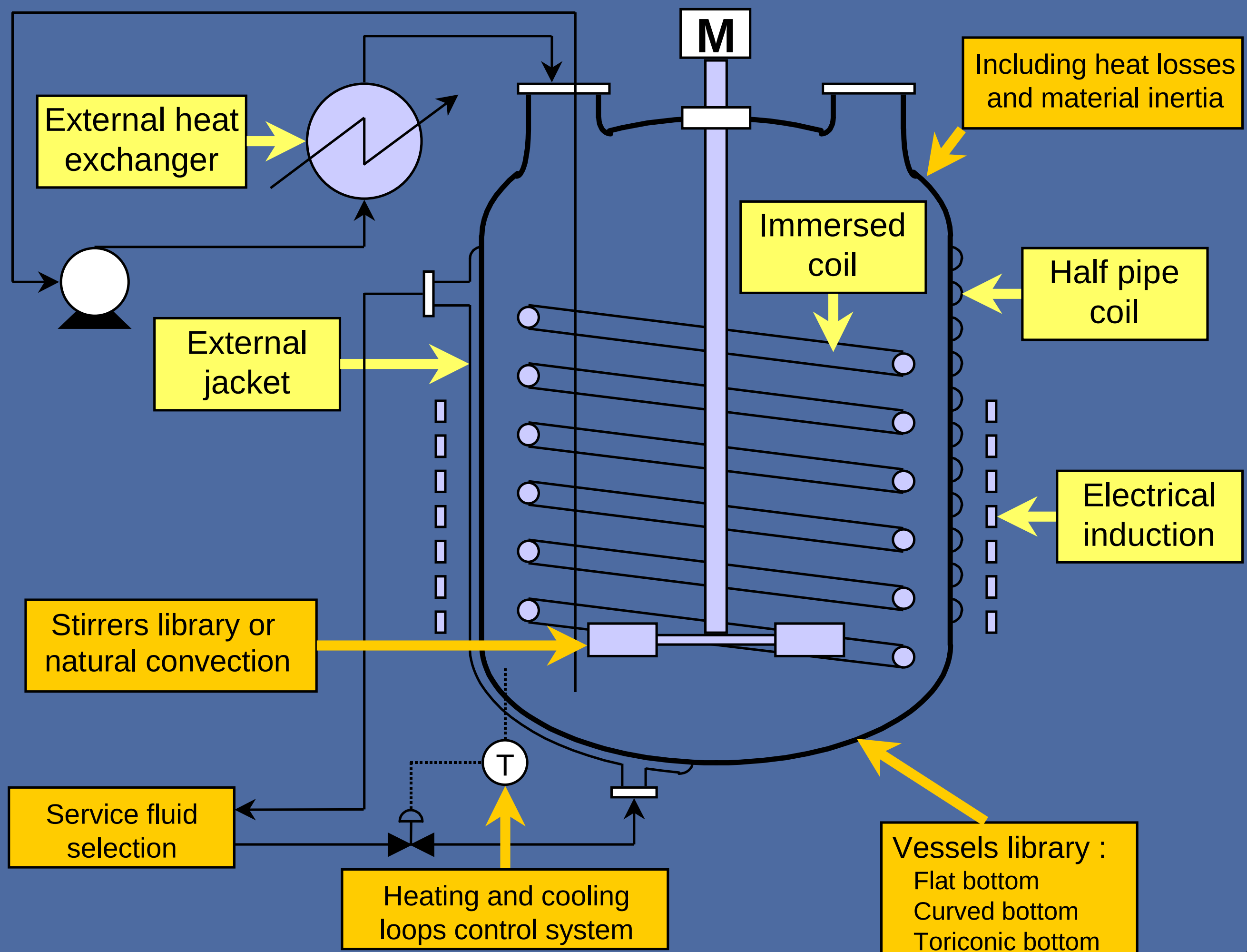


Evolution of parameters with time

Batch distillation columns simulator

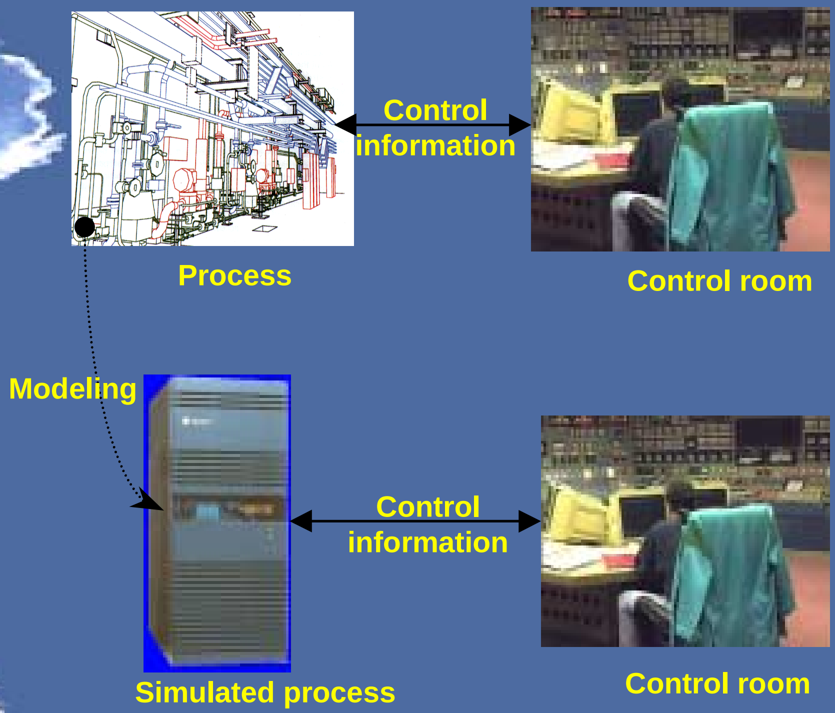
- Typical applications
  - improvement of scale-up phases
  - optimization of operating parameters: reflux ratio, boiler duty, cut-points,...
  - adaptation of an existing column to a new separation
  - definition of control strategies (control top ? bottom ?…)
  - safety studies (what-if the cooling fluid at the condenser stops, what-if the vacuum pump fails, VOC release…)
  - performance of cheap, quick and safe experiments
  - storage of knowledge and understanding
  - etc.

Batch chemical reactors simulator



Several models complexity to address different objectives

Dynamic simulation: example of operators training



- Trainee learn in a safe environment
- Instructor:
  - prepares several training scenarios
  - controls the simulation
  - introduces malfunctions
  - controls the reaction of the trainee
  - evaluates the trainee
- Training is:
  - accurate
  - complete (according to the plan)

