Process Simulation Fundamentals

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Agenda

- Process simulation goals and definitions
- Material and energy balances
- Degrees of freedom analysis
- Process simulation fundamentals,
- Process simulation in the life cycle of chemical processes
- Trends of process simulation
- Users guidelines
- Limitations and points of attention in process simulation
- Conclusions and perspectives

What is Simulation

- Simulation is the act of representing some aspects of the real world by numbers or symbols which may be manipulated to facilitate their study

Process Simulation

- Process: a group of operations that transform input streams into product streams by means of chemical-physical transformations
- Simulation: the mathematical representation of the reality by using a computer
- Dynamic process: a process which is studied in the time domain rather than in steady state

- Thermophysical properties: the crucial point
- Data Banks: the basic value
- Unit operations: mathematical modelling
- Other modules such as optimization, numerical procedures,...
- Cost estimation methods
- ....

What is a Process Simulator

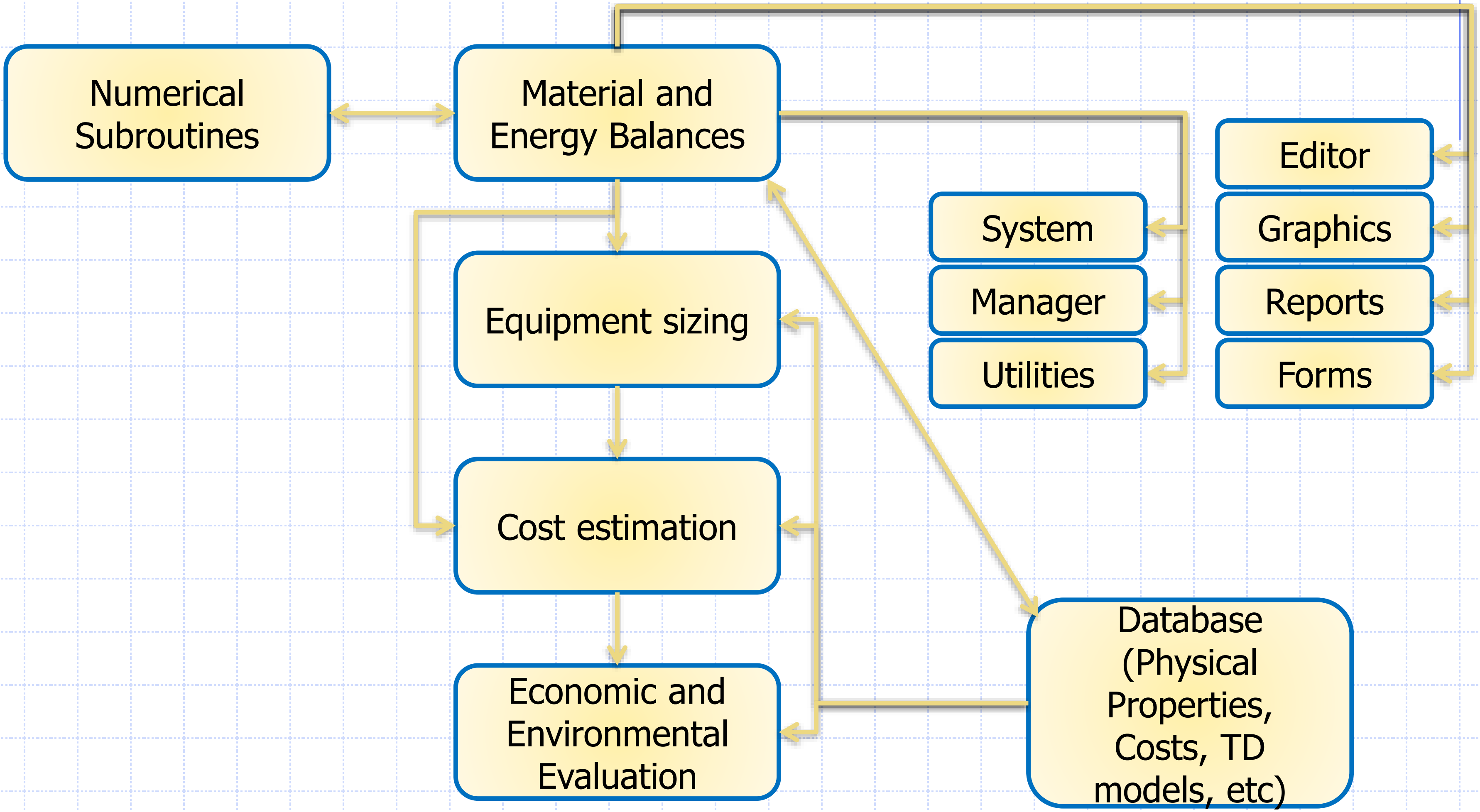
- An Engineering Tool which performs,
- Automated calculations
- Material and/or energy balances
- Physical property estimations
- Design/rating calculations
- Process optimization

It is not a Process Engineer!!

Flowsheet simulation

- What is a flowsheet simulation?
- It is a simulation in which a computer program solves quantitatively the mathematical model of the characteristics equations of a chemical process
- Is it realiable?
- The solution involves the adoption of underlying physical relationships:
  - Mass and energy balances
  - Equilibrium relationships
  - Reaction rate correlations
  - Mass/heat transfer
- What information will I obtain?
  - Stream flowrates, composition and properties
  - Operating conditions

A typical flow-sheeting code: steady state



Numerical Subroutines

Material and Energy Balances

Equipment sizing

Cost estimation

Economic and Environmental Evaluation

System

Manager

Utilities

Editor

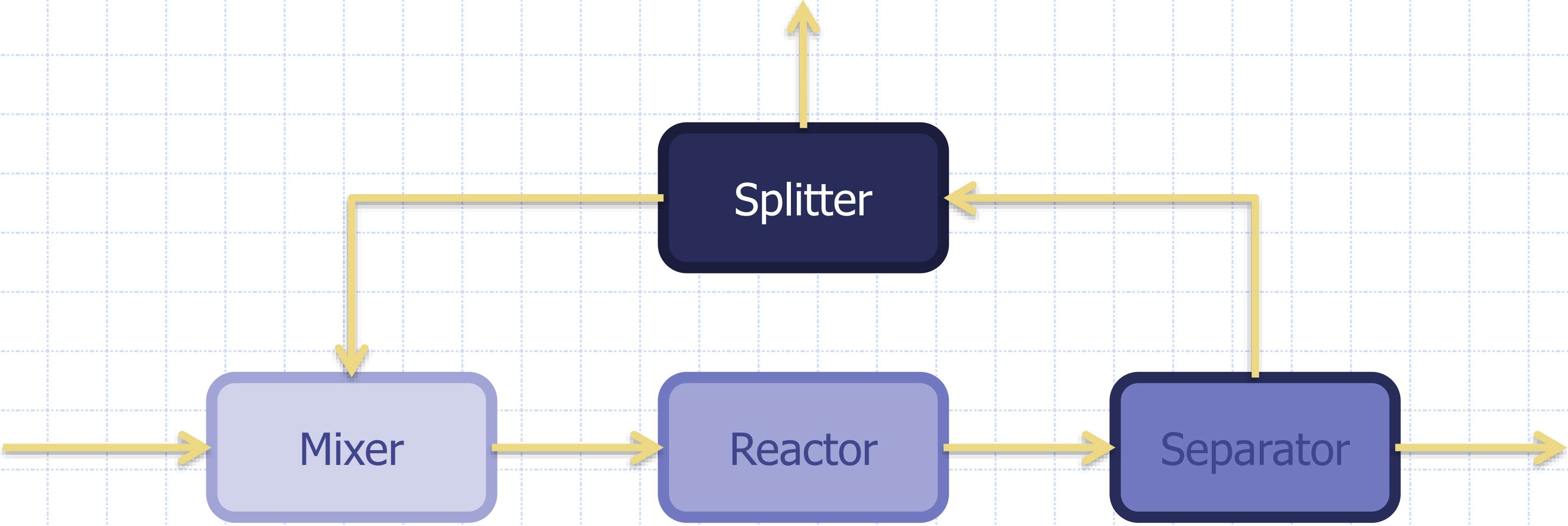
Graphics

Reports

Forms

Database (Physical Properties, Costs, TD models, etc)

Design & Analysis through process simulation/optimization



Splitter

Mixer

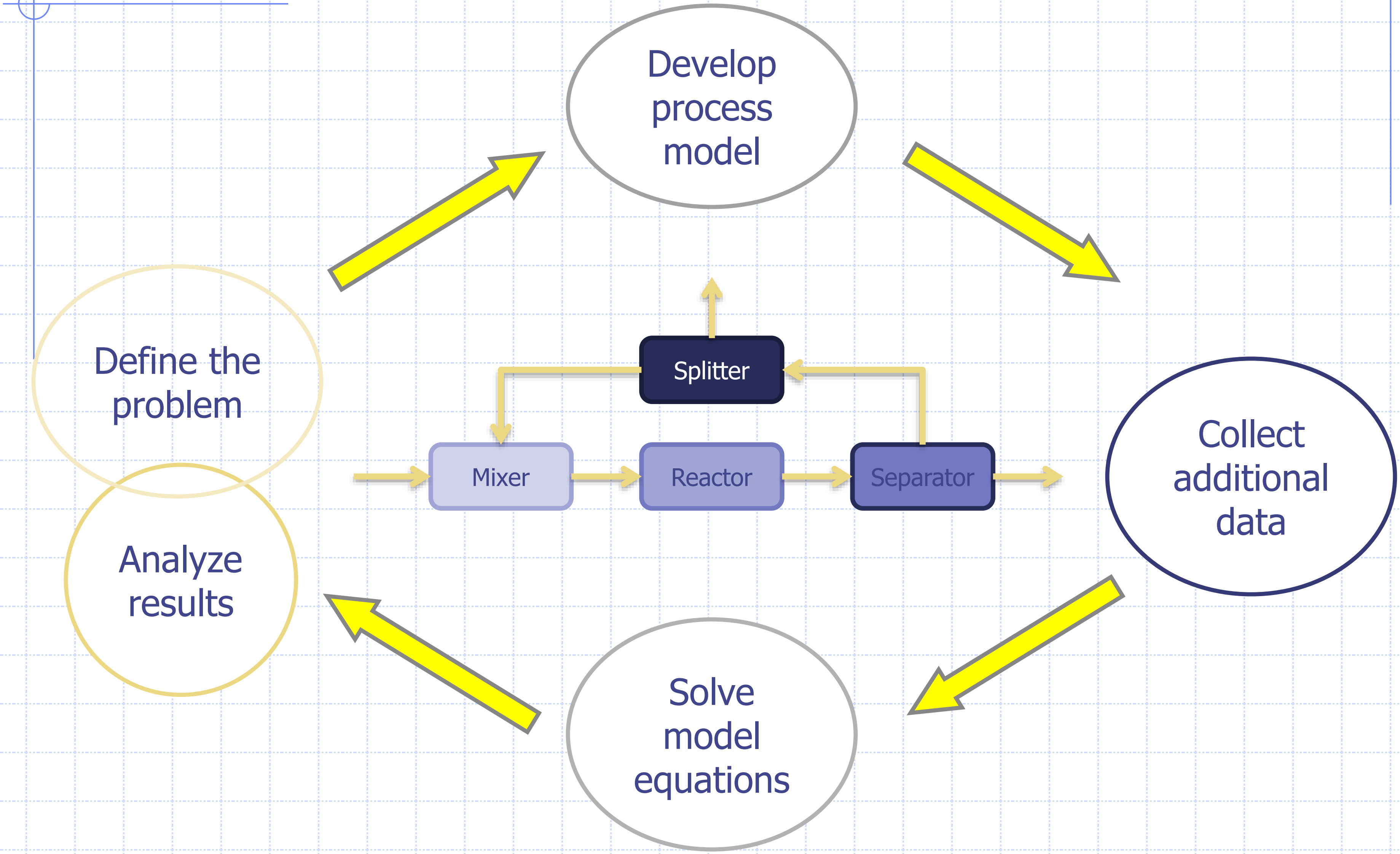
Reactor

Separator

What is our real world?

