# Process Simulation Techniques

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# Agenda

- Numerical strategies and types of process simulation
  - Equation oriented
  - Sequential modular approach
- Steady state process simulation
  - Procedure and structure of a steady state process simulator
  - Results obtainable and problems involved
- Dynamic simulation

# Numerical strategies and types of PSS

- Equation oriented
- Sequential modular approach

# Mathematical model of a process

Mass and energy conservation balances

$$\bar{f}\left(\bar{x}, \bar{a}, \bar{d}, \bar{p}\right) = 0$$

State variables

Feed variables

Degrees of freedom

System parameters

# Mathematically speaking

- n non linear material balances equations
- 1 energy balance non linear equation
- set of differential - algebraic equations (dynamic simulators)
- In presence of:
  - Many components;
  - Complex thermo-physical models for phase equilibria calculations
  - A high number of subsystems (equipment)
  - Rather complex equipment (distillation column,…)
  - Recycle streams
  - Control loops

# Numerical strategies

- Equation oriented strategy - simultaneous solution
  - Write down the entire set of equation
  - Identify the constraints
  - Solve the non liner system
- Sequential Modular approach
  - Each subsystem is solved independently, starting from the first one
  - Output streams for the solved subsystems are input streams for the next subsystem
  - Problems for the recycle streams (of material, energy and information)
- Combination of the two extreme approach
  - Equation can be lumped into modules
  - Modules can be represented by polynomials that fit input-output information

# Equation oriented (EO) flowsheeting …

- Solution of a set of non liner equations with constraints
- Definition of the matrix of the stream connection (process matrix)
- Definition of the inequality constraints
  - Linearization of non-linear equations
  - Process limits for Temperature, Pressure, concentration
  - Requirements that variable be in a certain order
  - Requirements that variables be positive or integer
- Define the procedure for determining the order in solving the equations
- The treatment of feedback (recycles)