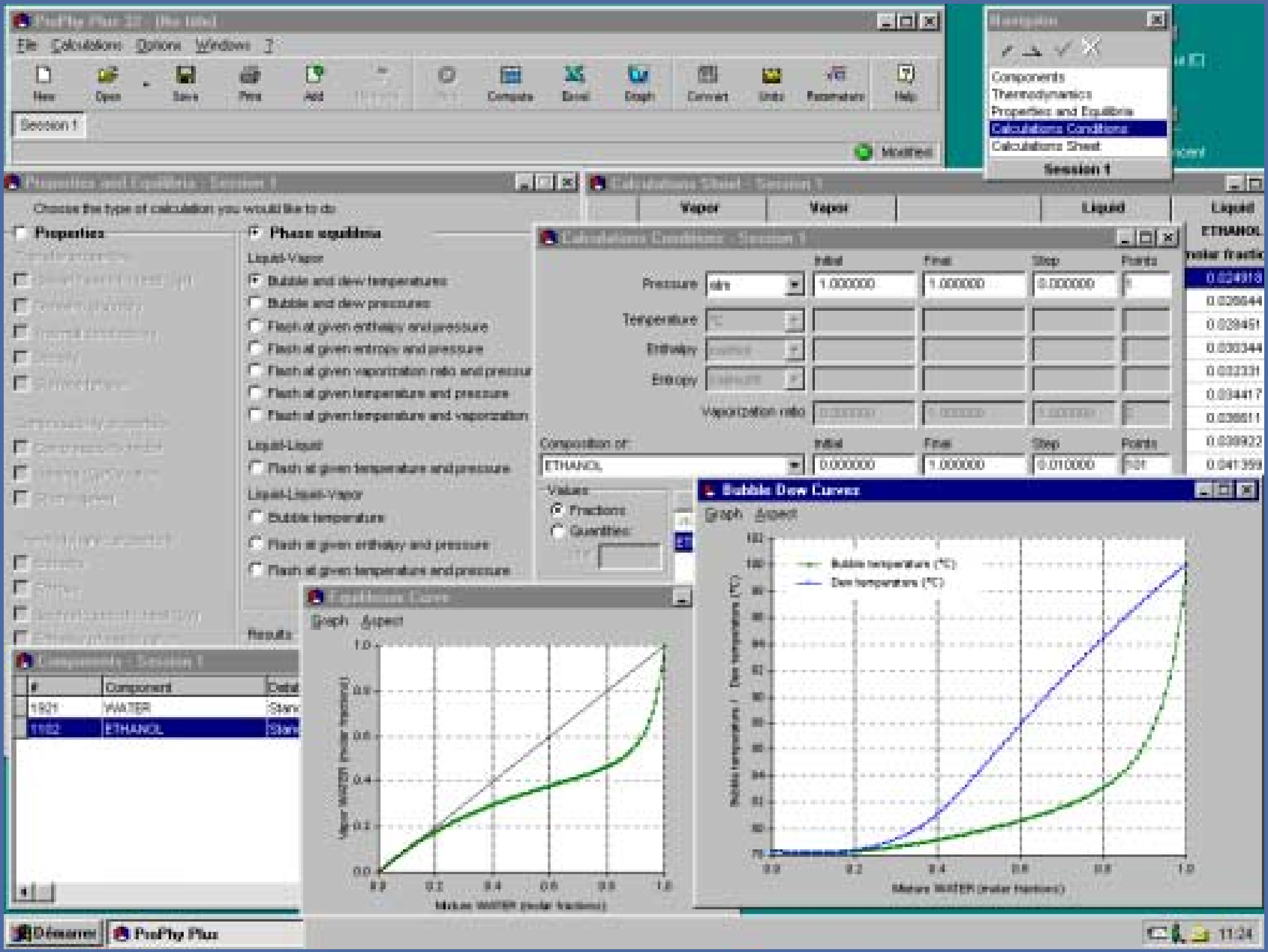
Main characteristics

High fidelity modeling of the whole process

Real time response

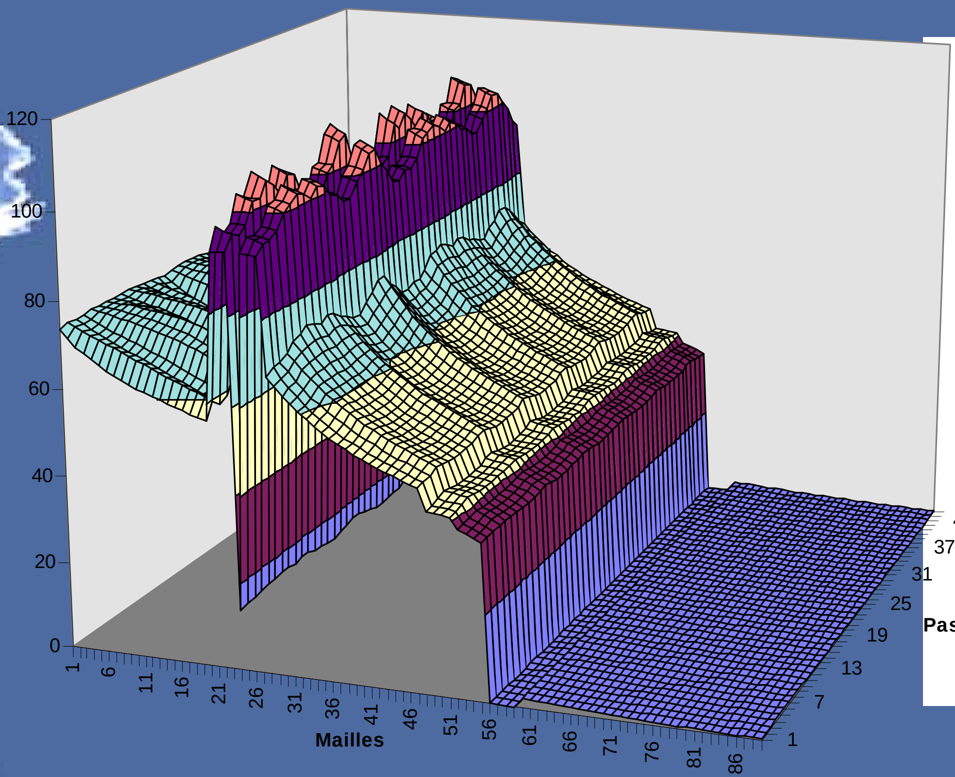
Realistic operating user interface (DCS)

