SPEED

Computer Aided Simulation of Chemical Processes: Day 1

Lecture 1: Introduction

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Computer Aided Simulation of Chemical Processes

Course Objectives

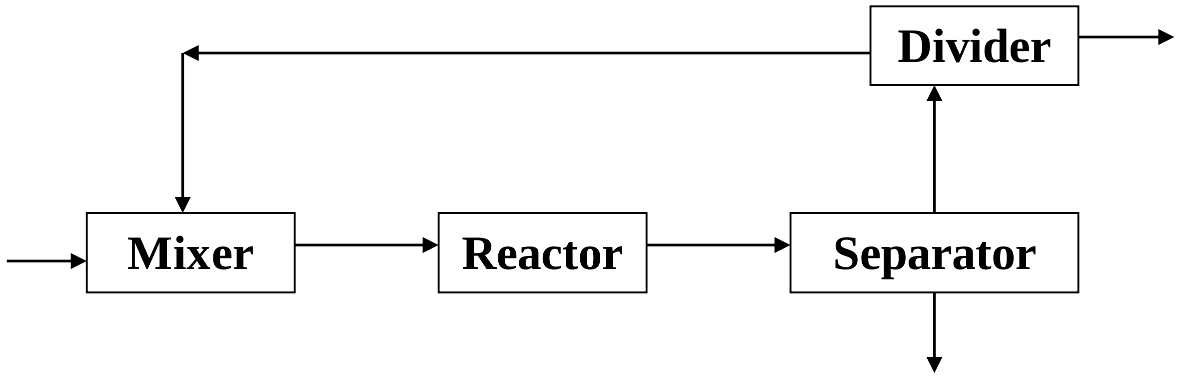
Provide the participants with a clear understanding of the main features of process simulation and how these and related tools (modelling, optimization, integration) can be employed to solve practical problems commonly encountered in process engineering.

Use of computer aided tools will play an important role

What is Simulation?

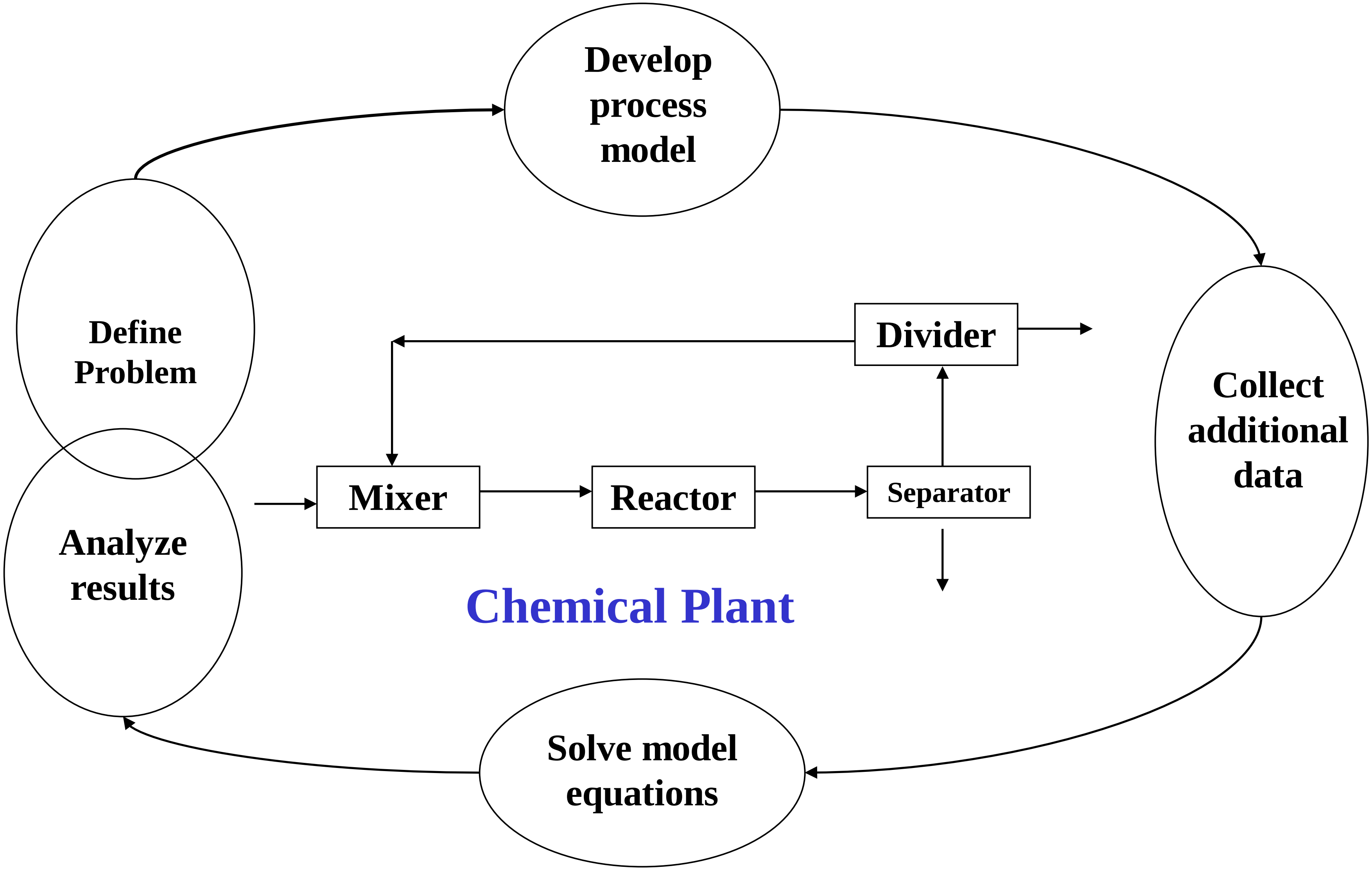
Simulation is the act of representing some aspects of the real world by numbers or symbols which may be manipulated to facilitate their study

Uses of process simulation: Design & analysis a process through simulation/optimization