A CHEMICAL PLANT

Main steps in process simulation



Develop process model

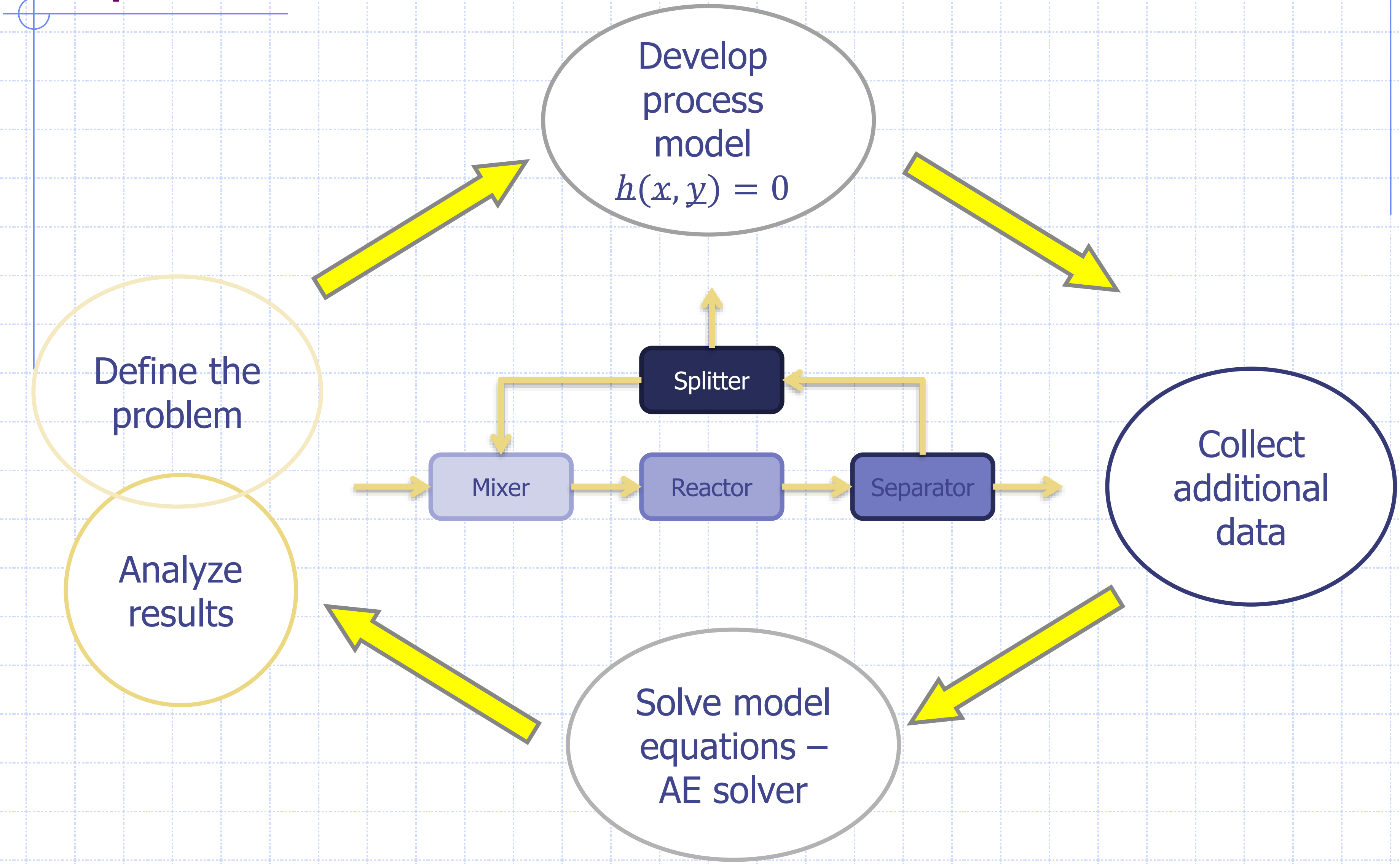
Collect additional data

Solve model equations

Analyze results

Define the problem

Steady state simulation – solve algebraic equations



Develop process model $h(x, y) = 0$

Collect additional data

Solve model equations – AE solver

Analyze results

Define the problem

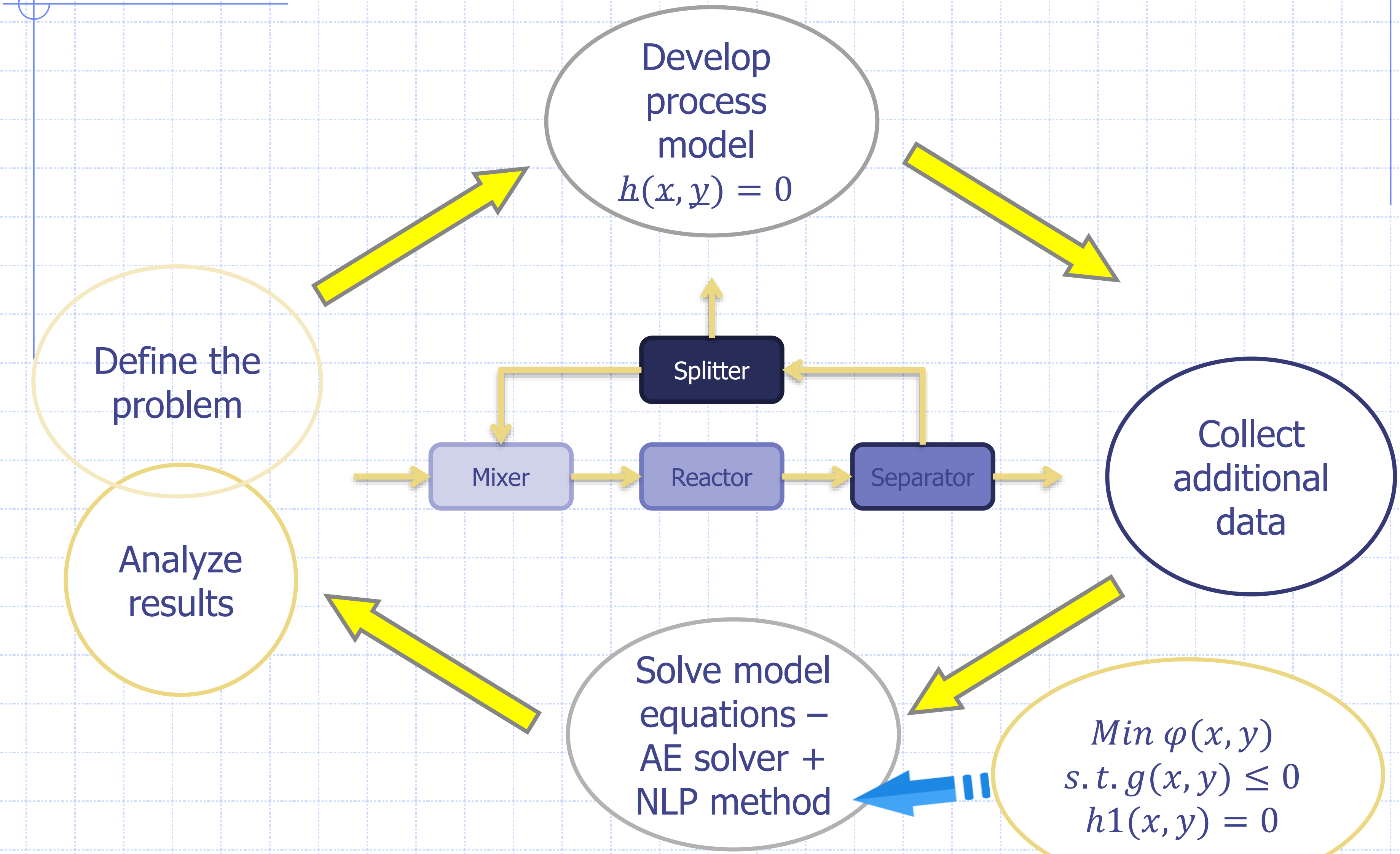
Splitter

Mixer

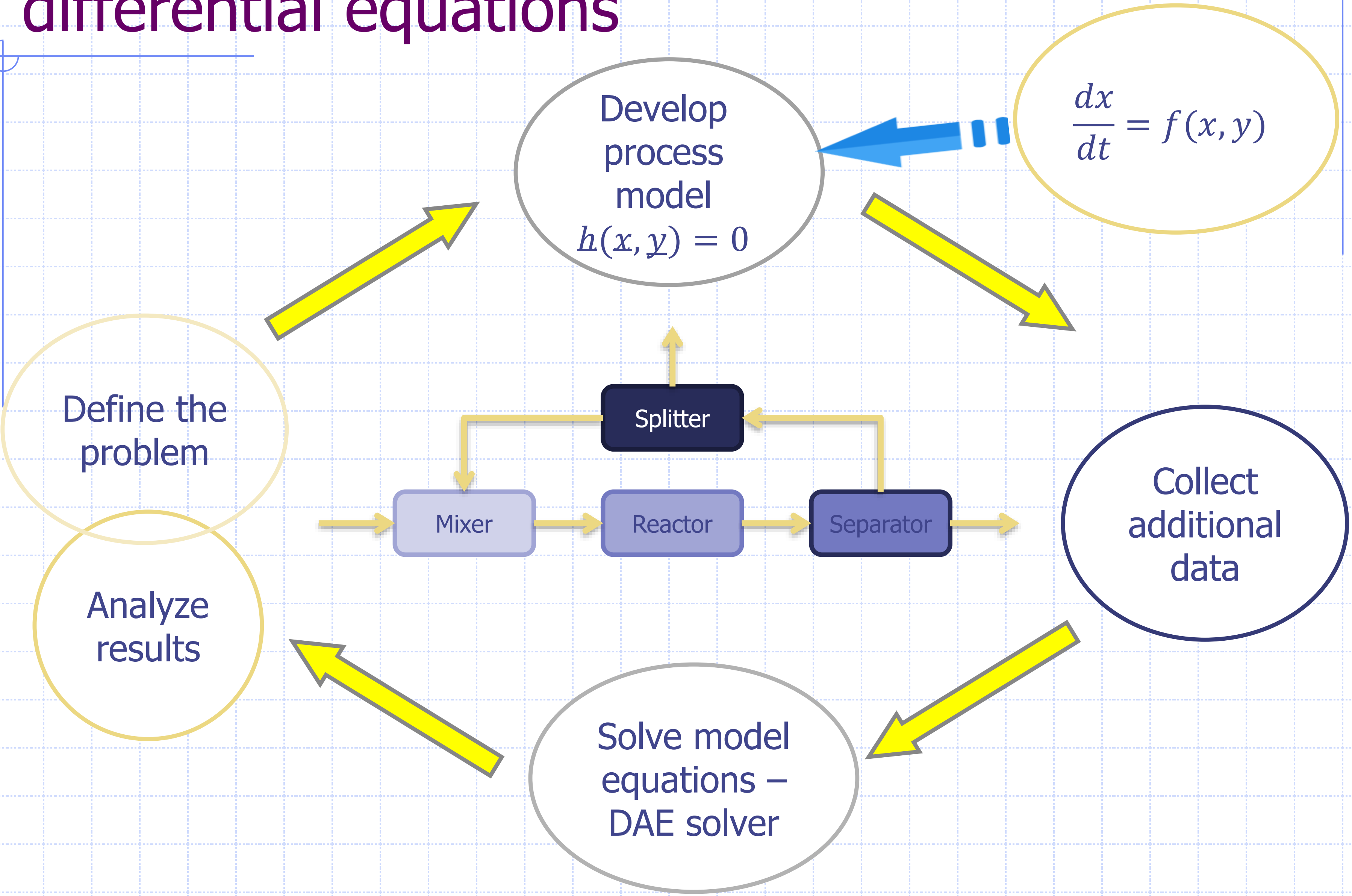
Reactor

Separator

Process optimization – minimize function s.t. constraints



Dynamic simulation– solve ordinary differential equations



Develop process model

$$h(x,y) = 0$$

$$\frac{dx}{dt} = f(x,y)$$

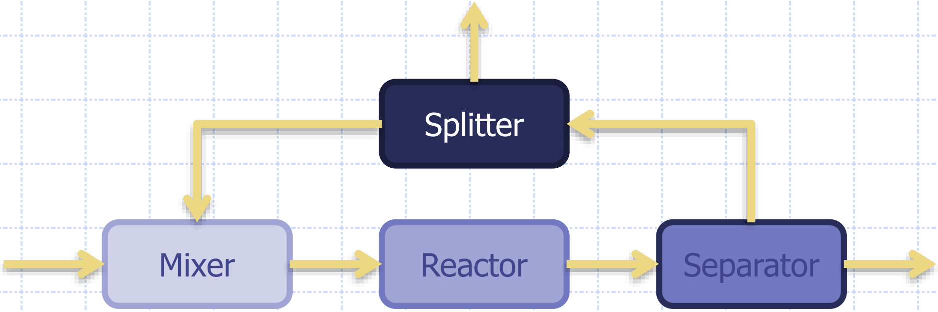
Collect additional data

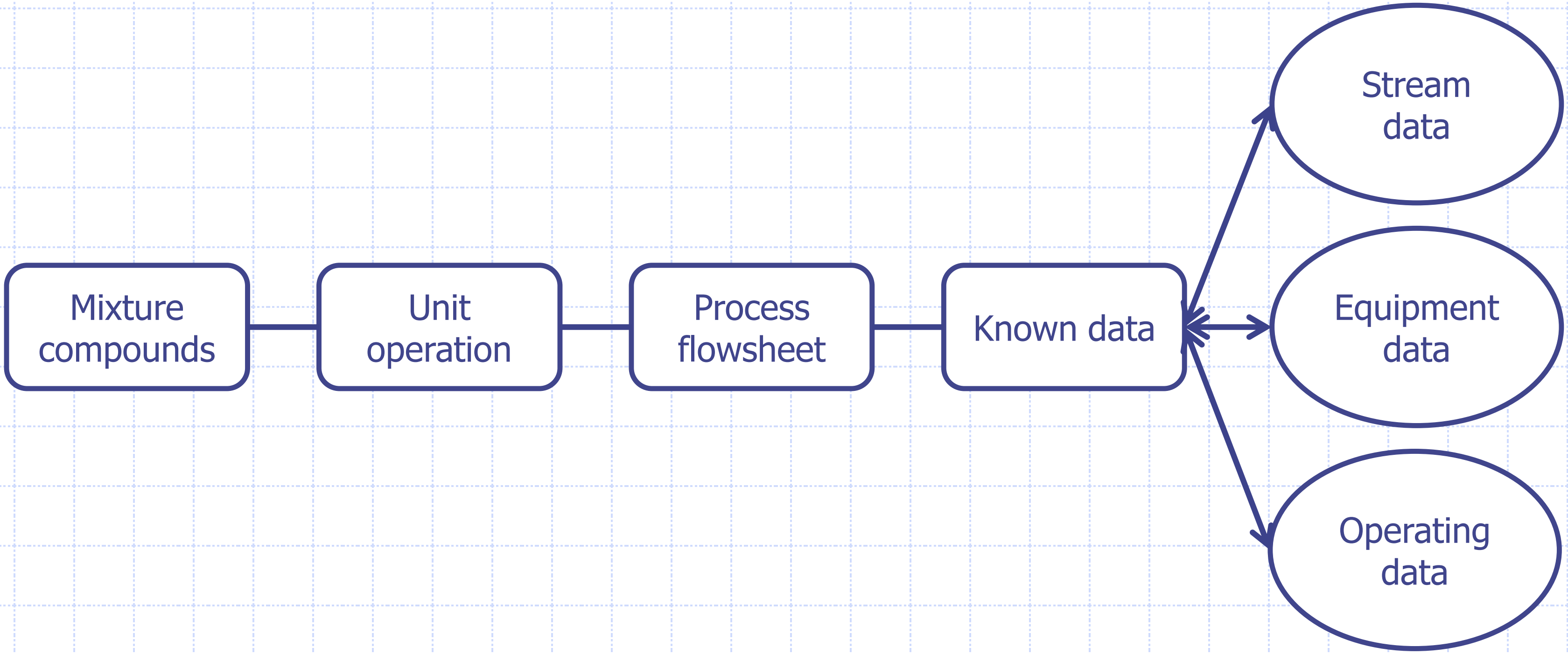
Solve model equations – DAE solver

Analyze results

Define the problem

Define the problem
What information do we need?