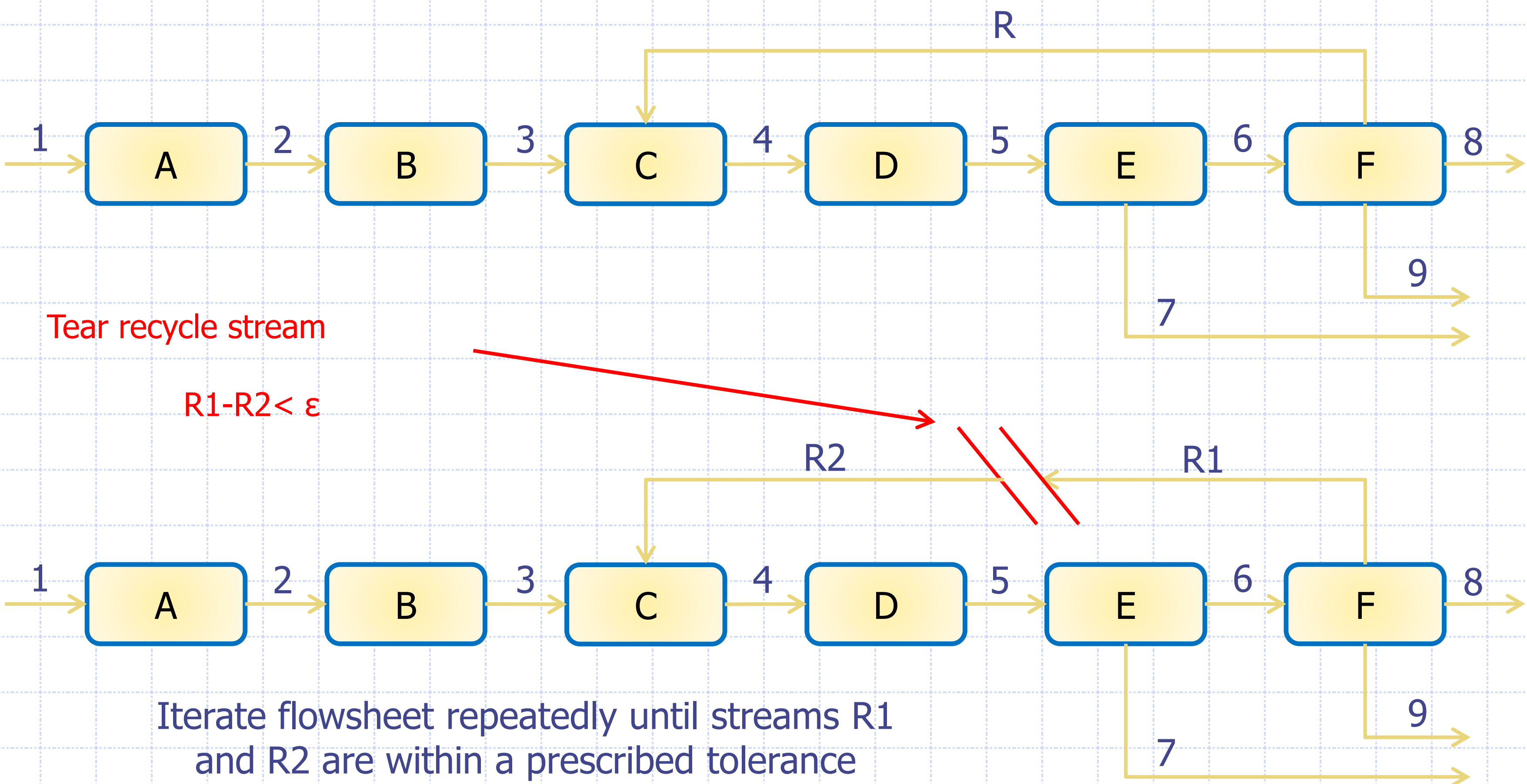
# Equation oriented (EO) convergence

- Method of solution
  - Newton Raphson
  - Secant
- Tearing = selecting certain output variables from a set of equations as known values so that the remaining variables can be solved by serial substitution
- Partitioning = partition of equations into blocks containing common variables
- Definition of initial guess
- Scaling the variables (the same order of magnitude)
- Scaling the equations (the same deviation from zero)

# Sequential modular approach (SMA)

- Most common approach
- Each unit operation is described by a subroutine
- The output of a module is the input of the next module
- Other subroutines take care of
  - equipment sizing and cost estimation
  - numerical calculations
  - handle recycle calculations
  - optimize and serve as controllers for the whole set of modules
- Tearing is the process of solving the recycles by deciding which stream should be interrupted and guessed
- Partitioning: grouping of equations for fast solving