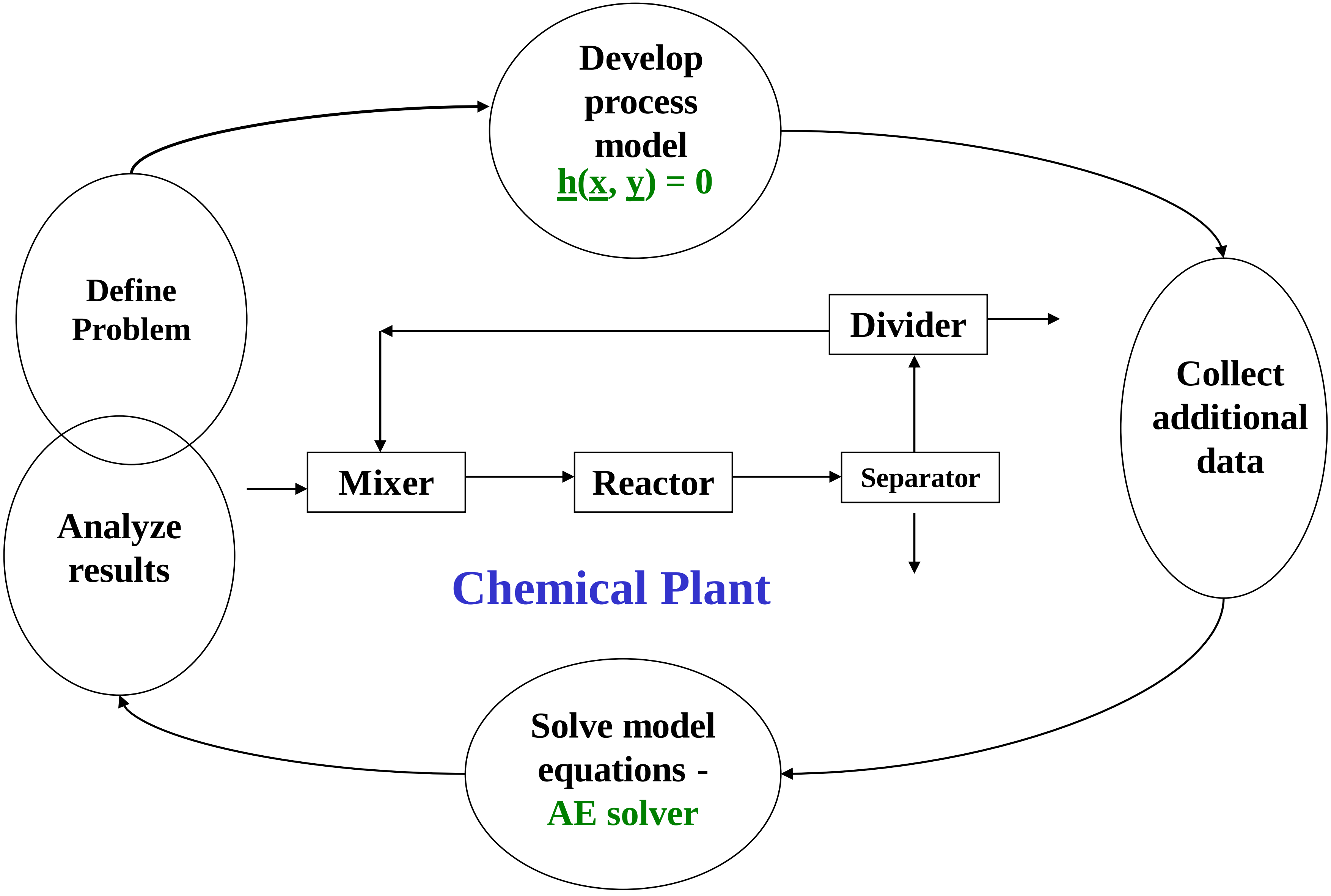


A chemical plant is our *real world*

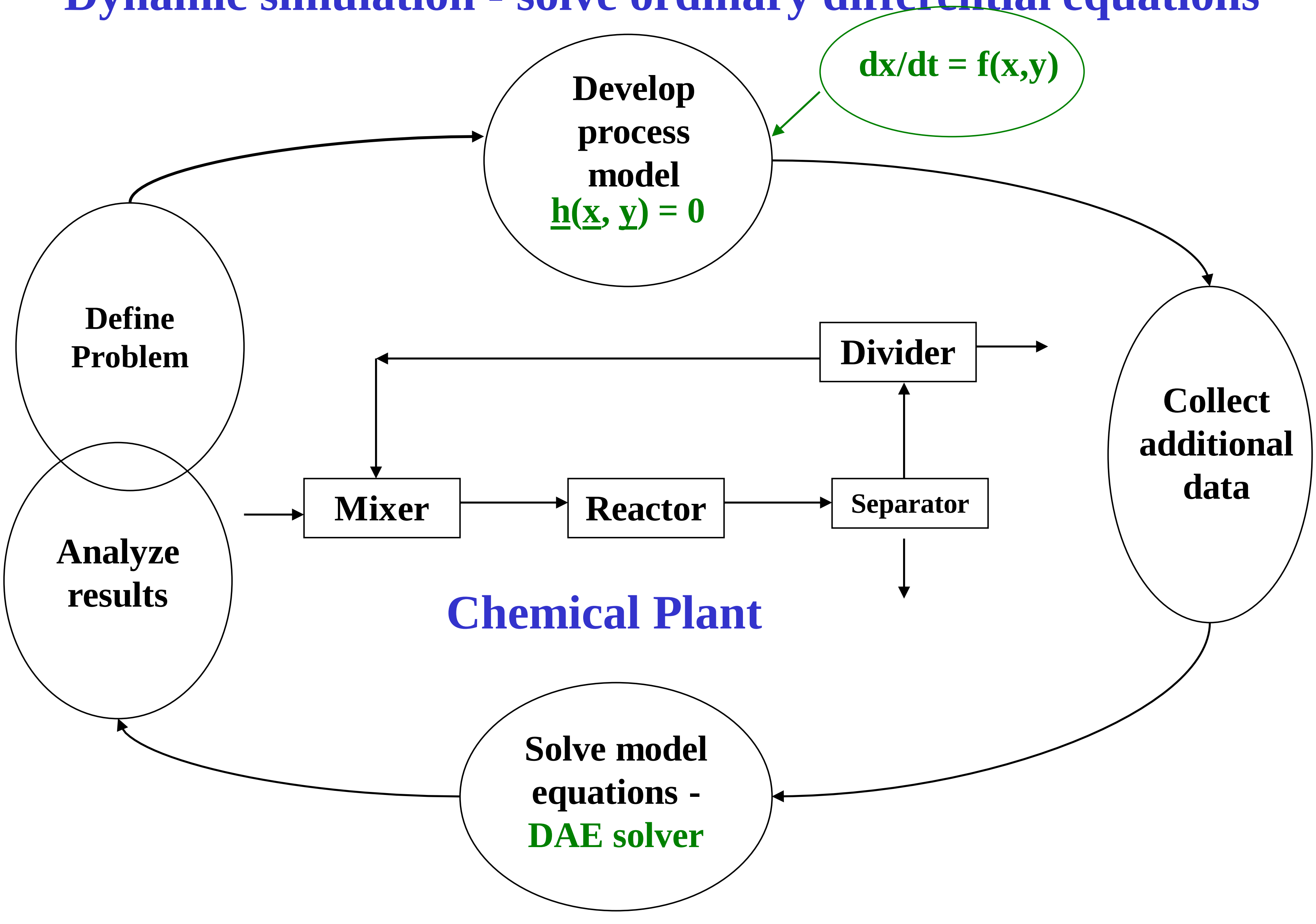
Main steps in process simulation



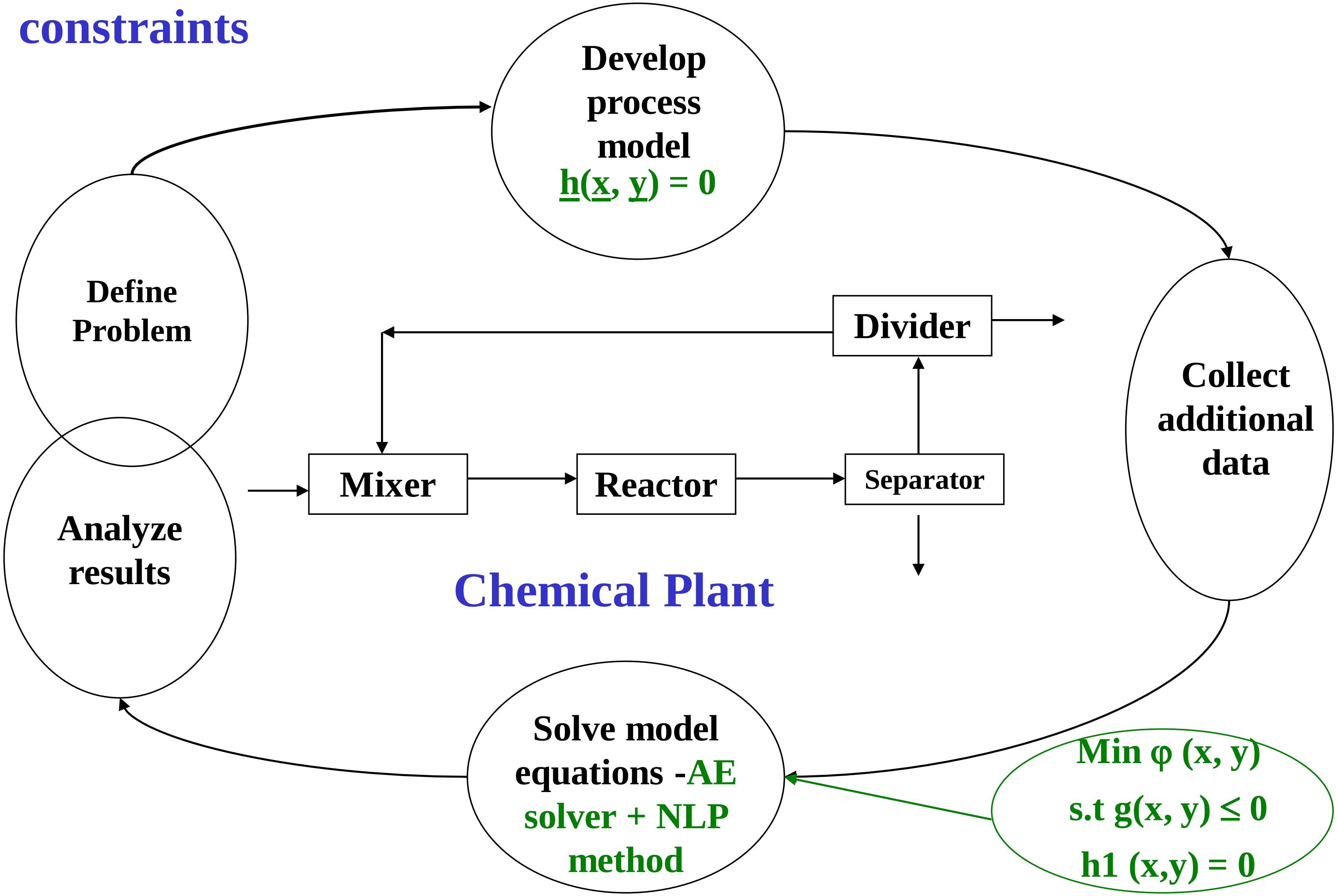
Steady state simulation - solve algebraic equations



Dynamic simulation - solve ordinary differential equations