Mixture compounds

Unit operation

Process flowsheet

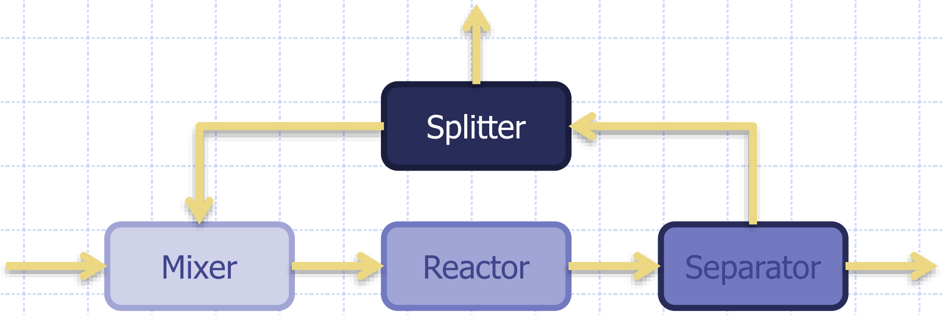
Known data

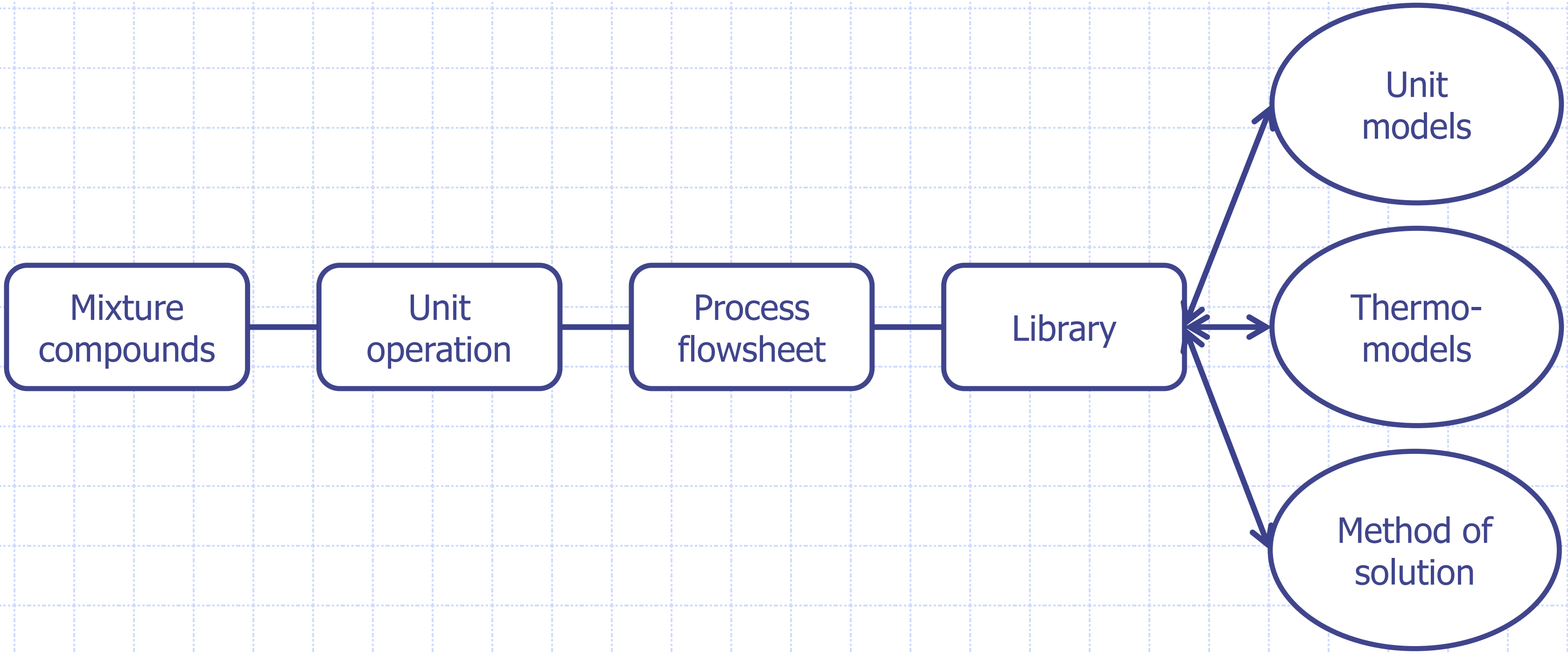
Stream data

Equipment data

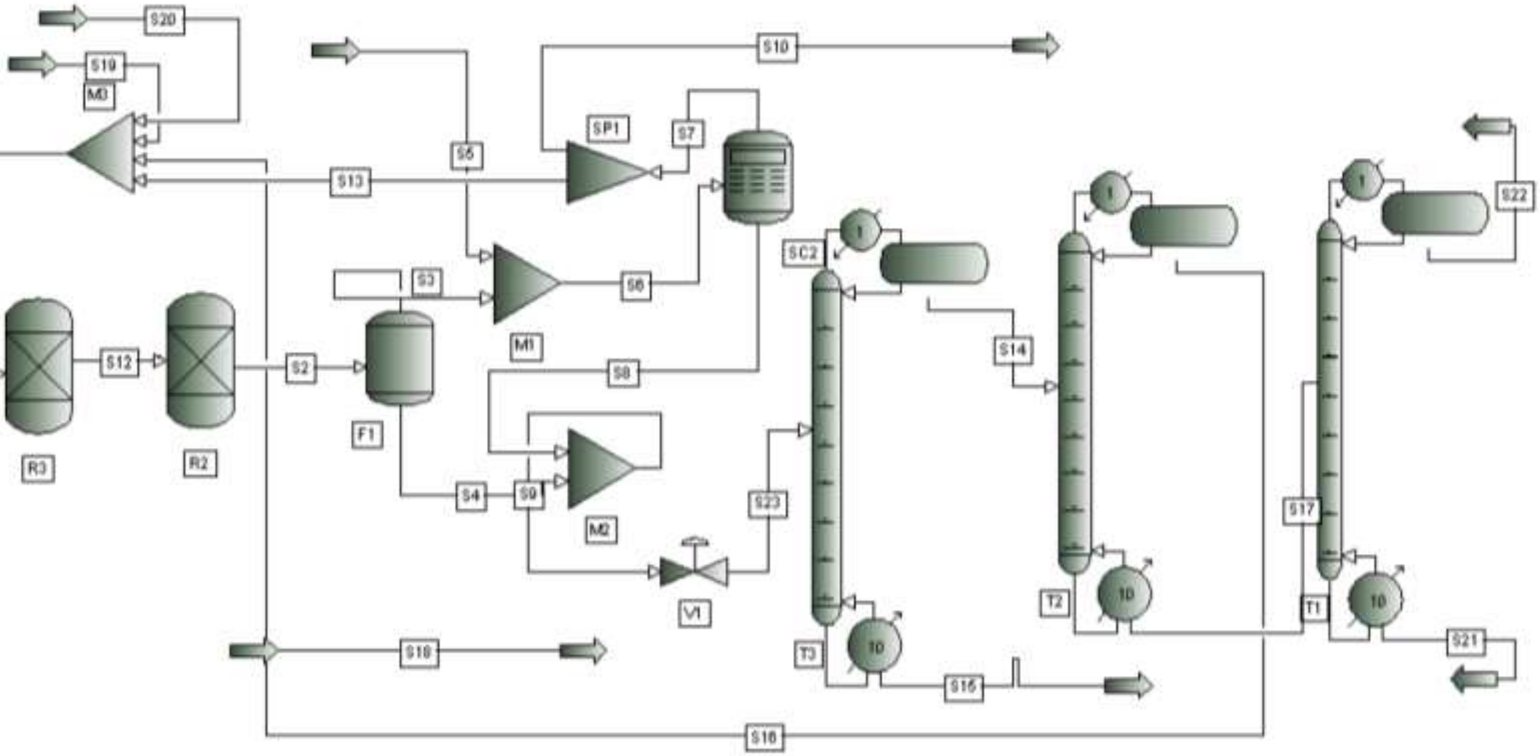
Operating data

Define the problem
What do we need to select from a simulator?



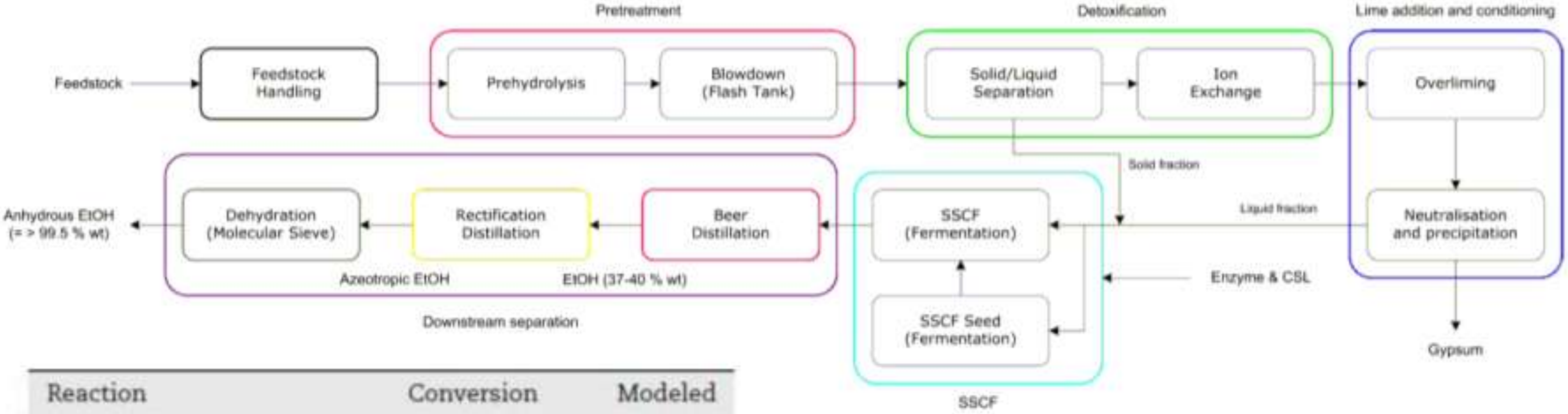


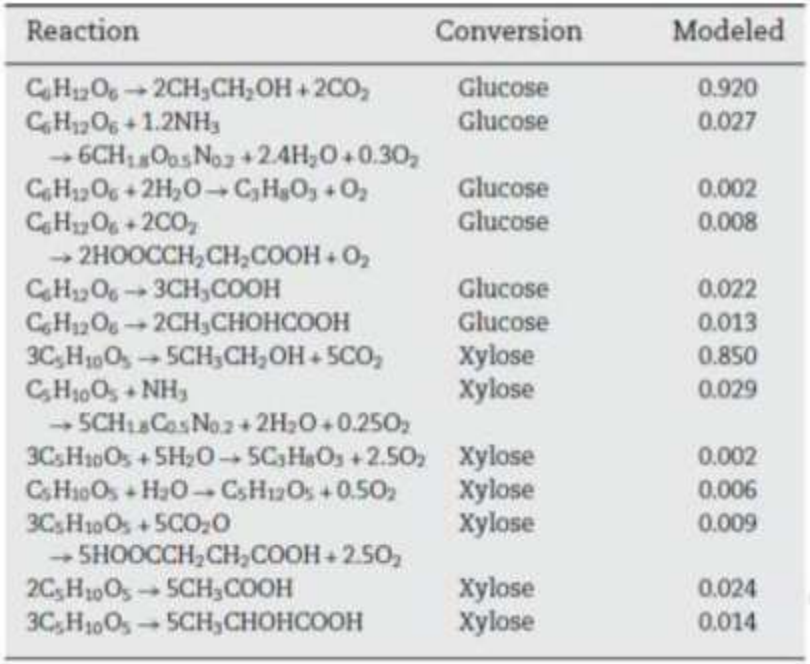
Example: ethanol production from ethylene



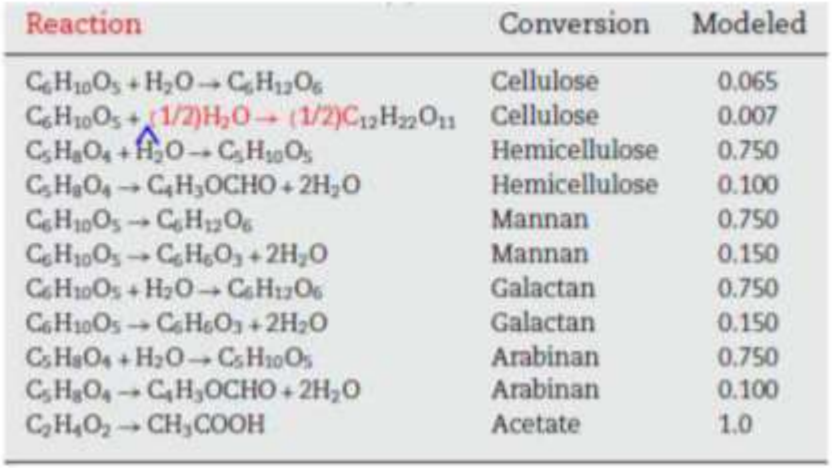
Almost all commercial process simulators can simulate this process in the steady state

Ethanol production from lignocellulosic material





Reaction	Conversion	Modeled
$C_6H_{12}O_6 \rightarrow 2CH_3CH_2OH + 2CO_2$	Glucose	0.920
$C_6H_{12}O_6 + 1.2NH_3 \rightarrow 6CH_{1.8}O_{0.5}N_{0.2} + 2.4H_2O + 0.3O_2$	Glucose	0.027
$C_6H_{12}O_6 + 2H_2O \rightarrow C_3H_8O_3 + O_2$	Glucose	0.002
$C_6H_{12}O_6 + 2CO_2 \rightarrow 2HOOCCH_2CH_2COOH + O_2$	Glucose	0.008
$C_6H_{12}O_6 \rightarrow 3CH_3COOH$	Glucose	0.022
$C_6H_{12}O_6 \rightarrow 2CH_3CHOHCOOH$	Glucose	0.013
$3C_5H_{10}O_5 \rightarrow 5CH_3CH_2OH + 5CO_2$	Xylose	0.850
$C_5H_{10}O_5 + NH_3 \rightarrow 5CH_{1.8}C_{0.5}N_{0.2} + 2H_2O + 0.25O_2$	Xylose	0.029
$3C_5H_{10}O_5 + 5H_2O \rightarrow 5C_3H_8O_3 + 2.5O_2$	Xylose	0.002
$C_5H_{10}O_5 + H_2O \rightarrow C_5H_{12}O_5 + 0.5O_2$	Xylose	0.006
$3C_5H_{10}O_5 + 5CO_2O \rightarrow 5HOOCCH_2CH_2COOH + 2.5O_2$	Xylose	0.009
$2C_5H_{10}O_5 \rightarrow 5CH_3COOH$	Xylose	0.024
$3C_5H_{10}O_5 \rightarrow 5CH_3CHOHCOOH$	Xylose	0.014