# Sequential modular approach (SMA)

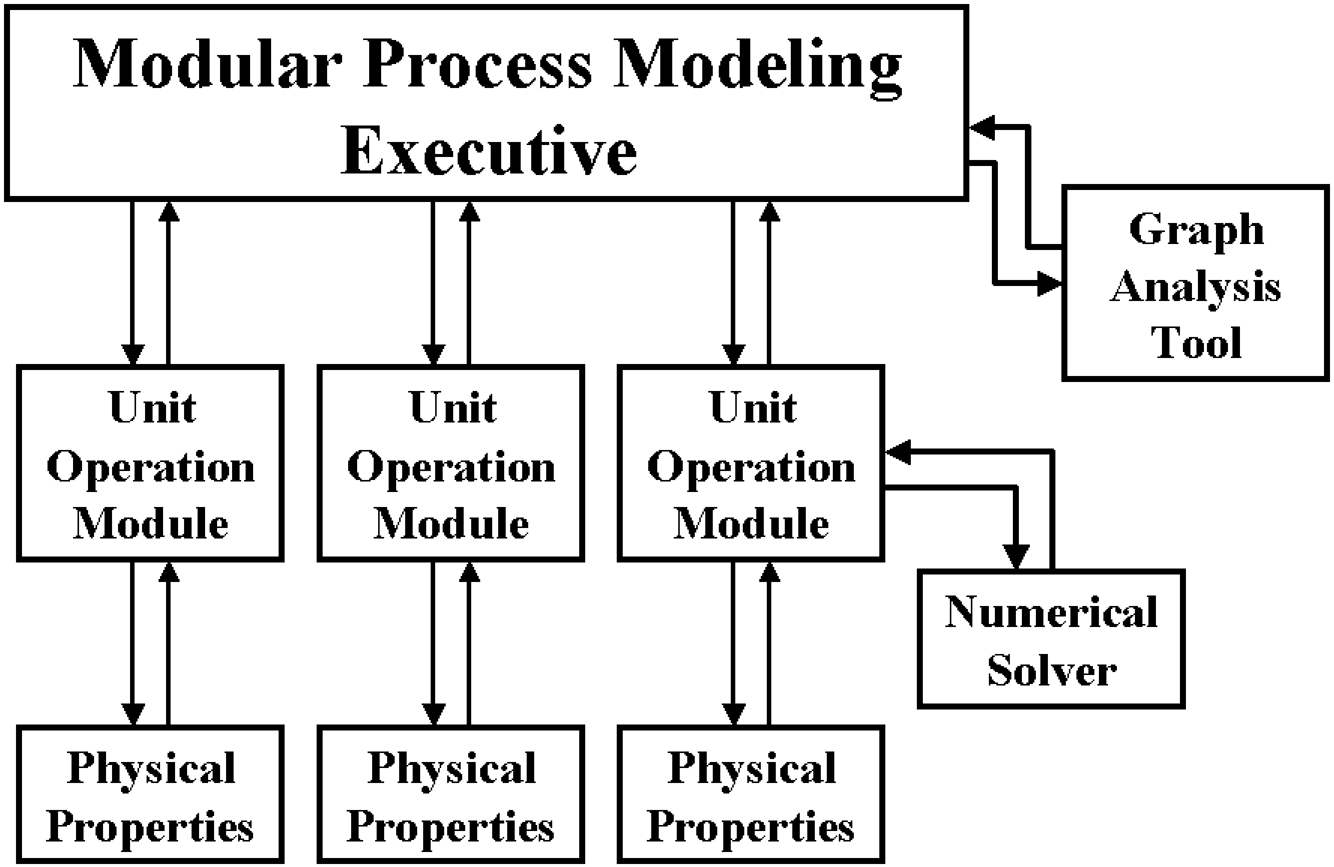



Iterate flowsheet repeatedly until streams R1 and R2 are within a prescribed tolerance