Simulation based process optimization: minimize function s.t. constraints



Four Types Computer Aided Process Engineering Problems solved through process simulation

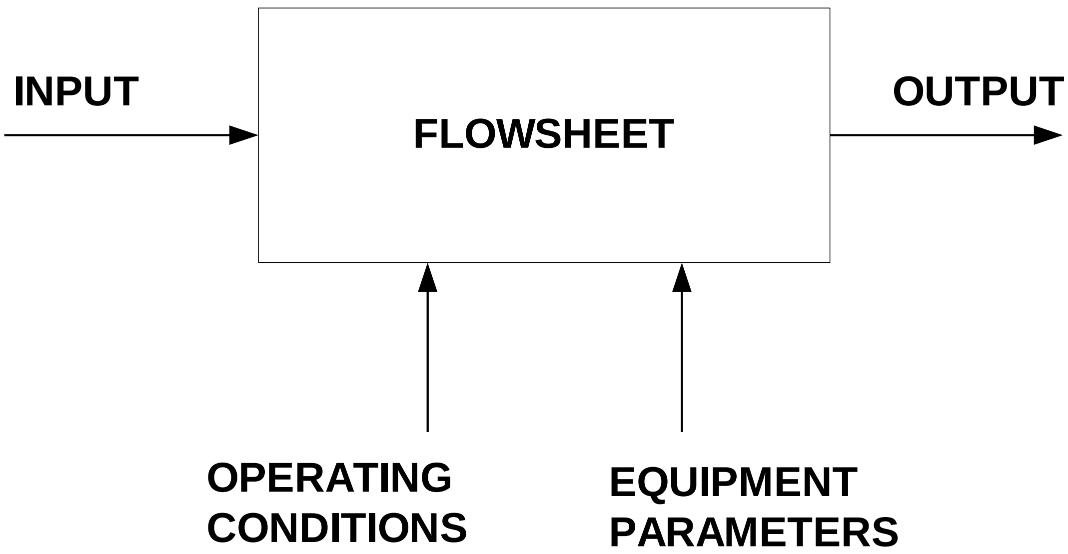
Flowsheeting

Specification (Design)

Optimization (Design)

Synthesis (& Design)