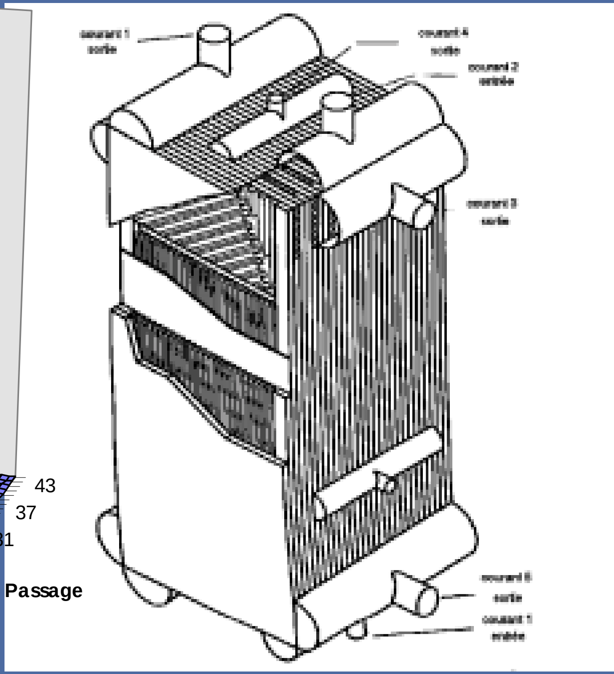
Thermodynamic properties and fluid phase equilibria calculations



Accurate physical properties are key to meaningful engineering results.
A library of models is required (EOS, activity coefficient models,…)