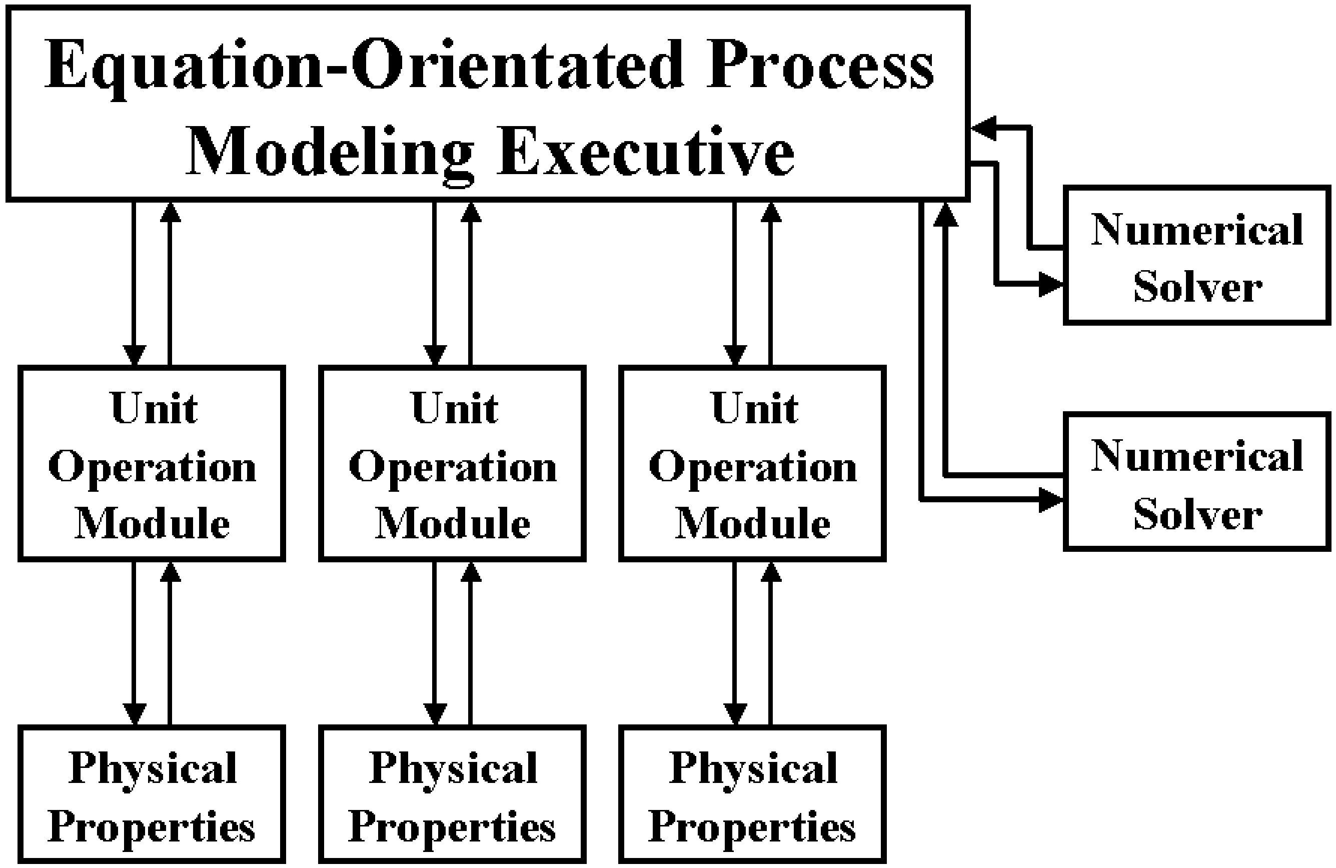
# SMA: Advantages and disadvantages

- Advantages of sequential modular approach
  - The flow-sheet architecture is easily understood because it closely follow the process
  - Individual modules can easily be added and removed
  - Modules of different levels of accuracy can be substituted
- Drawbacks of sequential modular approach
  - The input of a module is the output of a module: you cannot arbitrarily introduce an output or input
  - The modules need extra time to generate derivatives (perturbation of the input)
  - The modules may require a fixed procedure for the order of solution: slow convergence
  - Parameter specification is done with control loops: possibility of introducing nested loops
  - Phase equilibrium instability during the convergence of the process may lead to inconsistency in the process specifications
- SMA is the most popular approach,
  - but EO is the most applied in modern Process Simulators
  - SMA is adopted to initialize or get close to the solution, then EO to solve the model more precisely