Flowsheeting Problem



***Given* - all incoming information**

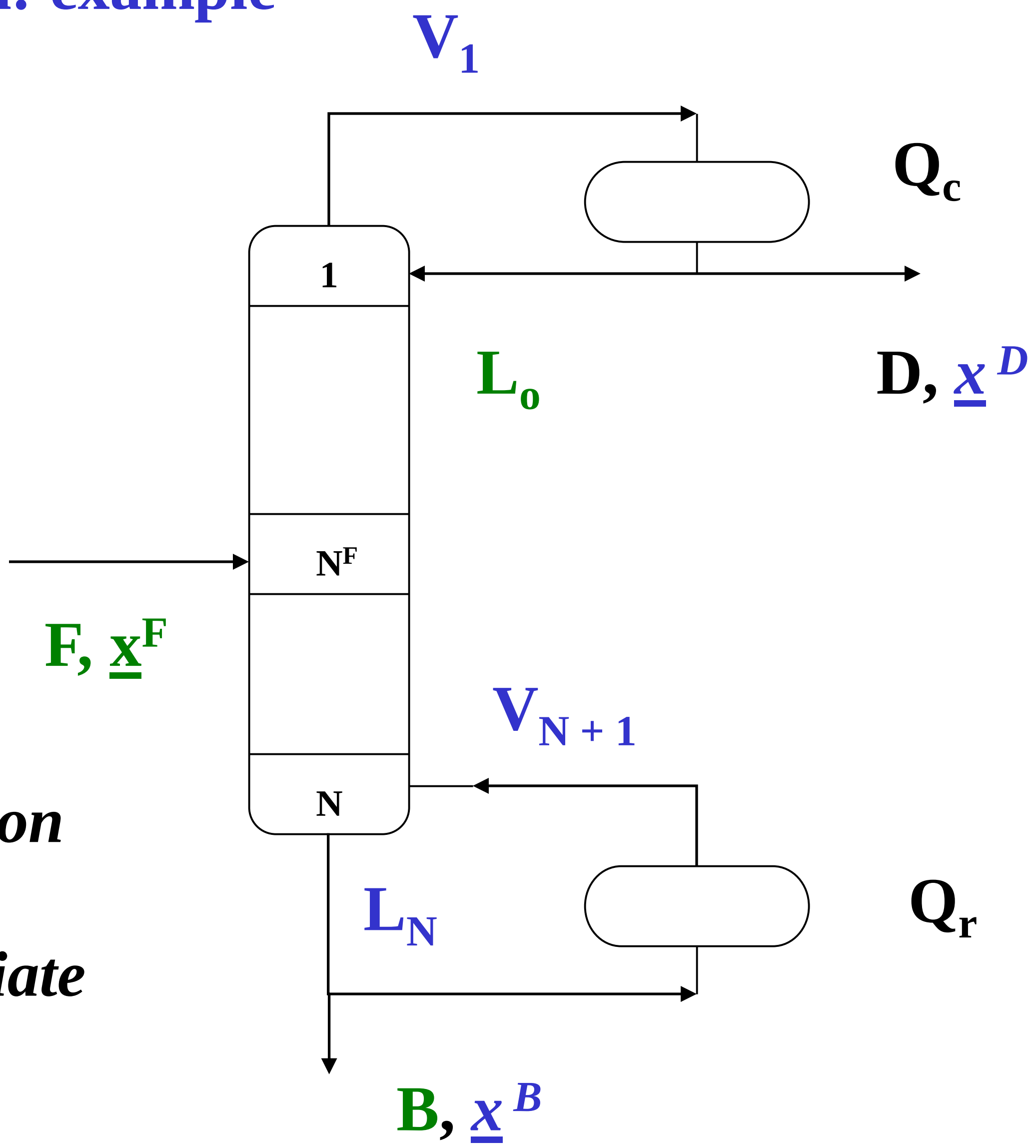
***Determine* - all outgoing information plus internal variables**

Flowsheeting Problem: example

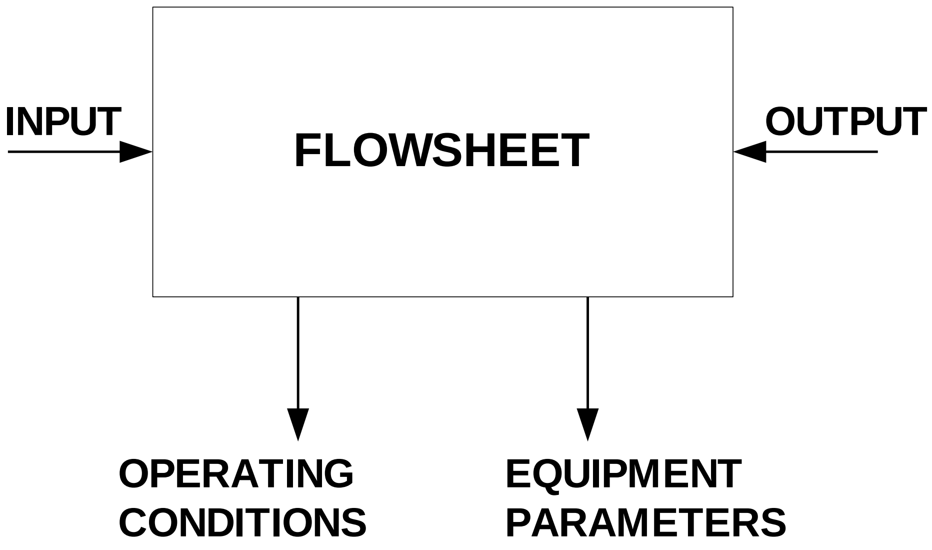
Given - F, $\underline{x}^F$, N, N^F, any one of reflux, Q_r or Q_c; D (or B), & $\underline{P}$

Determine - $\underline{V}$, $\underline{L}$, $\underline{T}$, $\underline{x}_p$, $\underline{y}_p$, $\underline{x}^D$, $\underline{x}^B$, *etc.*

All incoming information is specified while all outgoing and intermediate data is calculated



Specification (Design) Problem



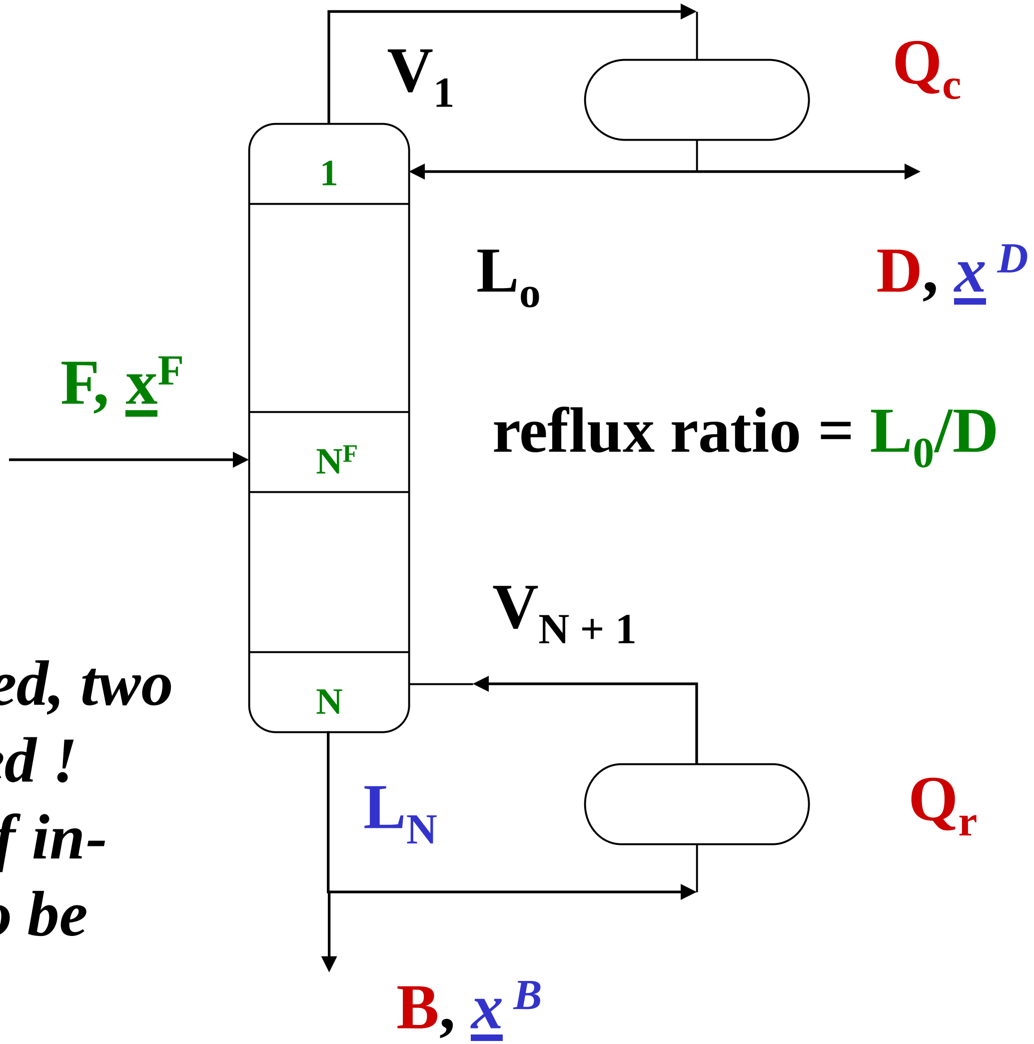
Compared to the flowsheeting problem, instead of all incoming information, some outgoing data is specified. Note that the degree of freedom remains the same !