Reaction	Conversion	Modeled
$C_6H_{10}O_5 + H_2O \rightarrow C_6H_{12}O_6$	Cellulose	0.065
$C_6H_{10}O_5 + (1/2)H_2O \rightarrow (1/2)C_{12}H_{22}O_{11}$	Cellulose	0.007
$C_5H_8O_4 + H_2O \rightarrow C_5H_{10}O_5$	Hemicellulose	0.750
$C_5H_8O_4 \rightarrow C_4H_3OCHO + 2H_2O$	Hemicellulose	0.100
$C_6H_{10}O_5 \rightarrow C_6H_{12}O_6$	Mannan	0.750
$C_6H_{10}O_5 \rightarrow C_6H_6O_3 + 2H_2O$	Mannan	0.150
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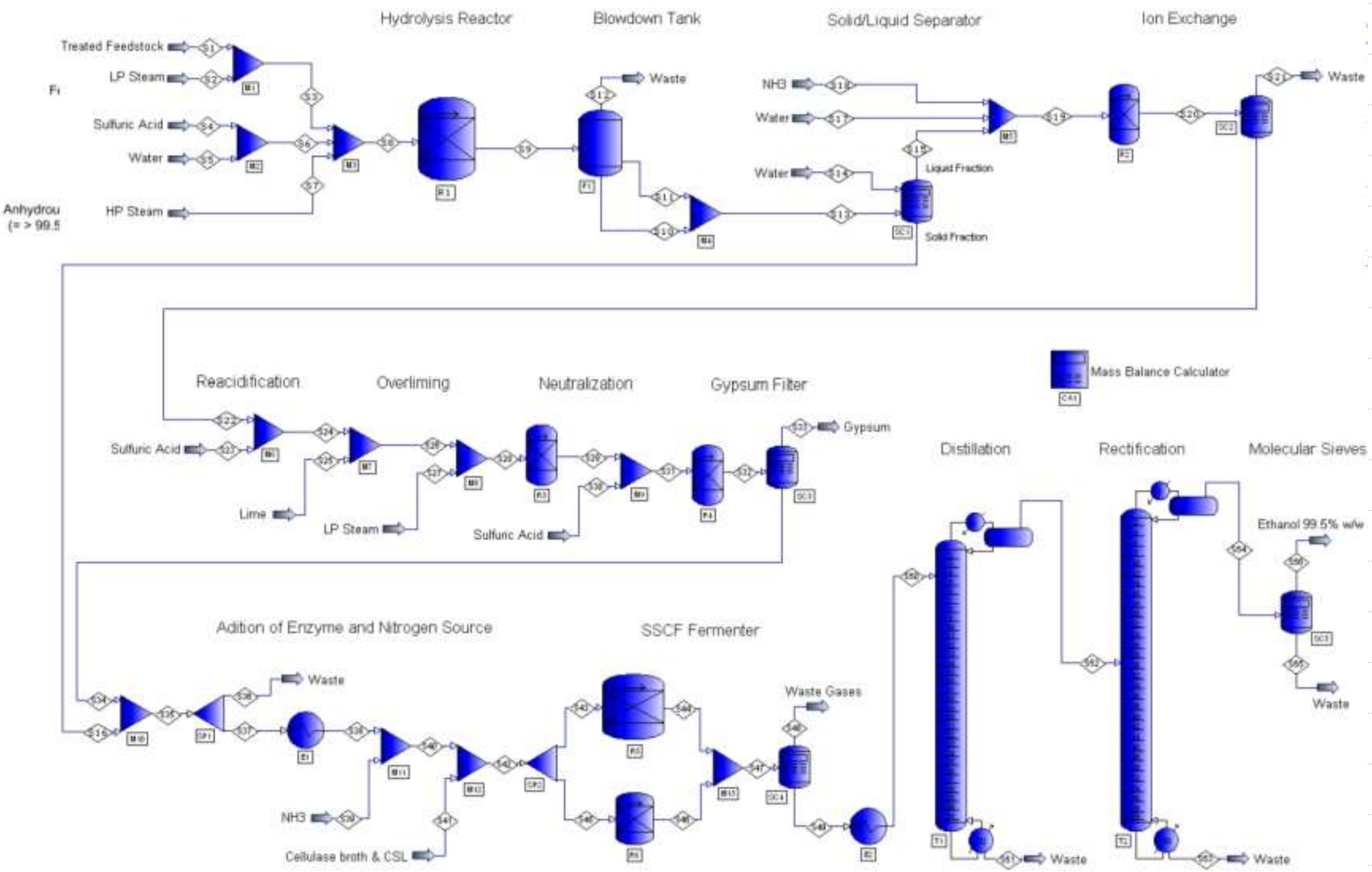
$C_5H_8O_4 + H_2O \rightarrow C_5H_{10}O_5$	Arabinan	0.750
$C_5H_8O_4 \rightarrow C_4H_3OCHO + 2H_2O$	Arabinan	0.100
$C_2H_4O_2 \rightarrow CH_3COOH$	Acetate	1.0

Ethanol production from lignocellulosic material



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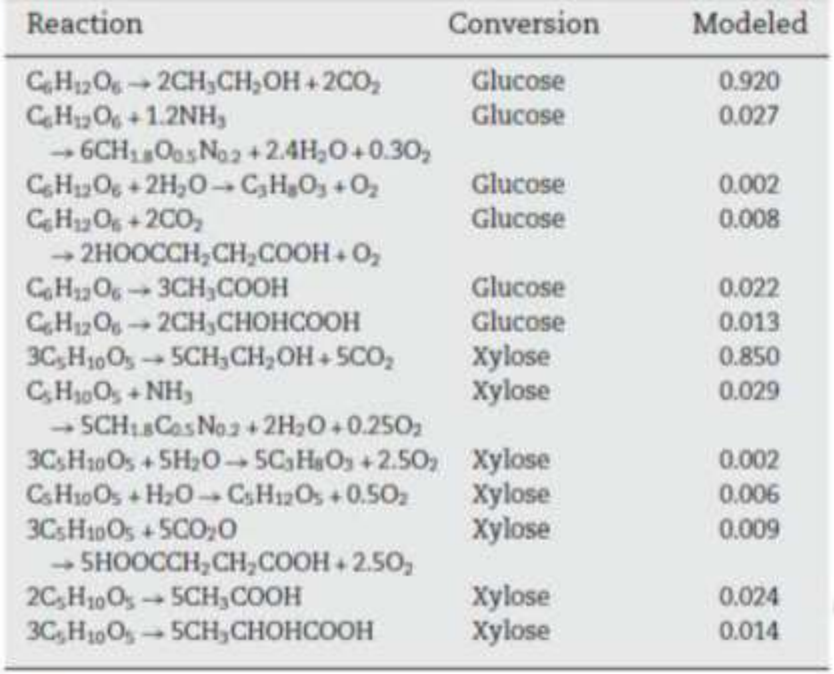

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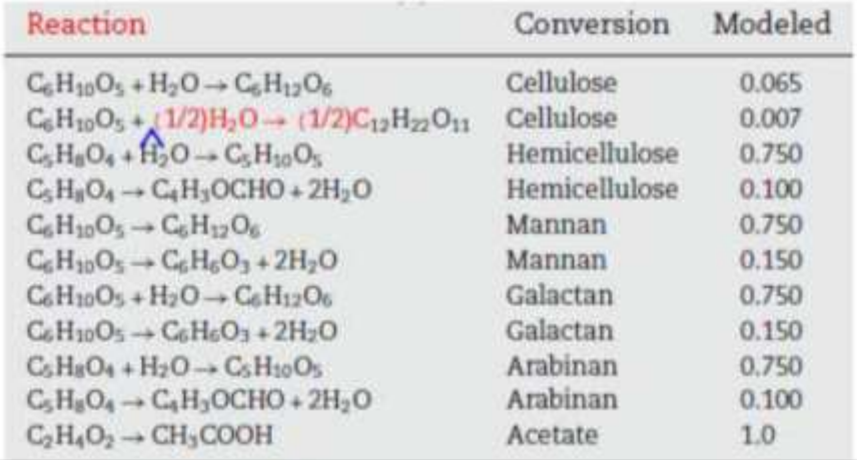

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$C_2H_4O_2 \rightarrow CH_3COOH$	Acetate	1.0

Compound	Pro II Library	User-defined
Ethanol	•	
Water	•	
Glucose		•
Xylose		•
Arabinose		•
Mannose		•
Galactose		•
Cellobiose		•
Acetic acid	•	
Lactic acid	•	
Succinic acid	•	
Glycerol	•	
Xylitol		•
Furfural	•	
Ethylene glycol	•	
HMF		•
Cellulose		•
Mannan		•
Galactan		•
Arabinan		•
Hemicellulose		•
Lignin		•
Z. Mobilis		•
Cellulase		•
Biomass		•
$[EMIM]^+[BF_4]^-$		•
Sulfuric acid	•	
Ammonia	•	
Ammonium acetate	•	
Ammonium sulfate	•	
Calcium hydroxide	•	
Calcium sulfate	•	

From Real life to Process Simulator

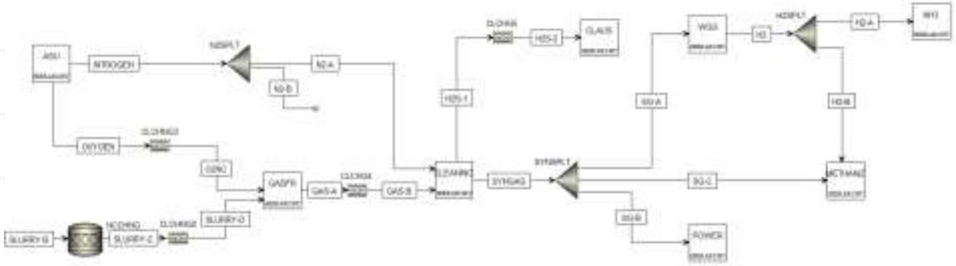
Unit operation (reactor)

Module (Rstoic)

Pipelines

Stream
s

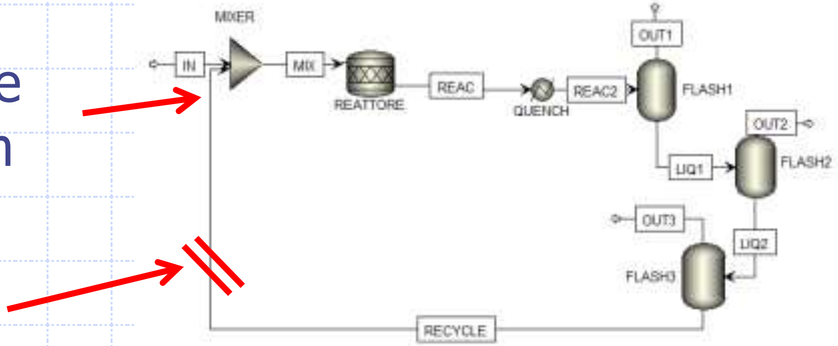
IGCC Plant



IGCC Flowsheet with decomposition

Recycle stream

Tear stream

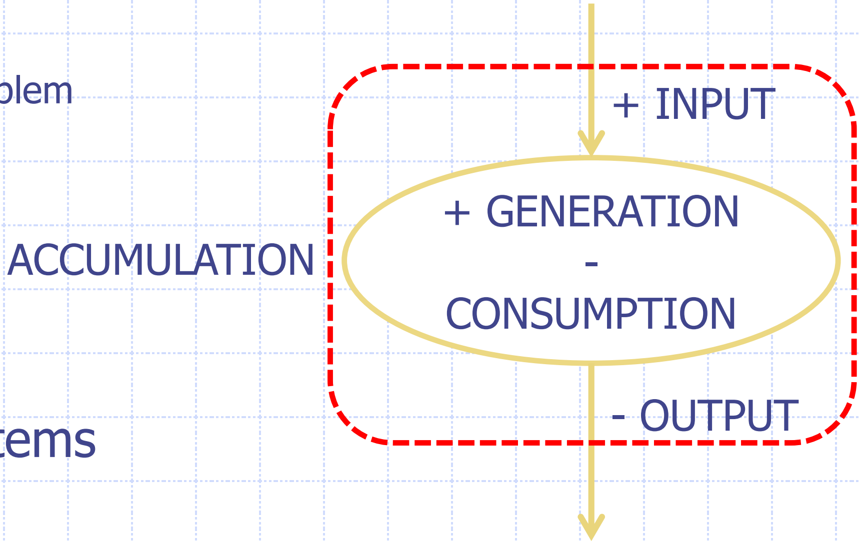


Material and energy Balances

- The general balance equation

$$input \; + \; generation - output - consumption \; = \; accumulation$$

- Valid for Batch, Continuous and Semi batch
- The procedure for a single unit
  - Define the basis
  - Write the flowchart ... write all the known variables, label unknowns
  - Convert all the data in consistent units
  - Perform the degree of freedom analysis
  - Write the equations in an efficient solver and solve the system
  - Calculate the quantities requested in the problem statement
- Balances on multiple-unit processes (recycle – bypass)
- Balances on reactive processes
  - Molecular or atomic species
  - Extent of reaction
- Single phase and multiple phase systems



ACCUMULATION

+ INPUT

+ GENERATION

\-

CONSUMPTION

\- OUTPUT

Degrees of Freedom (DoF)

- Intensive variables:
  - Temperature, Pressure, concentration, …
- Extensive variables
  - mass flow, energy flow, …
- Iterative variables
  - n° of stages in a distillation column

$$N_i = N_v - N_r$$

N_i = independent variables

N_v = total variables

N_r = independent equations

- Inherent relations (specific of the system)
- Mass balance relations
- Energy balance relations
- Phase equilibria relations
- Chemical equilibria relations

- $\boldsymbol{N\_i>0}$: "problem is underspecified and additional variables must be specified in order to determine the remaining variables"
- $\boldsymbol{N\_i=0}$: problem can be solved
- $\boldsymbol{N\_i<0}$: problem is overdetermined with redundant and possibly inconsistent relations

Stream

$$N_v = T, P, \dot{m}, H_{stream}, x_i = 1 + 1 + 1 + 1 + (c - 1) = c + 3$$
$$N_r = 1$$

Enthalpy is a function of composition, T and P

or

$$N_v = T, P, \dot{m}, H_{stream}, x_i = 1 + 1 + 1 + 1 + c = c + 4$$
$$N_r = 1 + 1$$

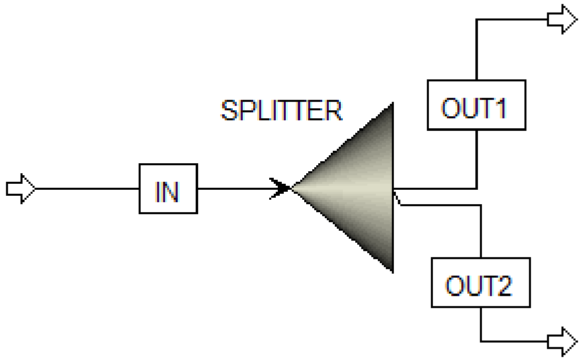
$$\sum_i^c x_i = 1$$

Enthalpy is a function of composition, T and P

$$N_i = c + 2$$

e.g.
c-1: components
1: temperature
1: pressure
1: mass flow

Splitter



$$N_v = 3 * (c + 2) + 1 = 3c + 7$$

Number of streams

Energetic balance

$$N_r = 2 + \underbrace{2 * (c - 1)} + 1 + 1 = 2c + 2$$

Inherent relations (constant T and P for inlet and outlets)