# Sequential Modular appoach

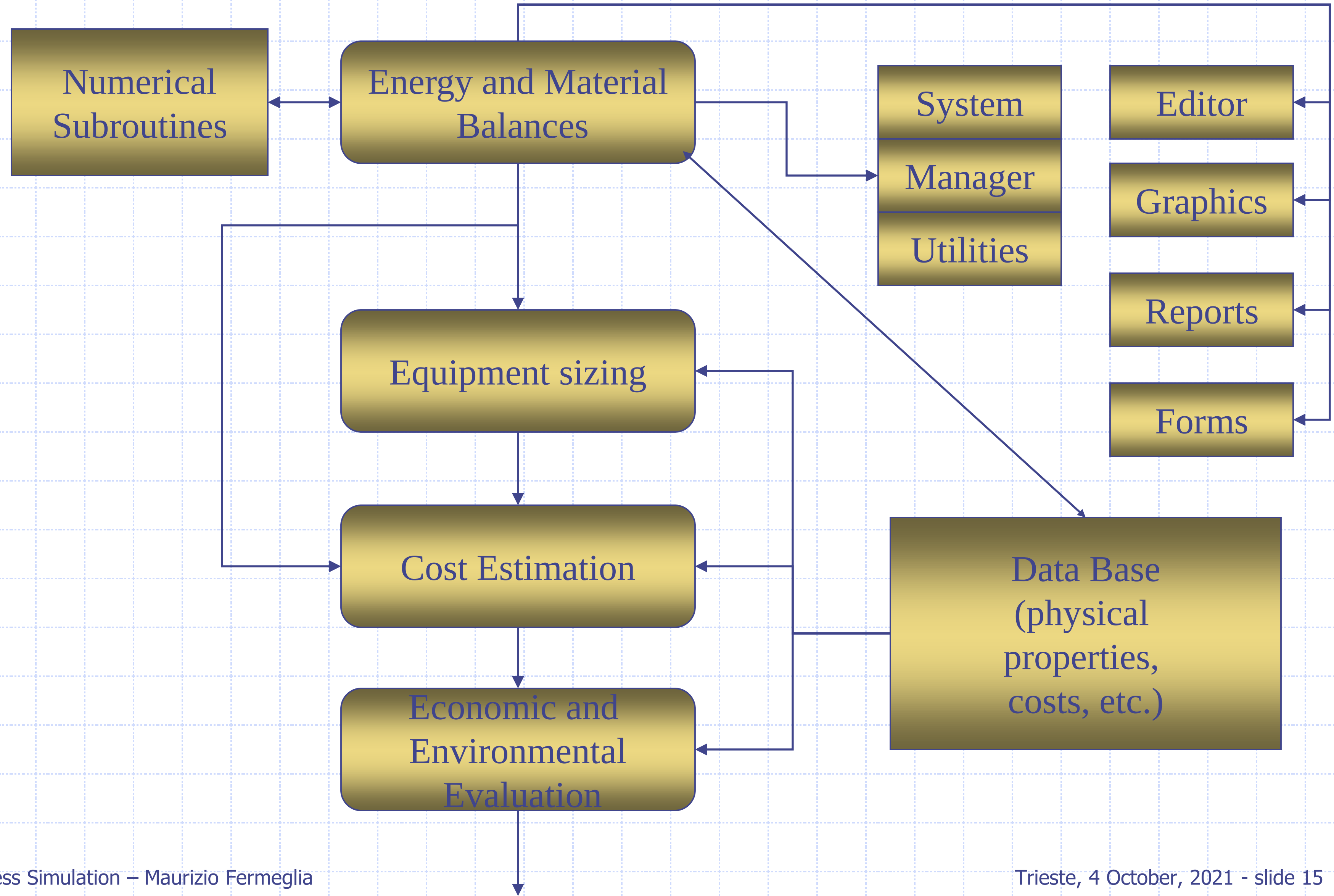


# Equation-Oriented approach



# Steady State process simulation

# A typical flow-sheeting code: steady state



# Steady State simulators: the core product

- Directly used in:
  - Process and equipment design
  - Evaluating process changes
  - Analyzing what-if scenarios
  - Sensitivity analysis
  - Optimization
  - Debottlenecking
- Basis for:
  - Dynamic simulation
  - Process synthesis
  - Detailed equipment design
  - Off-line and on-line equation based optimization
  - Application technologies for vertical markets, e.g. polymers

# Process simulation: the procedure

- Analysis: identify the problem
- Analysis: Obtain information
  - Get process data:
    - flow rates, operative conditions, concentrations
  - Get thermodynamic data:
    - In  house data or test run on pilot plant
    - Data Banks (Dechema, …) or literature
    - Via estimation methods (GC or MM)
  - Get kinetic data:
    - Directly from pilot plant or plant data
    - From excess Gibbs energy calculations (if possible)
    - Avoid a rigorous definition of kinetic model
    - Use concept of yield and conversion if possible
- Select the software and the hardware
- Run the base case
  - Degree freedom - convergency
- Adjust the base case
  - lumping, thermo, kinetic
- Assign Design Spec.
  - to each block
- Sensitivity analysis
  - Get process knowledge
- Assign Design spec.
  - to the global flowsheet
- Optimize the process
  - Define an OF
- Run the final simulation
  - With all the modifications included

# Steady State Process Simulation
# The Procedure …

- Identify the problem: perform a detailed analysis
- Obtain all the relevant information
  - Get process data: flow rates, operative conditions, concentrations
  - Get thermodynamic data:
    - In-house data
    - Data Banks (Dechema, …) or literature
    - Test run on laboratory / pilot plant
    - Via estimation methods (be suspicious on Group Contribution methods)
    - Via molecular modeling
  - Get kinetic data
    - Directly from pilot plant
    - from excess Gibbs energy calculations (if possible)
    - directly from plant data