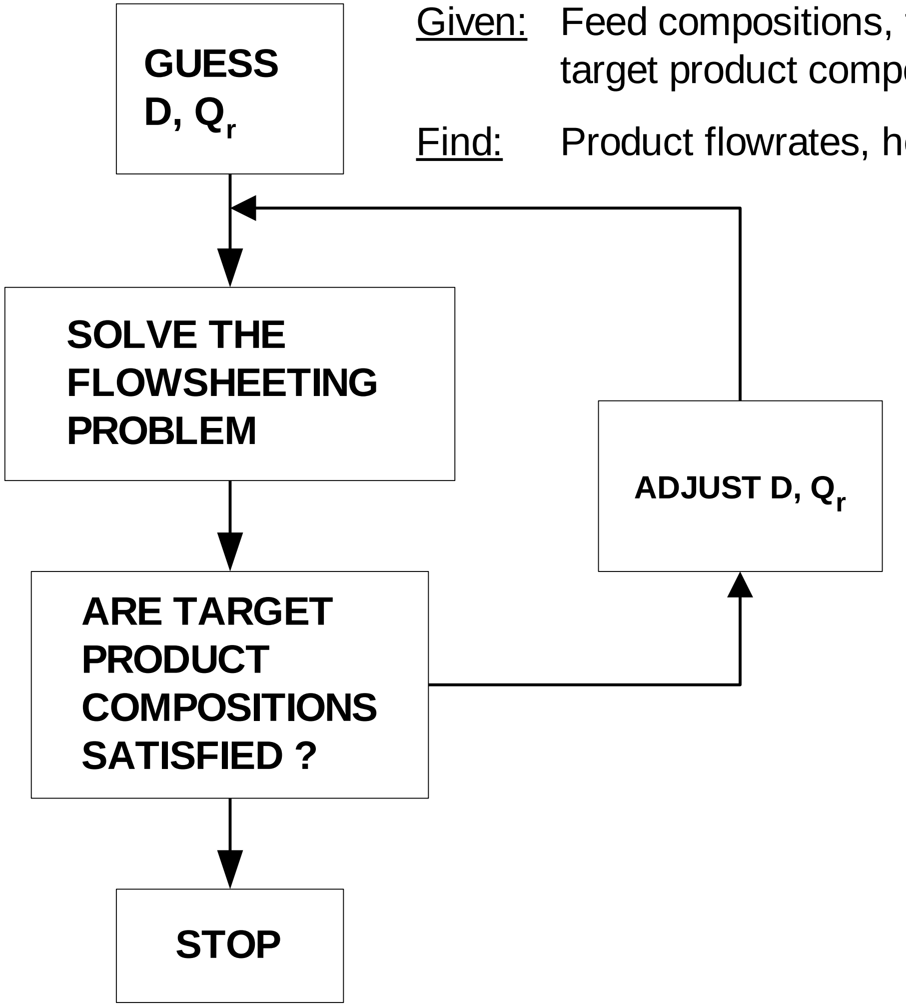
Specification (Design) Problem: example

Given - F, $\underline{x}^F$, N, N^F, x_1^D, x_2^B, $\underline{P}$

Determine - $\underline{V}$, $\underline{L}$, $\underline{T}$, x_p, $\underline{y}_p$, $\underline{x}^D$ (not x_1^D), $\underline{x}^B$ (not x_2^B), RR, D, B, Q_c, Q_r, etc

Instead of all incoming information being specified, two outgoing data are specified ! Thus, the same number of in-going information need to be determined.





Given: Feed compositions, feed flowrates, target product compositions

Find: Product flowrates, heating duties

Calculation procedure for specification problem

Optimization Problem

<u>Given</u>
Feed composition, feed flowrate

<u>Choose</u>
Target product composition
Number of trays, feed tray location

Minimize

Objective = f (yield, energy, capital cost, ….)

Optimization Problem: example

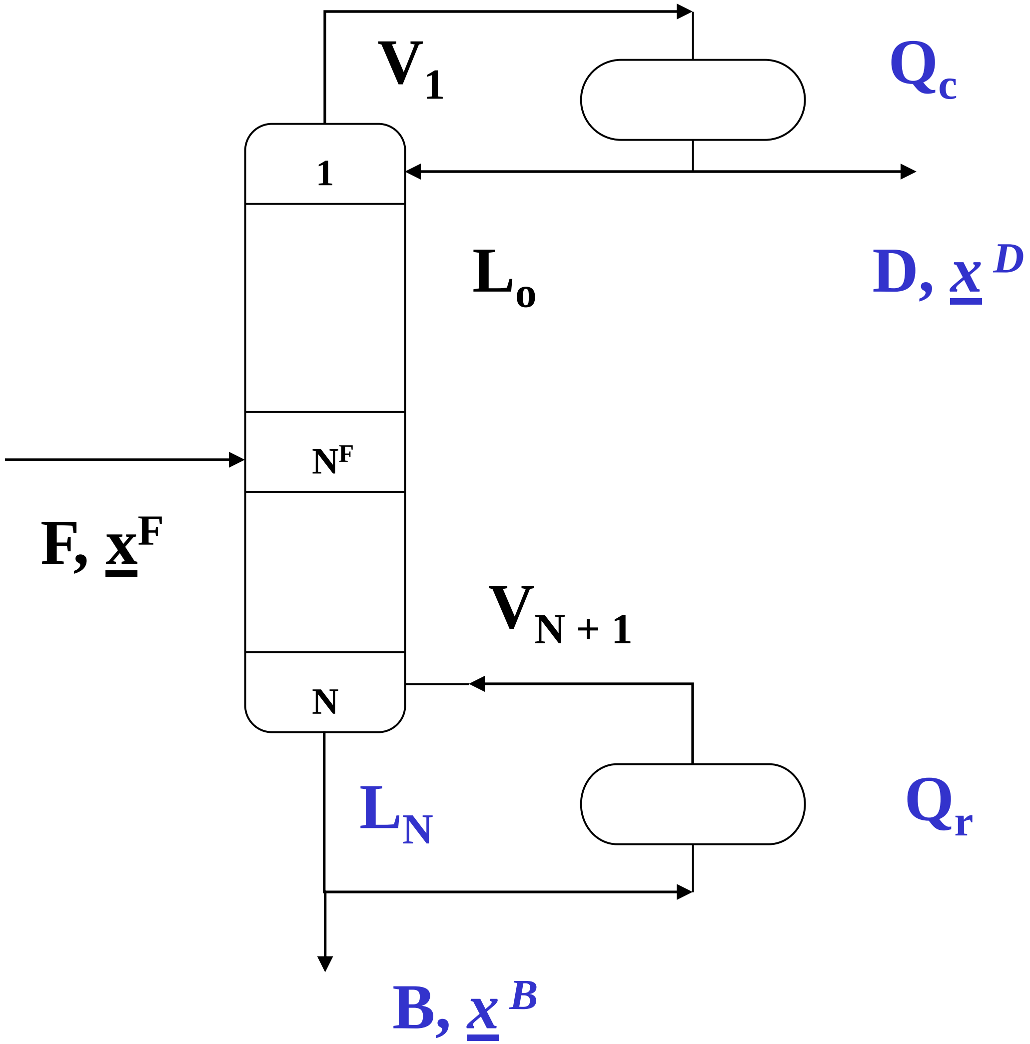
Given - F, $\underline{x}^F$, N, N^F, x_1^D, x_2^B, $\underline{P}$