Equipment design and rating: example of a plate-fin heat exchanger

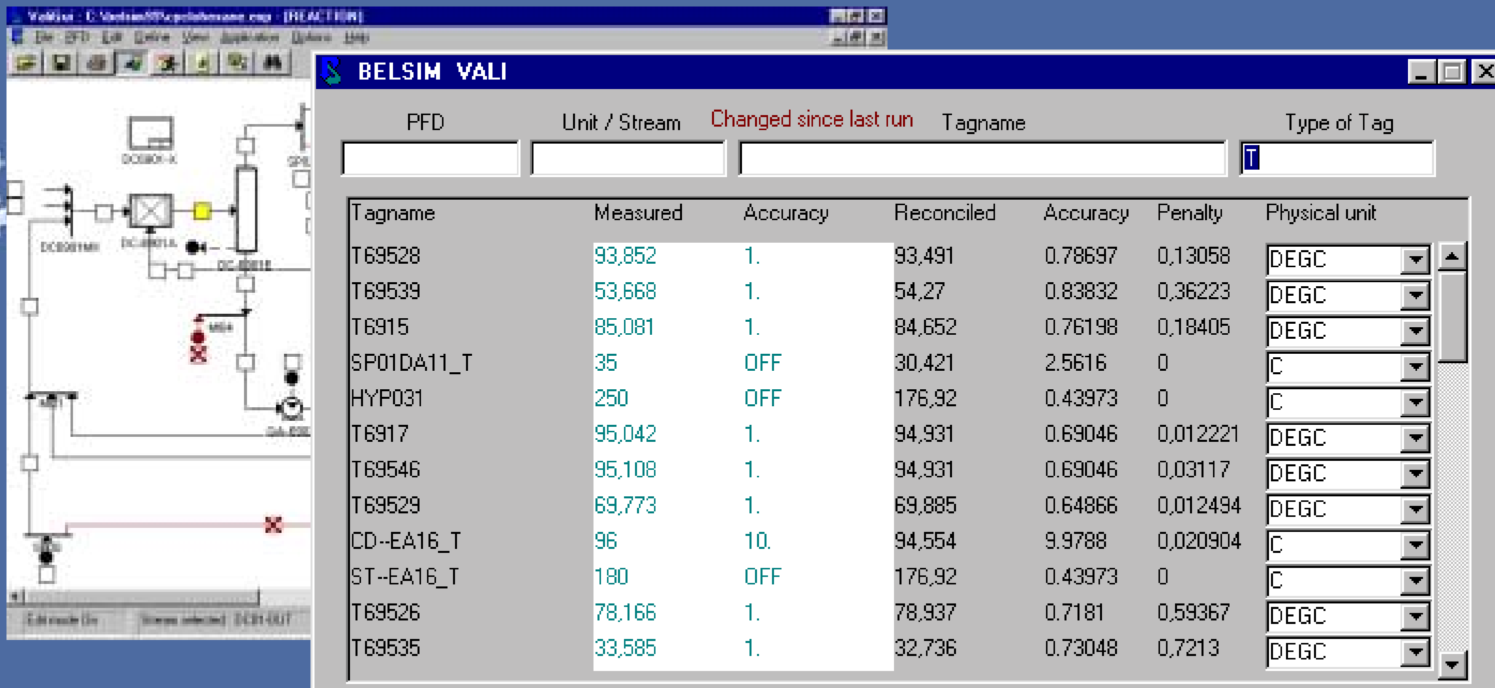




Typical output

- comprehensive information on temperature, pressure drop and flow-rates
- equipment datasheet
- setting plan for exchanger layout
- thermal and mechanical design