**TIP:** avoid a rigorous definition of kinetic model and use concept of yield and conversion wherever possible and reasonable, at least in the first stage of the development

# Steady State Process Simulation … The Procedure …

- Select the software
  - Steady state simulators
    - Aspen Plus (Aspentech)
    - SuperPro Designer
    - PRO II (Sim Sci)
    - Aspen HYSIS (AspenTech)
    - gPROMS (PSE)
    - …
  - Dynamic simulators
    - Aspen Dynamics (Aspentech)
    - Aspen Batch modeler (Aspentech)
    - Batch model and DynSim (Sim Sci)
    - gPROMS (PSE)
    - ABACUS (MIT)
    - .....
  - Integrated solution
    - Aspen Dynamic, Hysis, Pro II, …
- Select the Hardware

# Steady State Process Simulation … The Procedure …

- Training
  - Material and energy balances
  - Basic course on process simulation
  - Thermodynamic, phase equlibria and model selection
  - Specific topics in thermophysical property calculation
    - Electrolytes
    - Polymer systems
    - Kinetic data and kinetic modeling
  - Specific topics in unit operation modeling
    - heat exchangers design
    - Batch distillation and reaction
    - heat integration
  - Process dynamics and control and dynamic process simulation
  - Economic factors, cost analysis and energy consumption
  - Batch process modelling
  - Environmental impact and environmental evaluation
  - Control system

# Steady State Process Simulation
# … The Procedure …

- Run the base case that is:
  - a complete representation of the plant (or part of the plant) in which the goals are
    - the closure of the degree of freedom analysis
    - the convergence of all the variables
  - may not correspond to the goals to be achieved
  - the starting point of 'what if analysis'
  - validation procedure for thermodynamic models and for data used
  - the validation for the reaction modeling and for the kinetic assumption
  - the validation for the unit operation models used in terms of:
    - Reliability
    - Convergence and numerical methods
    - Completeness of the results
  - There is not a necessary one-to-one correspondence between pieces of equipment and a model block

# Steady State Process Simulation
# … The Procedure …

- Fine tune the base case by adjusting
  - Thermodynamic models and parameters (thermodynamic analysis)
  - Kinetic models
- Assign Design Specification to each block
  - Assign internal design specification which involves variables and equation of specific blocks, such as solvent recovery, outlet temperature, number of stages, reflux ratio,…
  - The simulator will close again the degree of freedom analysis by considering the new design specification
  - The simulator will solve the unit operation by varying an indicated variable so that the design specification is met
  - Different way of performing such task in different process simulators

# Steady State Process Simulation … The Procedure …

- Perform Sensitivity analysis
  - A sensitivity analysis is the observation of a process condition consequent to the variation of a single process variable (partial derivative)
  - One can perform one sensitivity per each variable
  - One can observe the effect of the variation in several process conditions
  - Sensitivity analysis is of paramount importance for determining the most 'sensitive' variables for an optimization of the process
  - Plot of the results are normally prepared

# Steady State Process Simulation … Sensitivity Analysis …

- Your most useful ally in identifying problems and assessing risk is the Sensitivity Analysis (Tony Perris)
  - "what if …?"
  - vary the input data ( and even the models)
  - explore the defaults
  - vary the assumptions
  - bound your region of confidence
  - explore combinations of uncertainties
- Sensitivity Analysis …
  - identify key sensitivities & their engineering consequences (efficiency vs. structure)
  - focus on what really matters (i.e. what has a serious effect)
  - allocate design margins accordingly

# Steady State Process Simulation … The Procedure…

- Design specification for the entire process
  - Is the natural result of a correct sensitivity analysis
  - Allows to define a given process condition by modifying a variable in any part of the process
  - IS a one – to – one relationship between specification and variable
- Case Studies
  - Run the simulation with different operating condition
  - Different from the sensitivity analysis
  - The simulation converges completely for each process condition