Determine - $\underline{V}$, $\underline{L}$, $\underline{T}$, $\underline{x}_p$, $\underline{y}_p$, $\underline{x}^D$ (not x_1^D), $\underline{x}^B$ (not x_2^B), RR, D, B, Q_c, Q_r, **etc**

Subject to,

$\varphi(\underline{x}^D, \underline{x}^B, Q_r, Q_c$, *cost data) = minimum, and,*

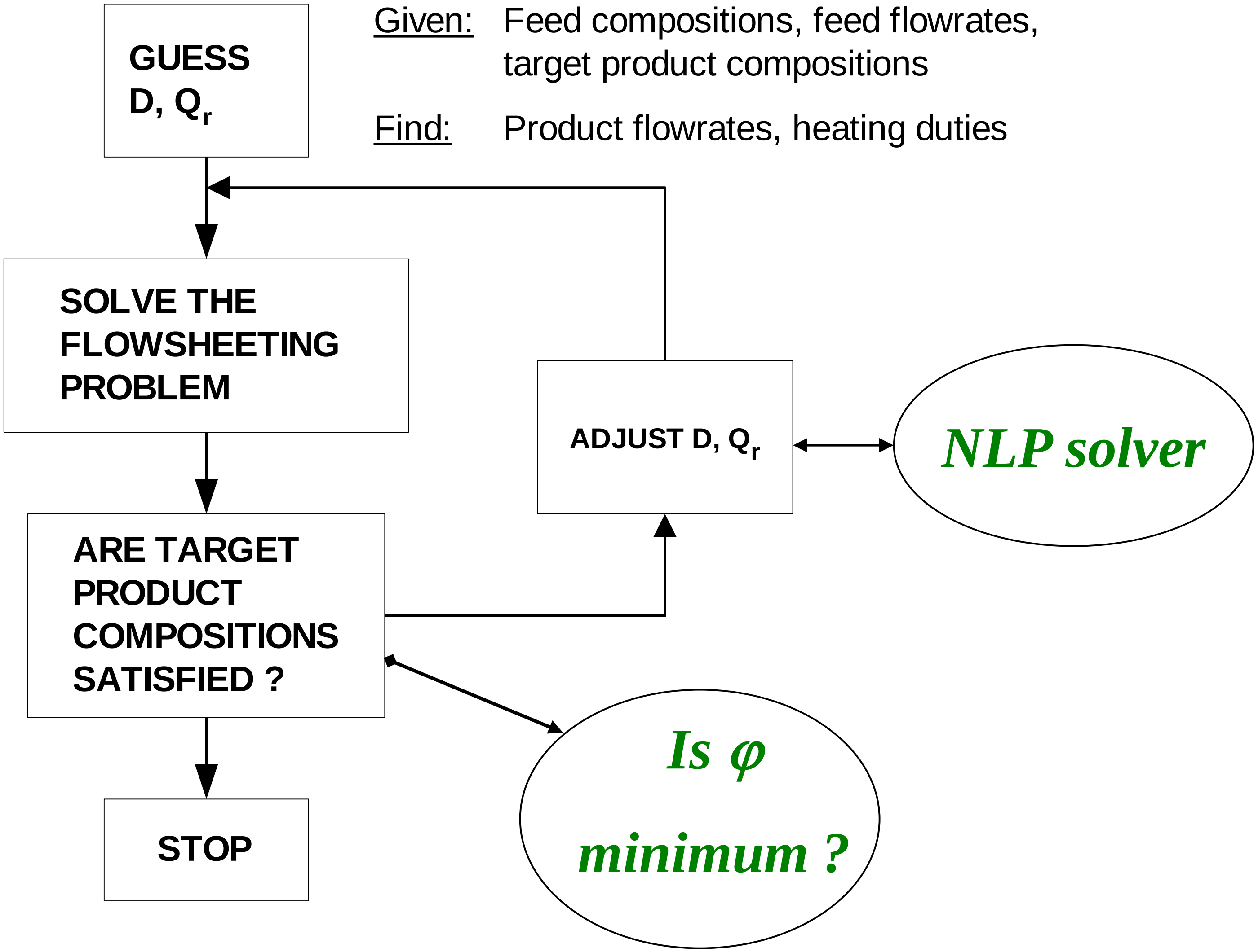
$x_1^D > 0.98$ & $x_2^B > 0.95$



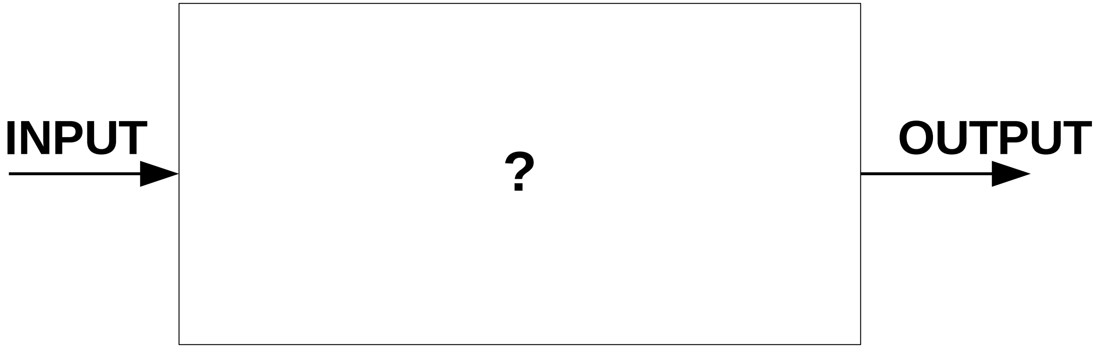
Calculation procedure for optimization problem