Data Validation

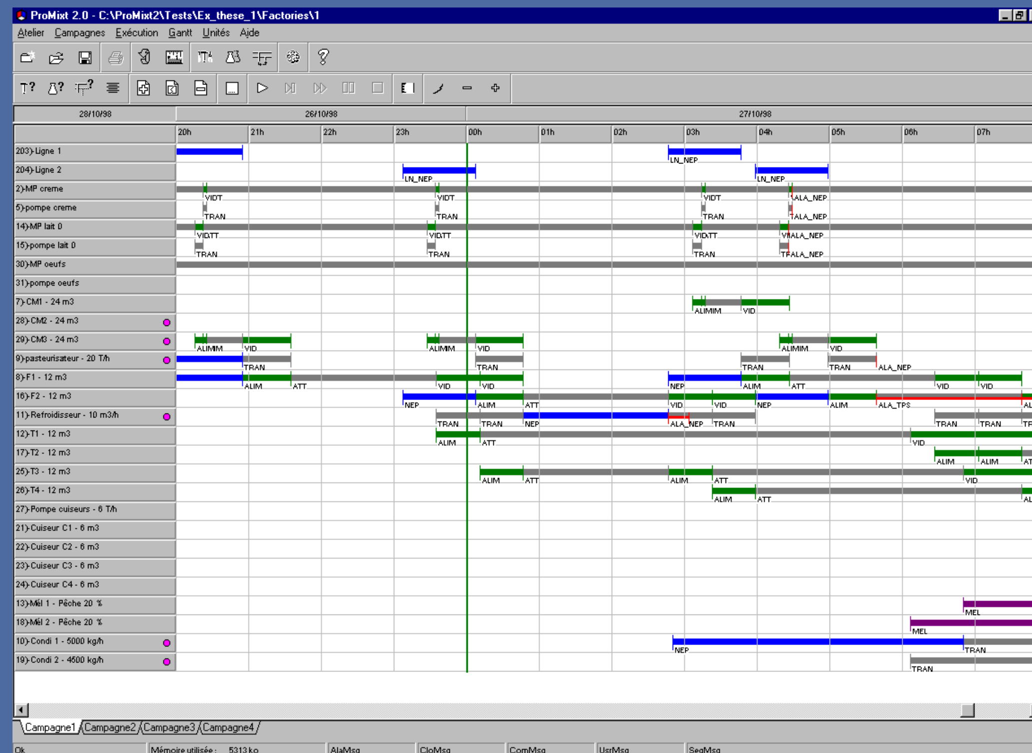


Application

- identification and quantification of instrumentation sensors errors
- access to data difficult or impossible to measure in the plant (soft sensors)
- reliable on-line monitoring of key process performance indicators
- safe operation closer to specifications and operating constraints
- required for on-line optimization

The data produced by the DCS needs to be reconciled

Scheduling

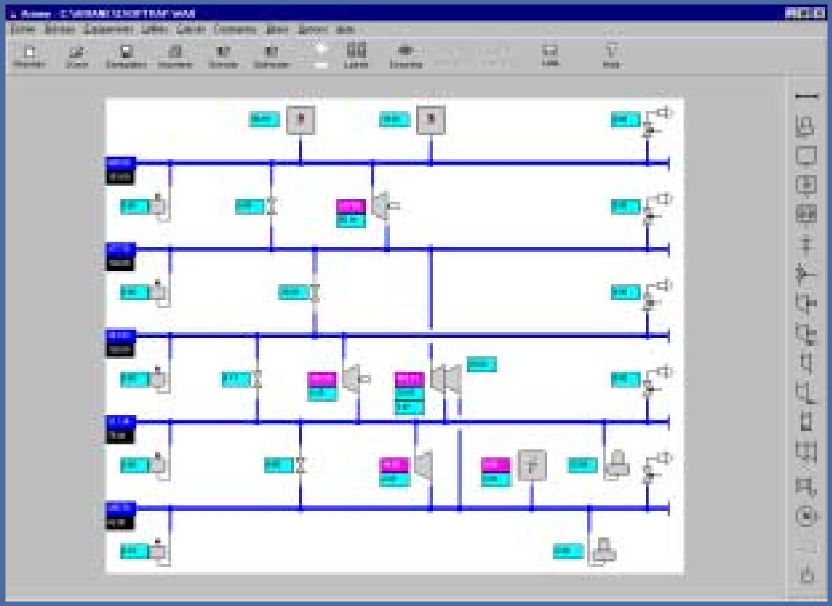


- **Application**
  - recipe-driven batch processes
  - multi-product batch plants
  - optimal schedule
  - analysis of alternative plans
- **Typical results**
  - Gantt chart graphics
  - Use of manufacturing resources: equipment, raw material, utilities,...

On-line process performance optimization

Application

- optimize plant profitability
- increase throughput
- improve quality
- lower operating costs
- minimize feed and processing costs
- operate closer to process constraints
- reduce process and product variability



Methodology

- Process modeling
- Validation of plant data
- Optimization of a technical or economical criteria
- The process model supplies new set points to the operators or directly to the DCS (closed-loop)

Conclusions

- A huge variety of CAPE tools
- CAPE tools are widely and routinely used in process design
- Current trends are toward:
  - re-use of models along the process life-cycle
  - more complex models
- Ready to investigate how micro-phenomena modeling can interface with the macro-level
- Partial answer to the title question *(The Use of CAPE tools: Why, How, for What purposes ?)*