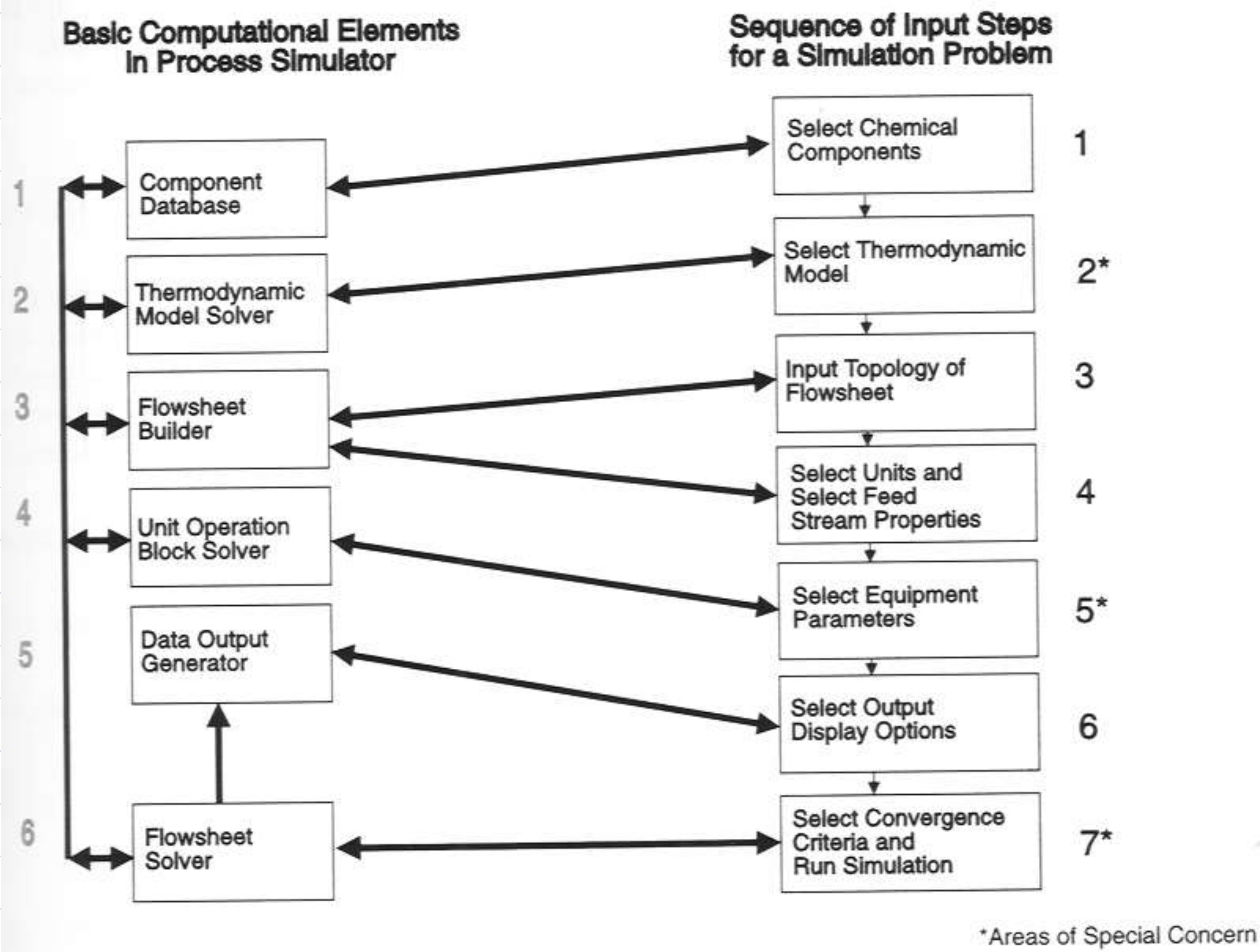
# Steady State Process Simulation … The Procedure.