Constant composition among inlet and 2 outlet streams

Mass Balance

Energy Balance

$$N_i = c + 5$$

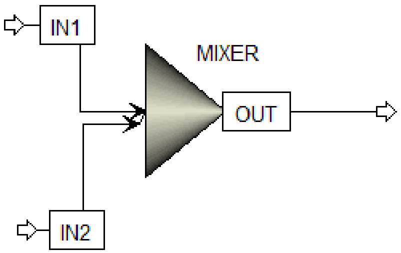
e.g.
c+2: definition of inlet stream
1: temperature
1: pressure
1: any composition or heat

Mixer

$$N_v = 3 * (c + 2) + 1 = 3c + 7$$

Number of streams

Heat exchanged



$$N_r = c + 1$$

Mass balance

Energetic balance

$$N_i = 2c + 6$$

e.g.
2*(c+2): definition of inlet streams
1: temperature
1: pressure

Pump, Heat exchanger

$$N_v = 2 * (c + 2) + 1 = 2c + 5$$

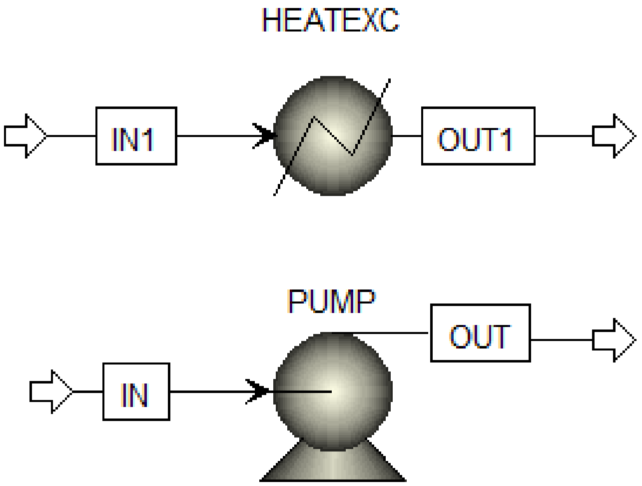
Number of streams

Energy/work balance

$$N_r = c + 1$$

Mass balance

Energy/work balance



$$N_i = c + 4$$

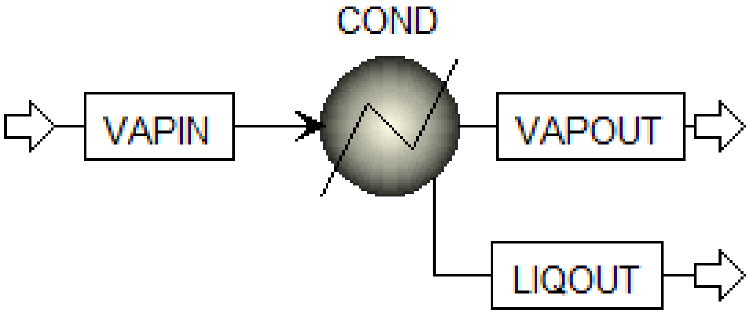
e.g.
(c+2): definition of inlet stream
1: temperature
1: pressure or heat

Partial Condenser/Reboiler/Flash

$$N_v = 3 * (c + 2) + 1 = 3c + 7$$

Number of streams

Energy/work balance



$$N_r = c + c + 1 + 2 = 2c + 3$$

Mass balance

Phase equilibrium

Energy Balance

T and P constant among outlet streams

$$N_i = c + 4$$

e.g.
(c+2): definition of inlet stream
1: temperature
1: pressure or heat

Reactor

$$N_v = 2 * (c+2) + 1 + n = 2c + 6$$

Number of streams

Energy/work balance

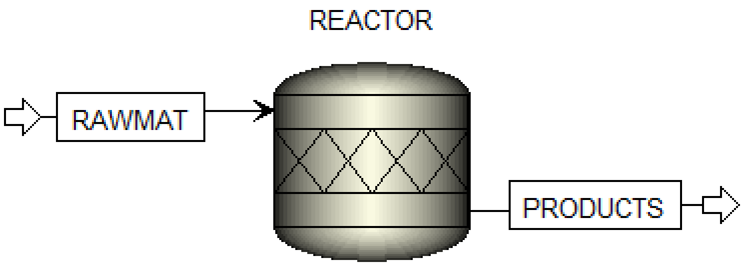
Stoichiometry of reactions

$$N_r = c + 1 + n$$

Equilibrium or conversion fixed

Mass balance

Energy balance



$$N_i = c + 4$$

If reactions are specified

e.g.
(c+2): definition of inlet stream
1: temperature
1: pressure or heat

$$N_i = c + 5$$

If reactions are not specified

e.g.
(c+2): definition of inlet stream
1: temperature
1: pressure or heat
1: equilibrium constant

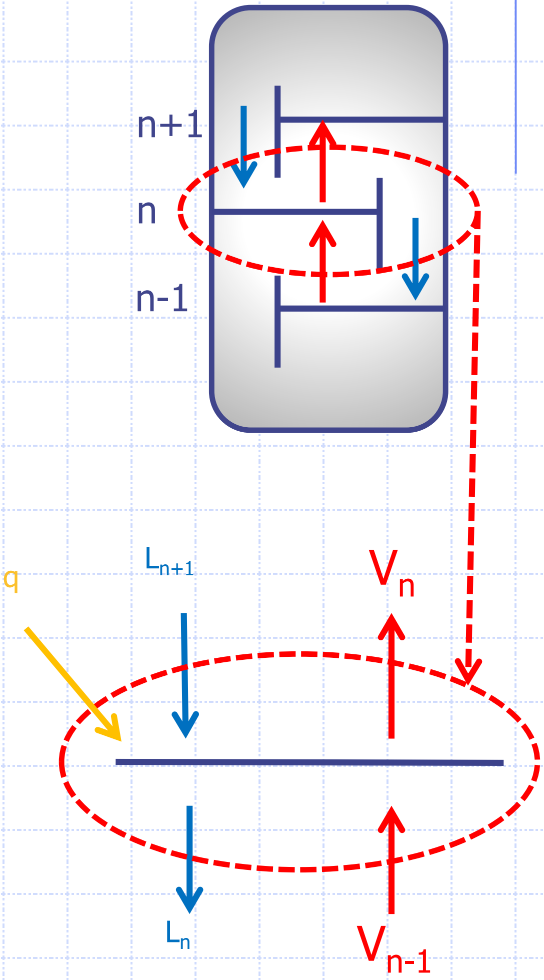
Separation column: Equilibrium stage

$$N_v = \underset{\substack{\uparrow\\ \text{Number of}\\ \text{streams}}}{4} * (c+2) + \underset{\substack{\uparrow\\ \text{Heat}\\ \text{exchanged}}}{1} = 4c + 9$$

$$N_r = \underset{\substack{\nwarrow\\ \text{Mass balance}}}{c} + \underset{\substack{\nwarrow\\ \text{Energy balance}}}{1} + \underset{\substack{\nwarrow\\ \text{Phase equilibria}}}{c} + \underset{\substack{\nwarrow\\ \text{T,P equivalence}}}{2} = 2c + 3$$

$$N_i = 2c + 6$$

e.g.
2(c+2): definition of inlet streams
1: temperature
1: pressure



Separation column: Feed stage

$$N_v = 5 * (c + 2) + 1 = 5c + 11$$

Number of streams

Heat exchanged

$$N_r = c + 1 + c + 2 = 2c + 3$$

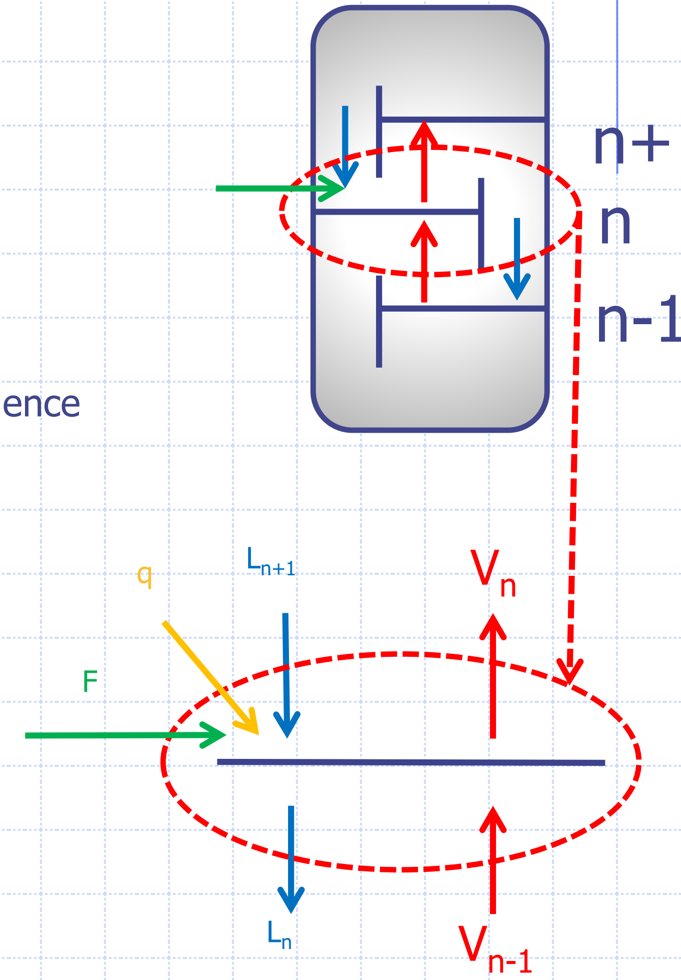
Mass balance

Energy balance

Phase equilibria

T,P equivalence

$$N_i = 3c + 8$$



e.g.
3(c+2): definition of inlet streams
1: temperature
1: pressure

Separation column: Side stream stage

$$N_v = 5 * (c+2) + 1 = 5c + 11$$

Number of streams

Heat exchanged

$$N_r = c + 1 + c + 4 + (c-1) = 3c + 4$$

Mass balance

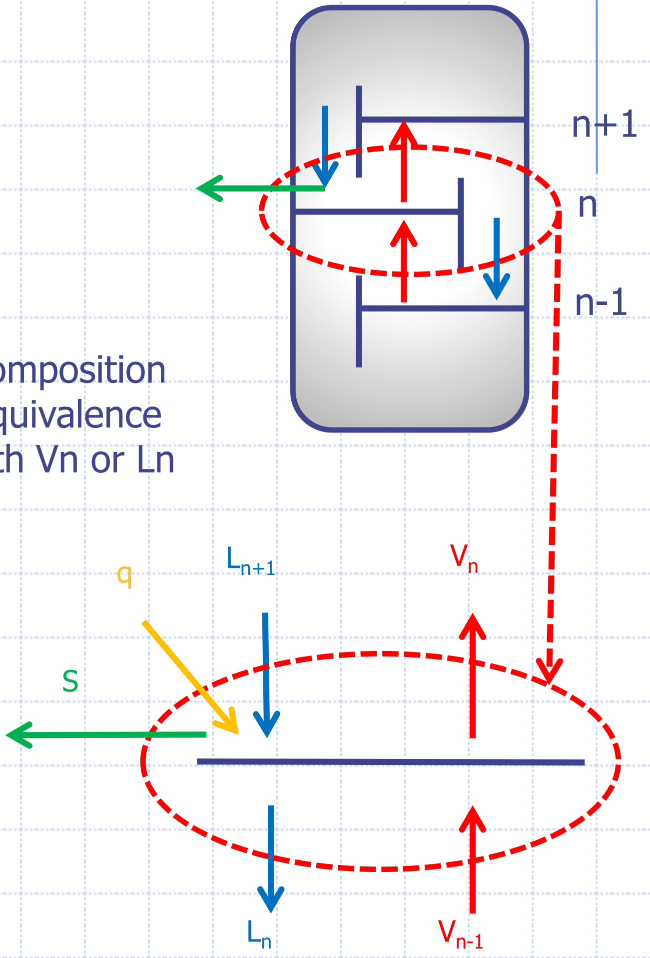
Energy balance

Phase equilibria

T,P equivalence for 3 outlet streams

Composition equivalence with Vn or Ln

$$N_i = 2c + 7$$



e.g.
2(c+2): definition of inlet streams
1: heat exchanged
1: pressure
1: mass flow of stream S

Absorption column

$$N_v = n * (2c + 6) + 1$$

Number of stages

DoF for each stage

Energy Balance

$$N_r = 2 * (c + 2) * (n - 1)$$

Streams ∀ stage

DoF for each stream

n-1 independent stages

$$N_i = 2n + 2c + 5$$

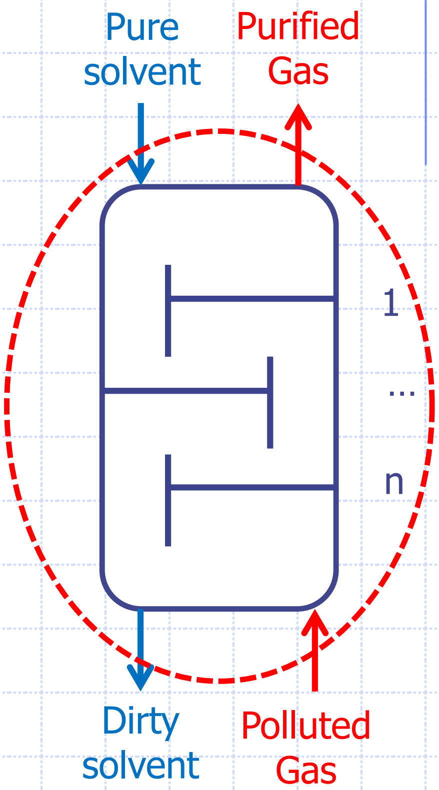
e.g.