Given: Feed compositions, feed flowrates, target product compositions

Find: Product flowrates, heating duties

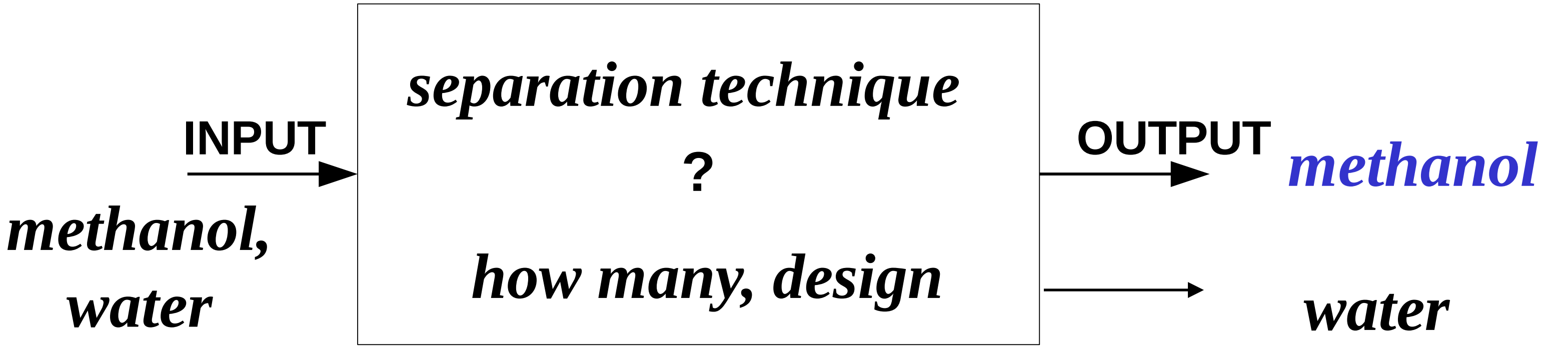


Synthesis (& Design) Problem



Inputs and outputs are known but flowsheet, equipment parameters and condition of operation are unknown !

Synthesis/Design Problem



Separation technique - distillation, flash, extraction, membrane-based separation?

How many unit operations are needed?

What is the design of each equipment?

Synthesis/Design Problem: example

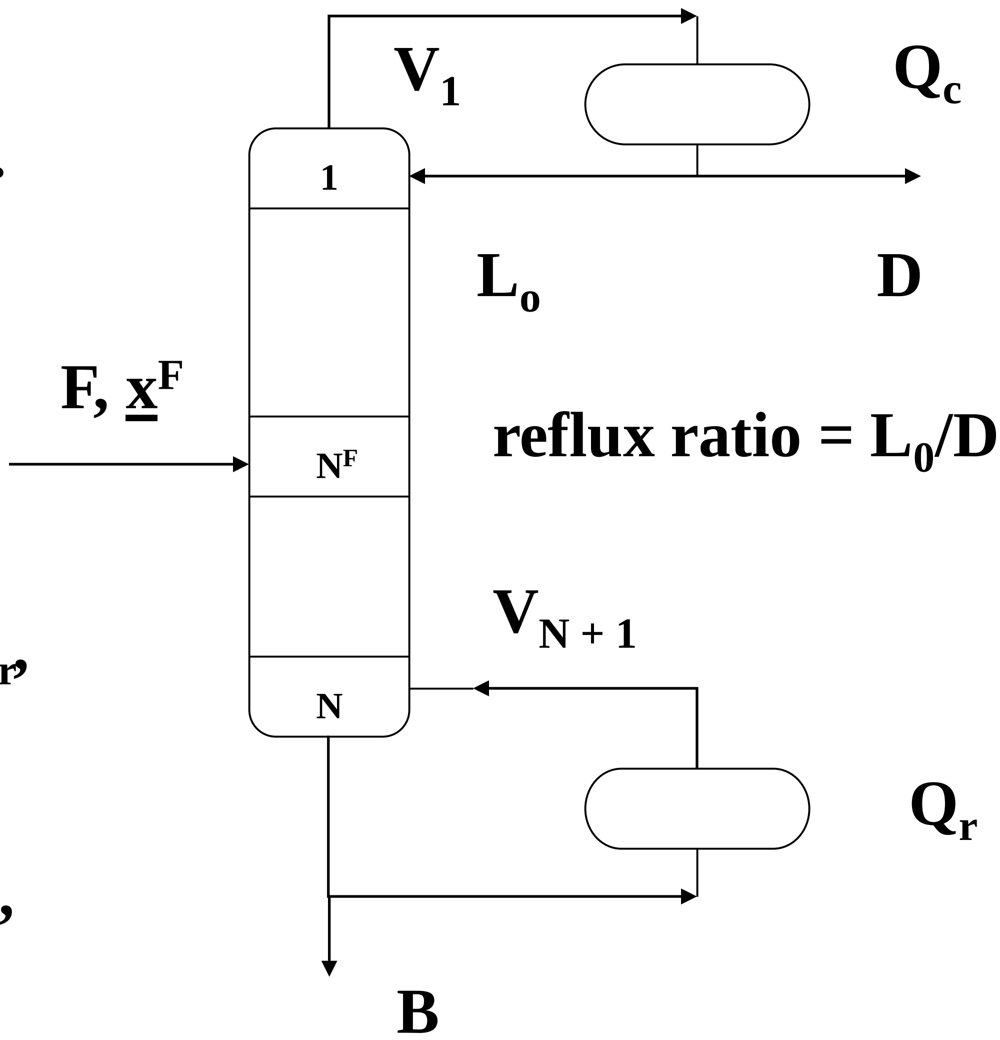
Given *- F, $\underline{x}^F$, x_1^D, x_2^B*

Determine ***- optimal separation unit operation.***

Assume ***distillation has been selected & only one needed***

***Determine**, N, N^F, $\underline{P}$, $\underline{V}$, $\underline{L}$, $\underline{T}$, $\underline{x}_p$, $\underline{y}_p$, $\underline{x}^D$ (not x_1^D), $\underline{x}^B$ (not x_2^B), RR, D, B, Q_c, Q_r,* **etc**