- Optimization
  - Is the procedure that allow to find the best conditions in terms of a well defined objective function
  - The objective function may be:
    - Energy consumption
    - Operating cost
    - Equipment cost
    - Environmental impact
    - …
  - The number of variables is more than one
  - Points of attention:
    - Multiple minimum
    - Feasible and non-feasible path
    - Numerical convergence

# Steady State Process Simulation The Recipe

- Components definition
- Physical - Chemical properties definition
- Choosing the proper unit operation models
- Design the flowsheet connectivity
- Feed conditions definition
- Unit operation internal definitions for each unit operation involved in the process
- Process specification definition (Design Specifications)
- Analysis tools
  - Sensitivity analysis
  - Case studies
  - Optimization
- Sustainability evaluation (Profit, Planet, People)

# Structure of a Process Simulator



# Results obtainable

- Verification of the process operating conditions
- Information on intermediate streams (not measured)
- Enthalpy balances information
- Verification of the plant specifications
- Validation of phase equilibrium models for the real system to be used in similar conditions
- Influence of the operative parameters on the process specifications
- Process De-bottlenecking for each individual section
- A priori Identification of process control strategies and tuning of instrumentation
- Possibility to verify security systems behavior for variation of process condition

# Problems involved

- Availability of all the required thermodynamic properties of the pure components involved
- Definition of an accurate thermodynamic model (Equations of state or Excess Gibbs energy model) for binary and multi-component mixtures
- Availability of all the necessary interaction parameters
- Availability of all the necessary unit operations modules
- Necessity of defining dummy operations, not always easy to identify
- Tear streams identification to achieve rapid convergence if in presence of recycles
- Necessity of defining user models and user thermo (in C++, FTN or VB - VBA)

# Dynamic Simulation

# Definitions

- What does “dynamic” mean?
  - Dynamic simulation accounts for process transients, from an initial state to a final (steady) state
- Why dynamic simulation?
  - predicted transient behavior of processes under different conditions can be used in different fields
- When adopting dynamic approach?
  - Whenever the process itself is dynamic (i.e. batch process), for start-up phase of steady state processes or in order to deal with non-predictable events, such as changing in environmental conditions, rupture of equipment/controllers, etc…

# Dynamic simulation
# Process design and development

- Gives the design engineers a tool to conceptualize and verify process design by simulating
  - different design alternatives
  - operative conditions
  - safer process design can be accomplished quicker and more cost-effectively
- On-line applications
  - Calculation of inferential measurements
  - Decision support
- developing and testing alternative control schemes used to model a chemical process in basic regulatory control schemes as
  - Internal Model Control (IMC)
  - Model Predictive Control (MPC)

# Features of Dynamic simulation

- Advanced control
  - Advanced control of processes includes
    - Regulatory mode: responsible for
      - disturbance rejection
      - bringing the process set point
    - Transition mode: responsible for manipulating setpoints for controllers
      - start up
      - shut down
- Training plant personnel
  - Disturbances can be modeled and operator response can be monitored in an easy, cost effective way
    - DCS systems - control panel simulated by an external dynamic simulator
    - networked workstation - central server provides access to problem data base
    - standalone PC (see above)

# Features of Dynamic simulation

- Optimizing plant operations
  - By using an appropriate objective function (product quality) dynamic simulation can optimize (off-line or real time):
    - operating efficiency
    - profit or cost
    - environmental impact
    - troubleshoot process operability
- Process reliability/availability studies
  - Determining
    - failure propagation speed
    - equipment reliability
    - equipment availability

# Characteristics of a dynamic simulator

- Components
  - Thermodynamic / Physical properties
  - Unit operation models
  - Numerical solvers
- Mathematically
  - Consist of large systems of ordinary differential and algebraic equations
- Computationally intensive
  - Solver issues: speed - robustness
  - Mathematical problems: non-linear - sparse - stiff
- Approaches
  - Equation based approach (the most popular approach)
  - Sequential modular approach
- Dynamic simulation in Aspen+
  - Aspen+ steady state→ batch processes (reactor, distillation)
  - Aspen Custom modeler
  - Aspen Batch Process developerAspen+ Dynamics
  - Aspen Chromatography
  - Aspen Operator training

# Benefits of Dynamics Modeling

- Capital avoidance and lower operating costs through better engineering decisions
- Throughput, product quality, safety and environmental improvements through improved process understanding
- Increased productivity through enhanced integration of engineering work processes