2(c+2): definition of inlet streams

n: P ∀ stage

n: Heat loss ∀ stage

1: number of stages



Distillation column

$$N_v = (c+4) + (c+5) + (2c+2n+5) + (3c+8) + (2c+2m+5) + (c+4) = 10c + 2m + 2n + 31$$

	Condenser	Splitter	Rectifying column	Feed stage	Stripping column	Reboiler	
Streams	2	3	4	5	4	3	Total = 21

Streams counted twice = 9

Streams independent = 12

$$N_r = 9 * (c+2)$$

$$N_i = 2 * (n+m) + c + 13$$

e.g.

c+2: definition of feed

n,m: P ∀ stage

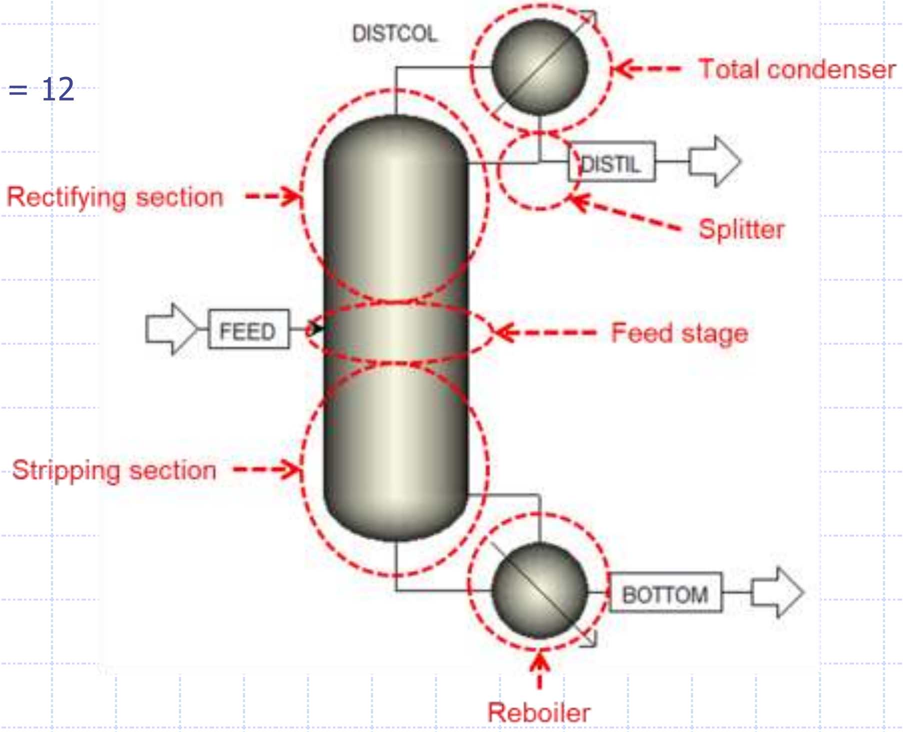
n,m: Heat loss ∀ stage

2: number of stages n,m

1: Reflux ratio

2: LK,HK recovery

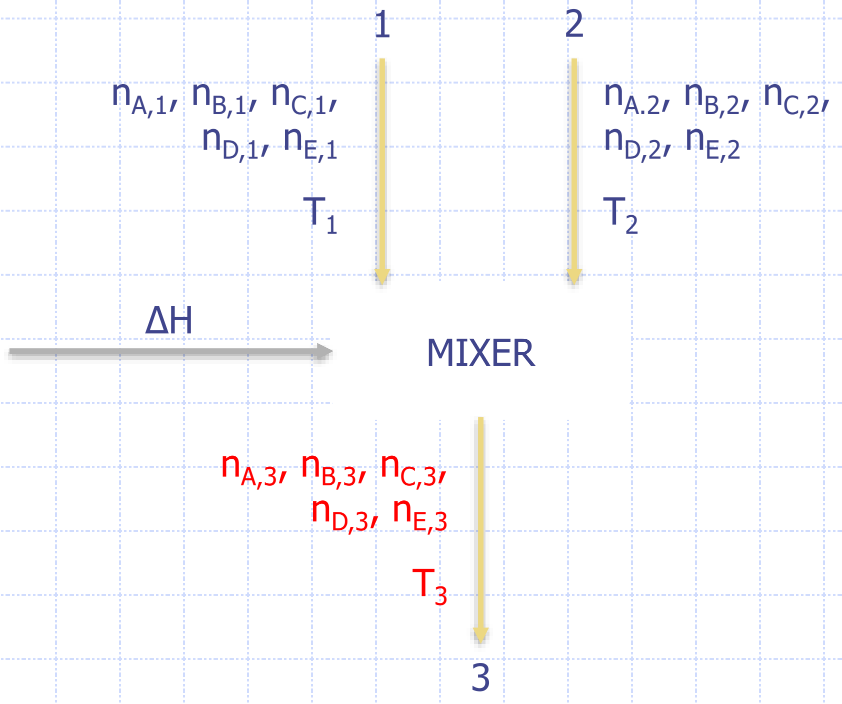
6: T,P condenser, reboiler, splitter



DoF Analysis of a Single Unit Operation

- Two streams (1,2) are mixed adiabatically
  - Each stream may contain any of five components (A, B, C, D, E)
  - No phase changes take place
  - The heat capacity of all components may be approximated as constants and the heat of mixing can be neglected
  - Calculate the component molar flow rates and T of the product stream from specified values of these quantities for the feed streams
- Solution
  - 5 + 1 (Temp) unknowns
  - 5 material balance equations
  - 1 energy balance ΔH = 0 equation

$$\Delta Q_2 = \Delta Q_{tot}$$



1

2

$n_{A,1}$, $n_{B,1}$, $n_{C,1}$, $n_{D,1}$, $n_{E,1}$

T_1

$n_{A.2}$, $n_{B,2}$, $n_{C,2}$, $n_{D,2}$, $n_{E,2}$

T_2

ΔH

MIXER

$n_{A,3}$, $n_{B,3}$, $n_{C,3}$, $n_{D,3}$, $n_{E,3}$

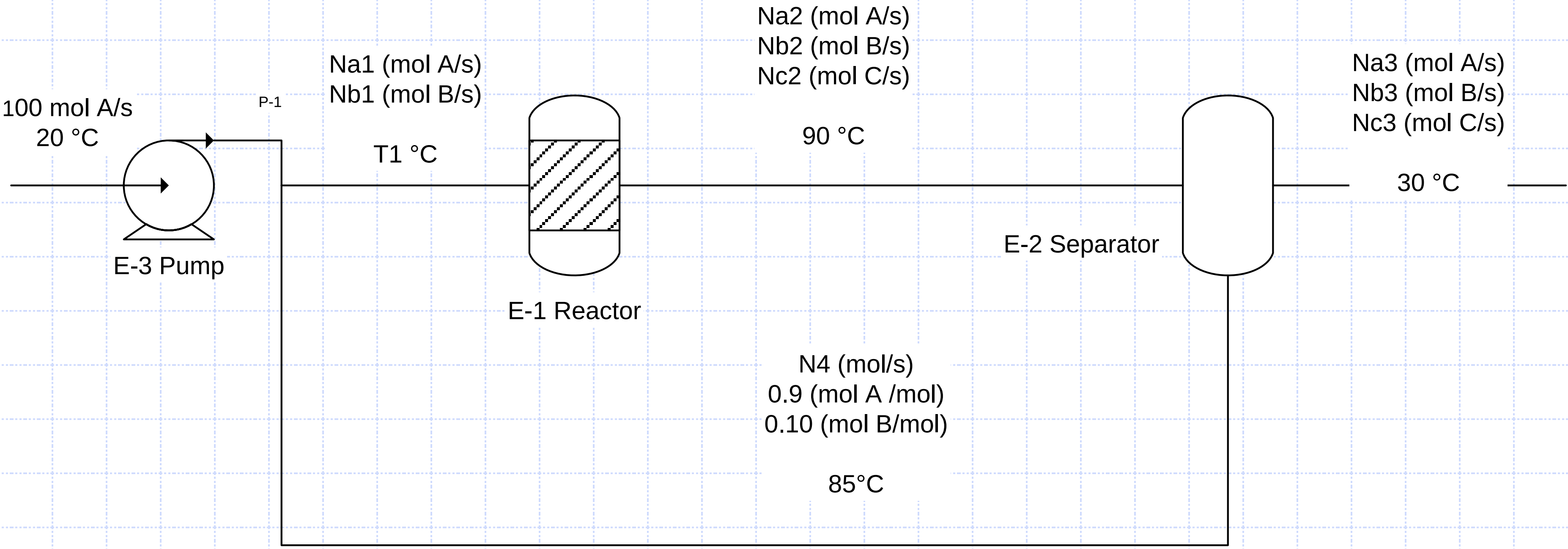
T_3

3

- MS Excel solution
- Process Simulator solution

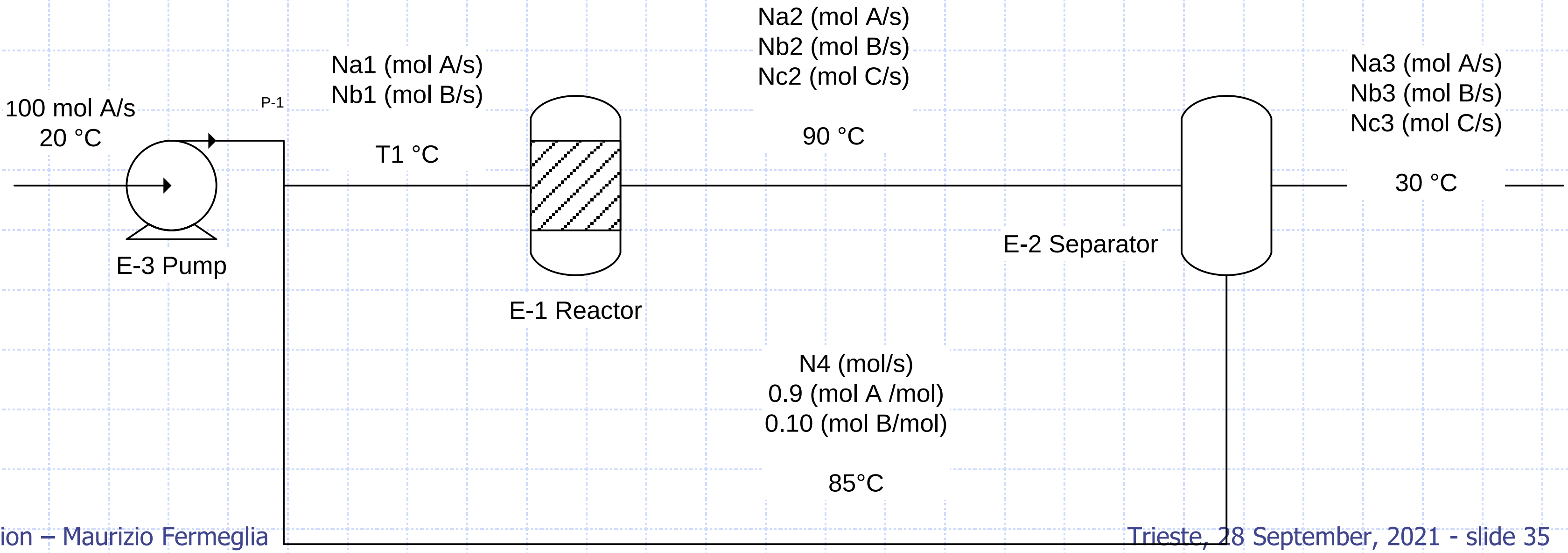
DoF of a Cyclic Process

- Gas-phase dehydrogenation of isobutane to isobutene
  - Reaction: A → B + C $C_4H_{10} \rightarrow C_4H_8 + H_2$
  - Pure isobutane (A) is mixed adiabatically with a recycle containing 90% mole isobutane and the balance isobutene (B)
  - Single pass isobutane conversion is 35%
  - All hydrogen (C) and 10% of the isobutane (as well as some isobutene) is sent to another part of the plant
  - Qr and Qs are the net rate of heat transfer in the reactor and separator



DoF of a Cyclic Process

- Unit operations
  - Mixing point:
    - Nv: 4 unknowns (Na1, Nb1, N4, T1); Nr: 3 eq. (2 Material Bal., 1 Energy Bal.) → **Ni: 1 local DoF**
  - Reactor
    - Nv: 7 unknowns (Na1, Nb1, Na2, Nb2, Nc2, T1, Qr); Nr: 4 eq. (2 Comp. Bal., 1 Energy Bal., 1 conversion spec.) → **Ni: 3 local DoF**
  - Separator
    - Nv: 8 unknowns (Na2, Nb2, Nc2, Na3, Nb3, Nc3, N4, Qs); Nr: 5 eq. (3 Material Bal., 1 Energy Bal., 1 split spec.) → **Ni: 3 local DoF**
- Overall process
  - 7 local DoF (1+3+3); 7 ties (Na1, Nb1, Na2, Nb2, Nc2, N4, T1 counted twice) → **0 DoF**

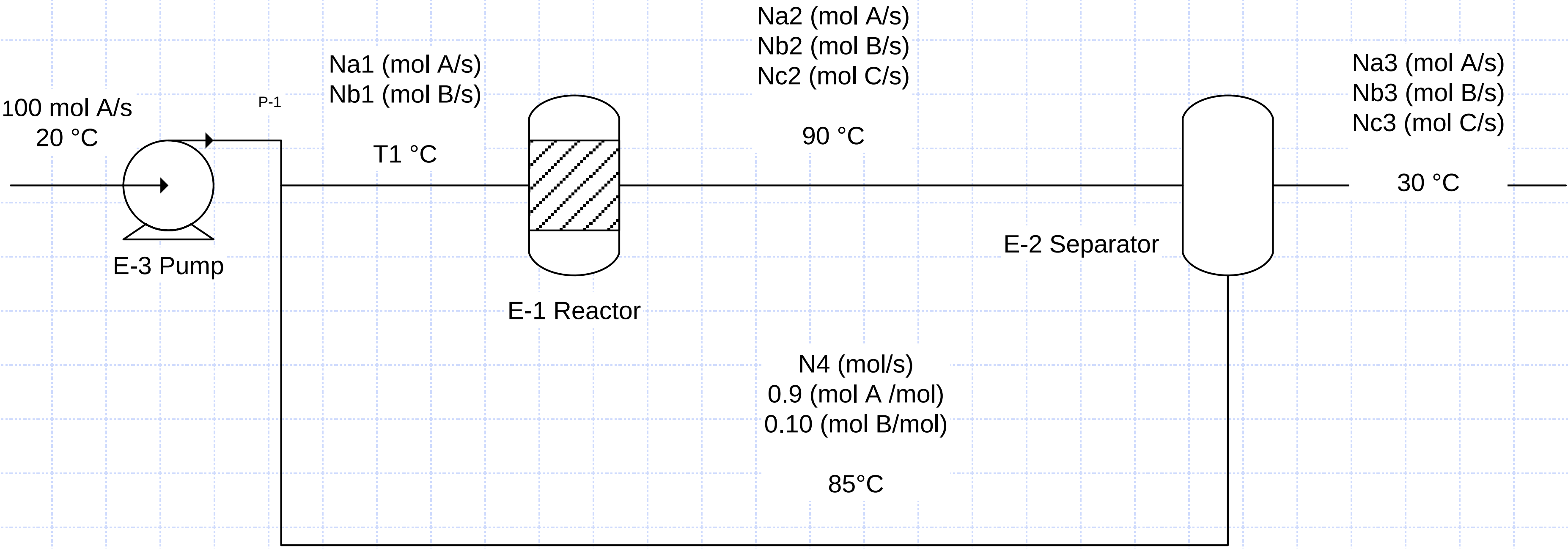


DoF of a Cyclic Process

MS EXCEL solution

- Initial estimate of the recycle set to 100 mol/s and assumed value of mixing point temperature of 50°C.
- The value of N4a is varied until the calculated recycle flow rate (N4c) equals the assumed value of N4a that drives the value of (N4a-N4c) to zero.
- Once the flow rates are correct, the mixing point temperature will be varied to determine the values that drives ΔH =0 for the adiabatic mixer

Process simulator solution



Spreadsheets: very tempting but be careful!

- Hidden equations?
- Range checking?
- Hidden/implicit defaults?
- Thermo physical properties?
- Do you REALLY know what it does?
- Has it really been validated on YOUR kind of problem?
- Has it been properly documented?

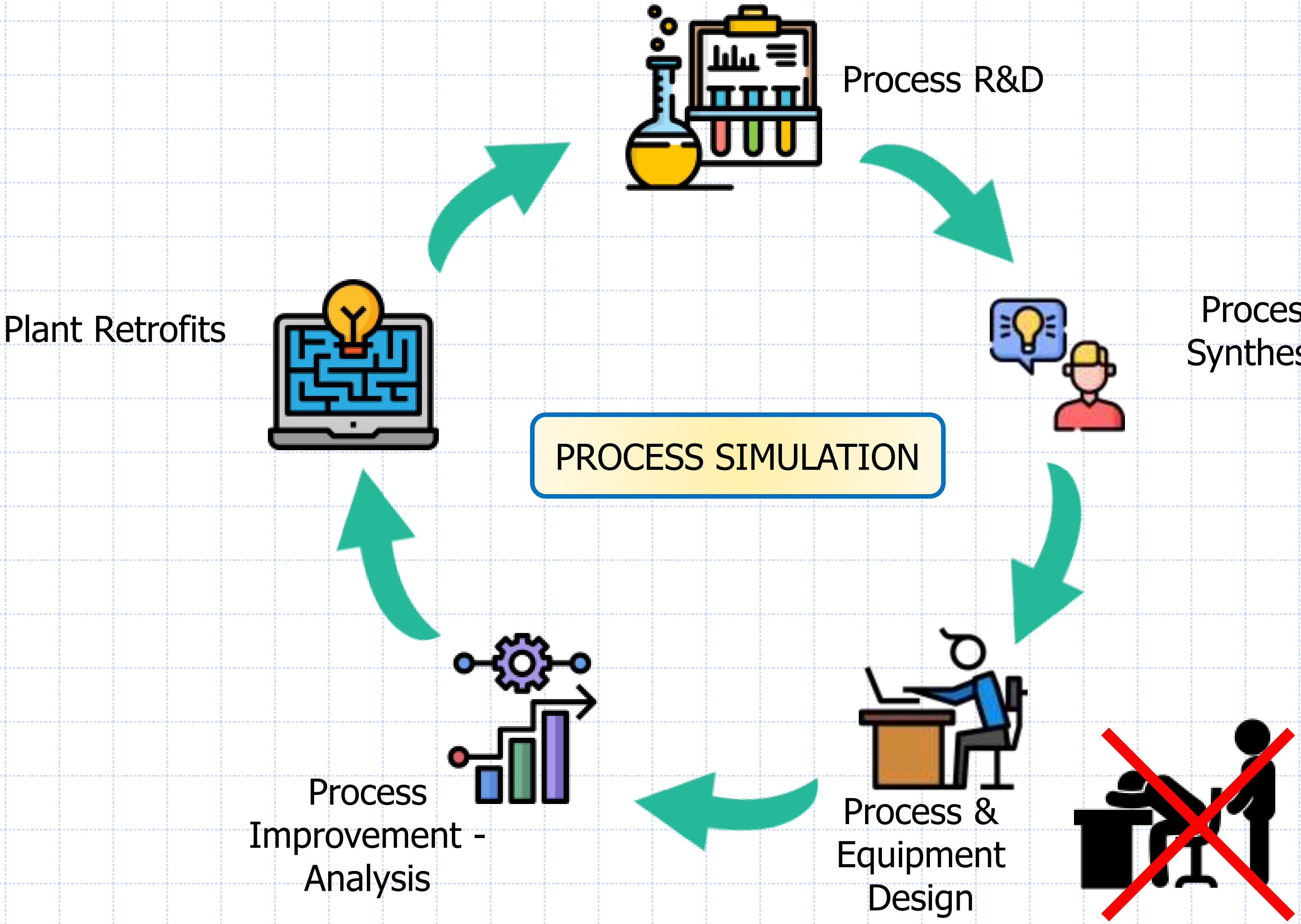
Spreadsheets vs Process Simulator

Easy to use	Requires a training
Free of charge (more or less)	License is usually needed
Shareable results	Export of results
Self-implemented system	Use of existing unit operation
Simple systems	Complicated flowsheets
Basic Thermophysical prop	Advanced Thermophys prop
Lack of Thermodyn models	Plenty of Thermodyn models
Limited to user knowledge	Experts’ know-how
Simple convergence	Sensitivity, Optimization
Info not available	Documentation
Not validated	Numerous validation

Fundamentals

- Different possibilities for process simulation
  - Steady state simulation
  - Dynamic simulation
  - Integrated steady state - dynamic simulation (new feature)
- Different stages in process design
  - Process synthesis: identification of the optimal choice of units and the connection between them, selection of solvents,…
  - Process design and simulation: establishment of the optimal operating conditions and definition of each unit operation
  - Process analysis: study the effectiveness of design in the light of operational consideration (flexibility, controllability, safety, environmental effects, …)
- Process simulation impact on industry
  - The way engineering knowledge is used in processes
  - The design procedure of the process (plant)

Process simulation and the Engineering Work Process



Process R&D

Process Synthesis

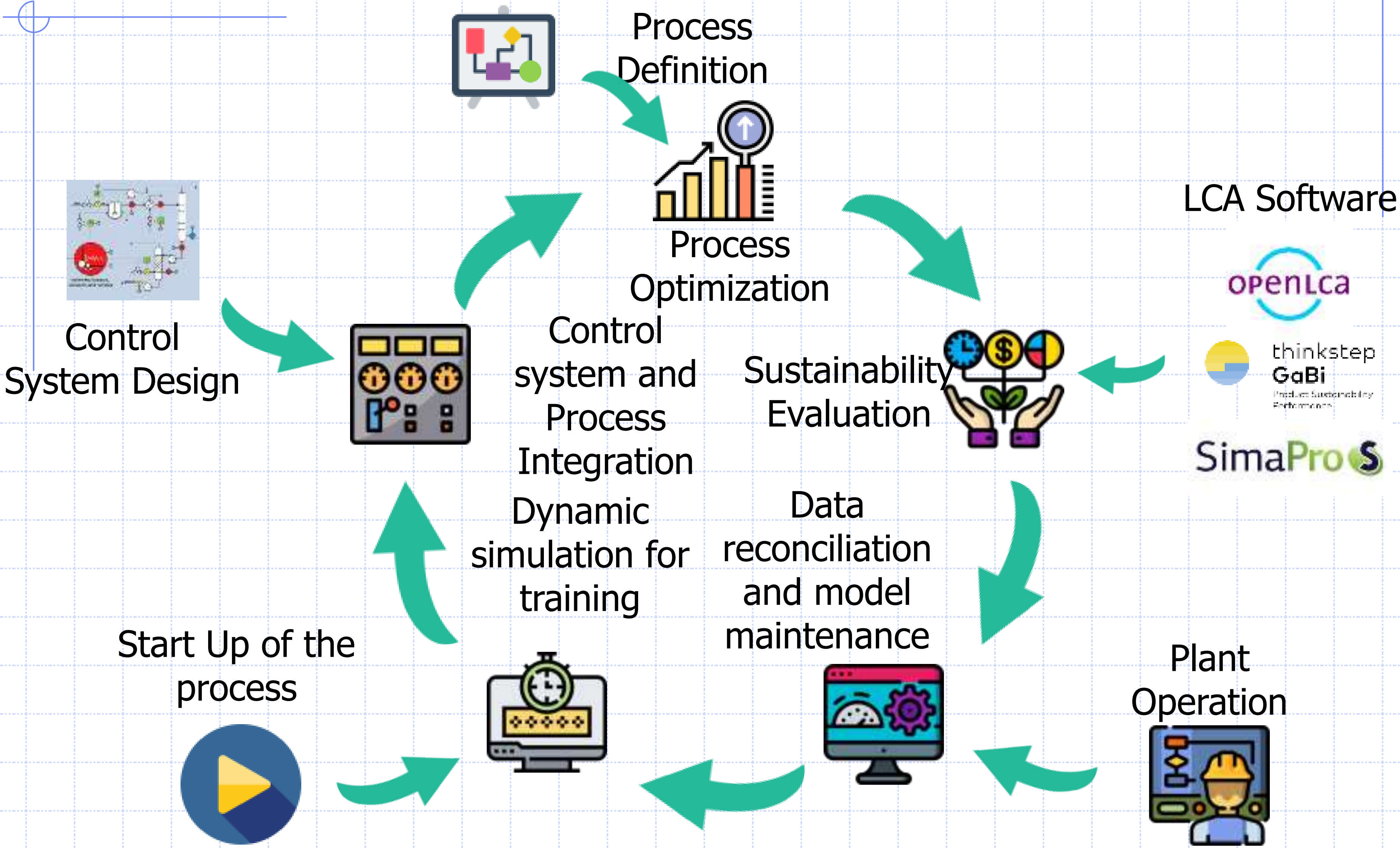
Process & Equipment Design Simulation

Process Improvement - Analysis

Plant Retrofits

PROCESS SIMULATION

The “Life Cycle” of a process



Process Definition

Process Optimization

Sustainability Evaluation

LCA Software

openLCA

thinkstep GaBi

SimaPro

Data reconciliation and model maintenance

Plant Operation

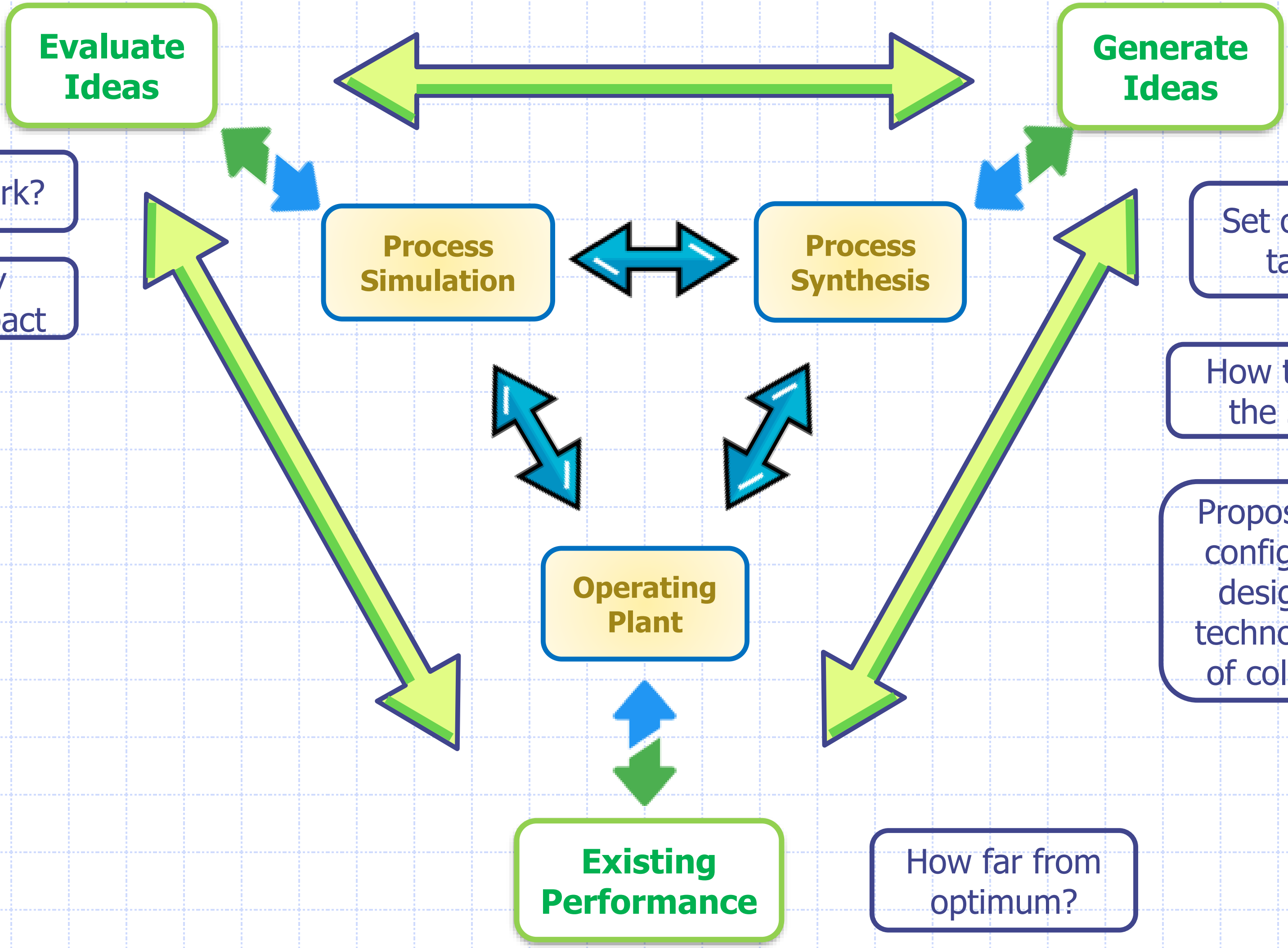
Dynamic simulation for training

Start Up of the process

Control system and Process Integration

Control System Design

Integration of Process Synthesis & Process Simulation



Evaluate Ideas

Generate Ideas

Process Simulation

Process Synthesis

Operating Plant

Existing Performance

Does it work?

Quantify «real» impact

Set objective targets

How to change the system?

Propose process configuration & design (Pinch technology, train of columns, …)

How far from optimum?

A new paradigm

From a traditional use of Process Simulation …

- Flowsheet Design
- Physical properties and phase equilibria
- Equipment critical parameters definition
  - distillation column stages,
  - column diameter
  - Reactors
- Material and energy balances

… to the comprehensive use of Process simulation in the entire 'life' of the plant.

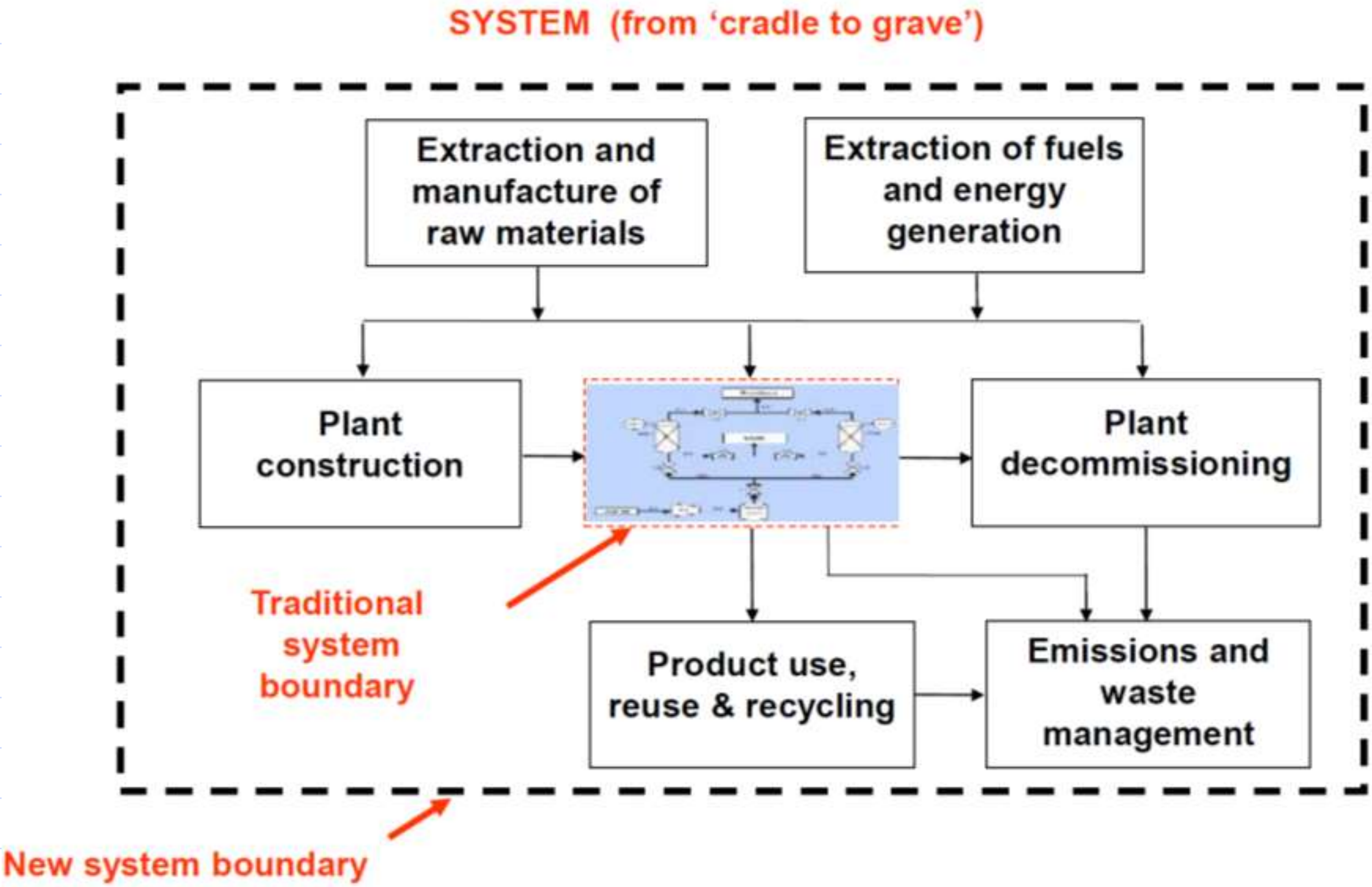
- Control strategies design
- Process optimization (better processes)
- Time evolution of the process
  - start up and shut down
- Risk Analysis
- Operator training
- Reduce the unsteady state operations
- Process synthesis and design
- Maintenance optimization

Model perspectives

The details of the model depend on the scope of the model itself

- Project Design Model
  - Provides Mass and Energy balances for equipment design
  - The main target is the achievement of a desired plant capacity
  - Not suitable for on-line optimization or plant studies (fixed flowrate)
  - Adopts rigorous unit operations
- Plant Operation Model
  - The main goal is the optimization of a single or a few unit operations
  - Rigorous model for key unit operations only
  - Easier to create and to tune up
- On-line Optimization Model
  - The scope is the optimization of plant operations on a wide perspective
  - Can handle a plethora of operating conditions
  - Rigorous approach for unit operations with high economic impact
  - Rather complex to create and handle
  - Have to run efficiently in order to provide reliable on-time information regarding process set point

Issues: system boundary definition



SYSTEM (from 'cradle to grave')

Extraction and manufacture of raw materials

Extraction of fuels and energy generation

Plant construction

Plant decommissioning

Product use, reuse & recycling

Emissions and waste management

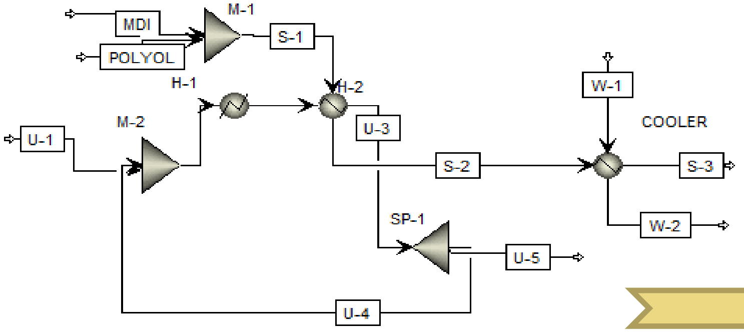
Traditional system boundary

New system boundary

Process simulation, multiscale modeling and life cycle assessment

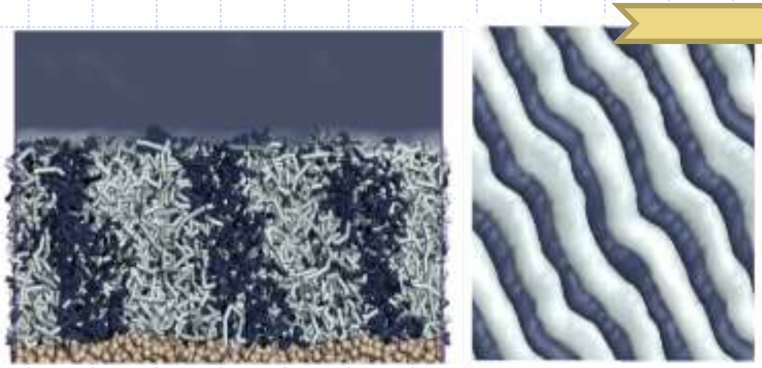
Process design

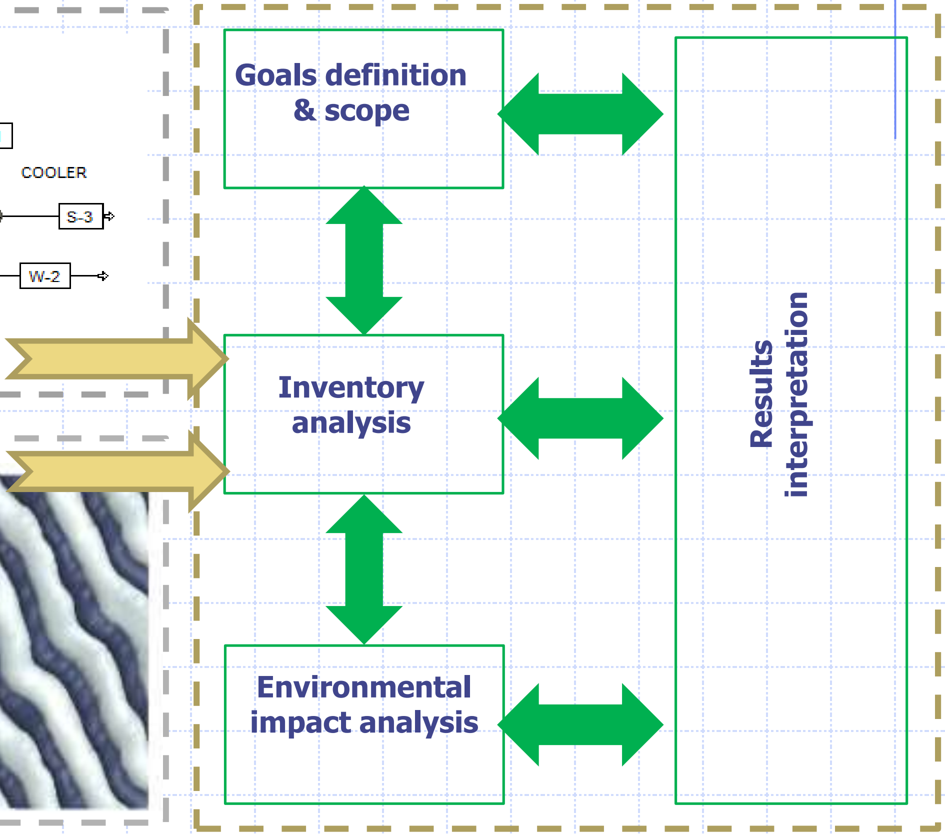
Material and energy balances



Product design

Multiscale modeling for material properties





Goals definition & scope

Inventory analysis

Environmental impact analysis

Results interpretation

Benefits of process simulation

- Partial or total replacement of Pilot Plant operations
  - Reduction of the number of runs
  - Runs planning
- Reduction of Time to market for the development of new processes
  - New processes
  - Modification of existing processes (different solvent,...)
  - Production of new materials
- Fast screening of process alternatives to select the best solution
  - What-if analysis
  - economic aspects
  - environmental aspects – emission studies
  - energy consumption aspects
  - flexibility of the proposed process – MOC (Management of Change)

Simulation Trends

- Move to increase simulation usage in operating environment
- Increased trend to integrate and link applications
- Desire for common interfaces to reduce learning curve
- Linking of simulation technology to control systems and plant data
- Integration of steady state, dynamic and real time optimization technologies
- Support of enhanced engineering workflow and productivity
- Enables economic analysis and optimization
- Enhances design and operational decisions
- Use web infrastructure to improve/monitor process

Some VERY IMPORTANT Principles:

- the program is an AID in making calculations and decisions: YOU must ensure that it is "fit for purpose"
- YOU are responsible for any results you generate and for any use which you make of them
- It is your PROFESSIONAL, ETHICAL & LEGAL RESPONSIBILITY to take care and to exercise good judgement
- In essence a program is no different to a pencil & paper

User’s Guidelines: Some Very Basic Advice!

- Think very hard about your OBJECTIVES
  - Your objective is NOT to develop a model, it is to solve an engineering problem? Never lose sight of this!
- Keep it SIMPLE
  - Start EXTREMELY simple: this needs less data, is easier to get going, provides a sound basis for anything more complex and may even satisfy your objectives
- Explore SENSITIVITIES
- Add detail SELECTIVELY
  - ONLY where you NEED it and only a bit at a time: adding detail means adding problems! Detailed models need more data, which you often don’t have and have to guess anyway. So use rigorous model only when necessary or feasible

User’s Guidelines: Solving the equations

- Have you achieved calculation conversion?
  - check what that actually means: converged doesn’t necessarily mean right!
  - Any sign of asymptotic behaviour?
- Make sure you understand any error/warning messages
- Any problems?
  - check the input data again
  - is the combination of specifications physically realistic?
  - could you use a simpler model to “get things moving in the right direction”?

User’s Guidelines: Checking the results

- Assess the results against your defined objectives:
  - do they make engineering sense?
  - are they within expected bounds?
  - are they within valid ranges of (eg) thermo?
  - can all “surprises” be explained in engineering terms?
- Check sensitivity of your results to input data, assumptions, etc
- Add detail where NECESSARY

Q: Why PS is important?

- Because it represent with high accuracy the real world
- Because it allows to focus on the interpretation of the results rather than on the methods for obtaining the results
- Because it allows a global vision on the process engineering by assembling theories and models
- Because it is essential in the design of new and existing processes
- Because it is a simple tool for treating real cases

User’s Guidelines: Input data: KIS

- Get the units of dimension right!
- Make sure the specifications are consistent and feasible!
- Does the program correctly understand your problem definition? (check any data-reprint/summary very carefully)
- Does it use any default values & are they suitable for your problem?
- ESPECIALLY check the thermophysical property data (and then check it again!)
- Old models & data for a new problem? Be careful!

Q: Which are the limitations?

- No equipment design nor momentum balances
- Models of some important units missing
- Multiple solutions for flowsheeting and poor recycle convergence
- PS is a tool: it cannot interpret results
- Thermodynamic modeling is of paramount importance (accuracy and reliability is still questionable…)
- Kinetic models
- Availability of parameters must be checked
- Calibration of the results versus existing data is necessary
- Time scale of some phenomena are still crucial (reaction, fluid dynamic,..)
- Changing results depending on simulators release data

- Avoid the GIGO….. Approach = garbage in gospel out

Q: Common Sources of Problems?

- model/program does not apply to your problem
- errors in input data, inappropriate defaults
- over-complication: Keep It SIMPLE!
- units of measurement
- convergence problems: ignoring error & warning messages
- applying models or data outside their range of validity
- failure to consider transients

Q: Common Sources of Problems?

- Thermophysical Properties
  - Basic validity of model?
  - Data from different sources (especially mixture data)?
    - Is the data valid for YOUR mixture under YOUR conditions?
    - Potential Azeotropes (real or imaginary!)?
  - Extrapolation properties:
    - Ranges of validity (composition too)?
    - Anywhere near any of the critical points?
    - Transients?
    - Convergence paths?
  - Trace components can be important
- Sensitivity analysis
  - "Pre-flight drill"!

Industrial Processes are complex

To get benefits from process simulations one must
CRITICALLY SIMPLIFY THE PROCESS

⬇

The need of engineering knowledge and experience.

Process simulation is a simple and helpful tool…

…

… to be used by chemical engineers that fully
understand the process!!!

Process simulation is a simple and helpful tool…

… to be used by chemical engineers that fully understand the process

When using a mathematical model, careful attention must be given to the uncertainties in the model – *Richard Feynman*

… Never let a kid play with a Kalashnikov (AK37)….

Conclusions

- Process simulation is a powerful methodology for
  - Material and energy balances in steady state conditions
  - Material and energy balances in dynamic condition
  - Investigation of process dynamics and batch process
  - Implementation of a control strategy
- Process simulation is applicable in different field of the process engineering
  - Analysis of existing processes (optimization, de-bottlenecking,...)
  - Synthesis of new processes (solvent selection, environmental impact,...)
  - Operator training, process dynamics start up and shut down
- Process simulation is applicable in the framework of environmental impact study and sustainable development
  - What if analysis
  - Safety analysis
  - Environmental evaluation
  - New and cleaner processes investigation

DEMO time

Process simulators

- ASPEN+
- COCO- COFE

Home Work

- Install Aspen+ following the procedure reported in the manual
- Install COCO from the link to the SW distribution
  - Available here: https://www.cocosimulator.org/