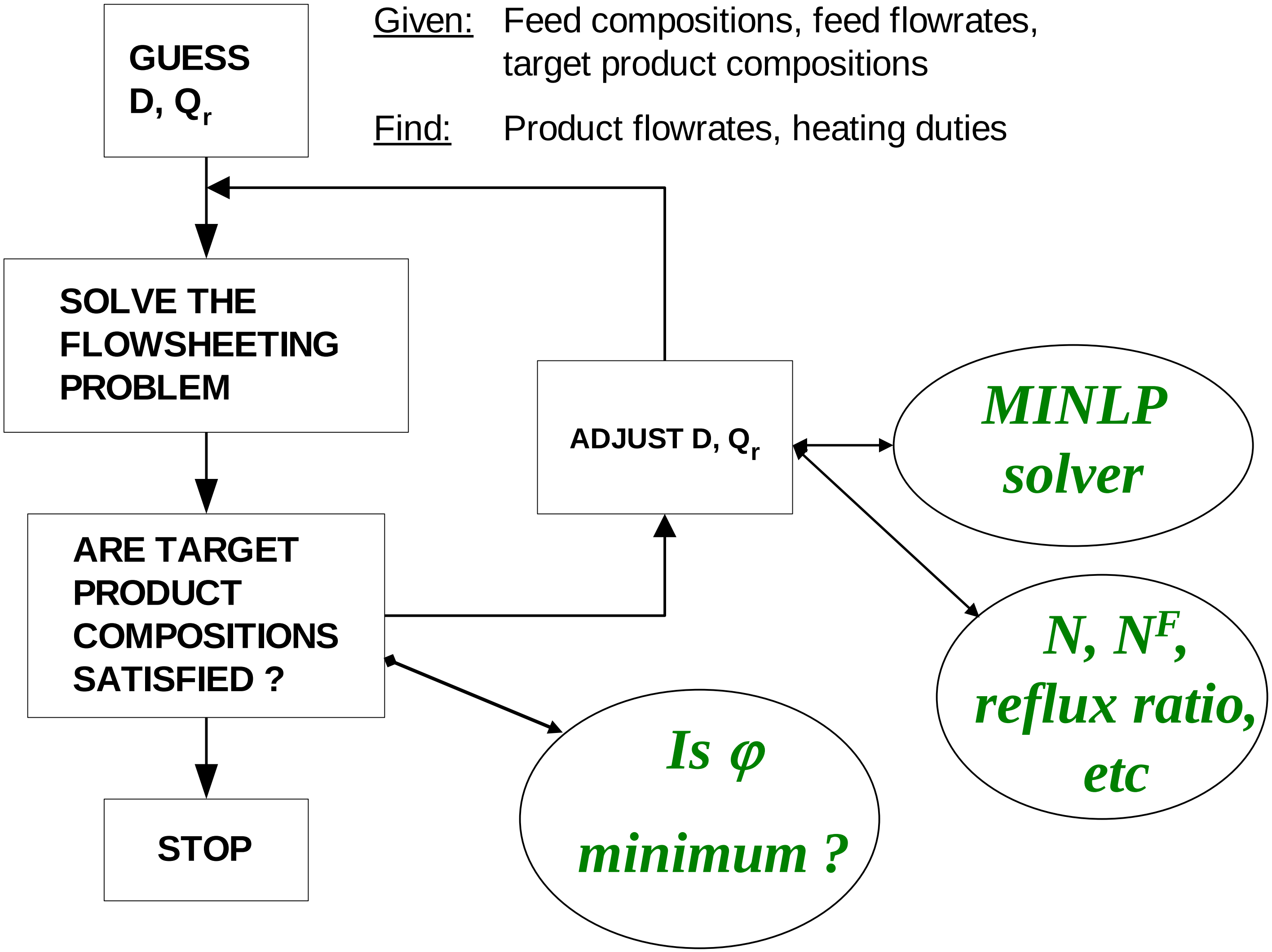
Subject ***to, φ ($\underline{x}^D$, $\underline{x}^B$, Q_r, Q_c, cost data) = minimum, and, $x_1^D > 0.98$ & $x_2^B > 0.95$***



Calculation procedure for synthesis problem

<u>Given:</u> Feed compositions, feed flowrates, target product compositions

<u>Find:</u> Product flowrates, heating duties



What is a Process Simulator?

An *Engineering Tool* which performs,

*** Automated calculations**

*** Material and/or energy balances**

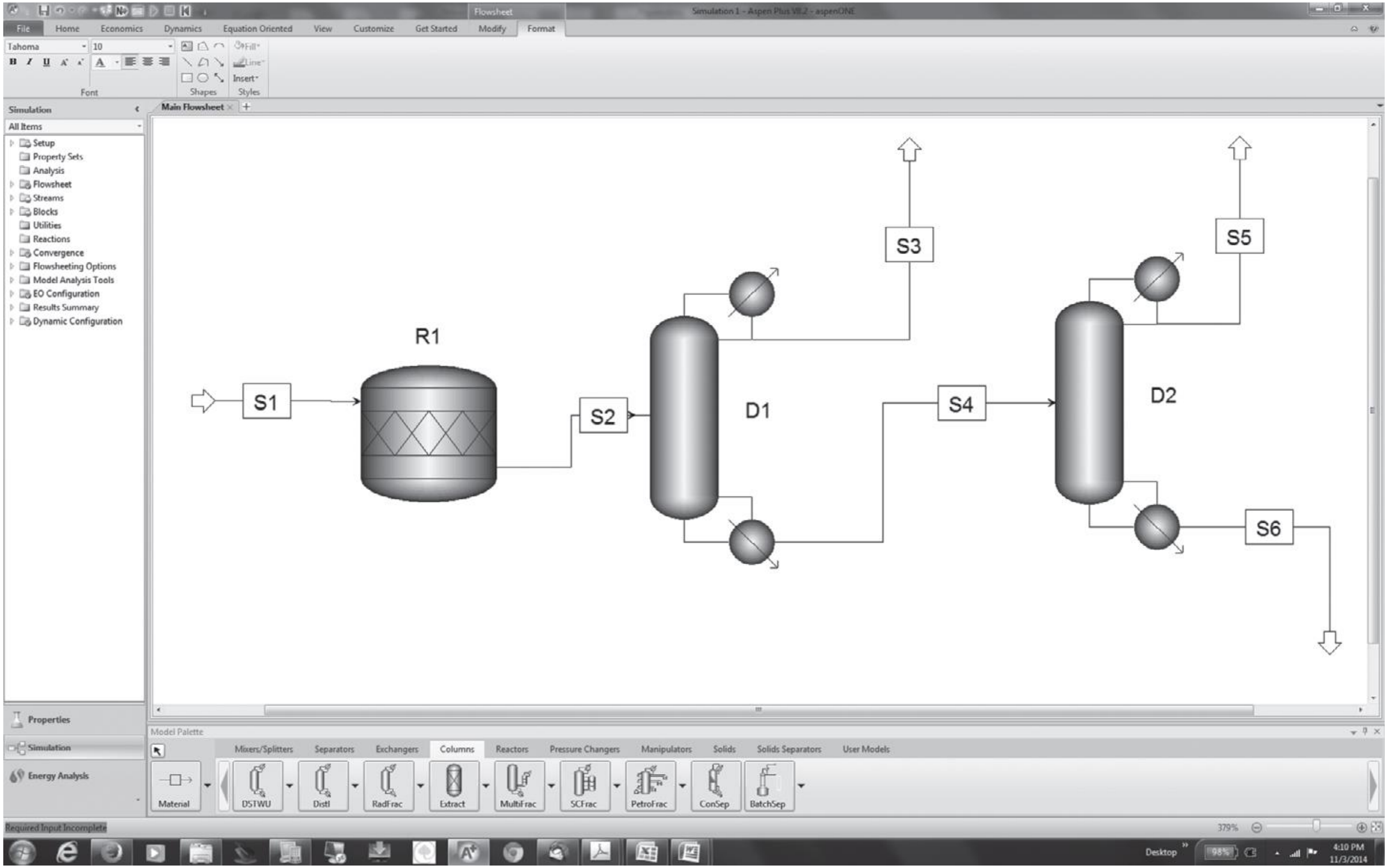
*** Physical property estimations**

*** Design/rating calculations**

*** Process optimization**

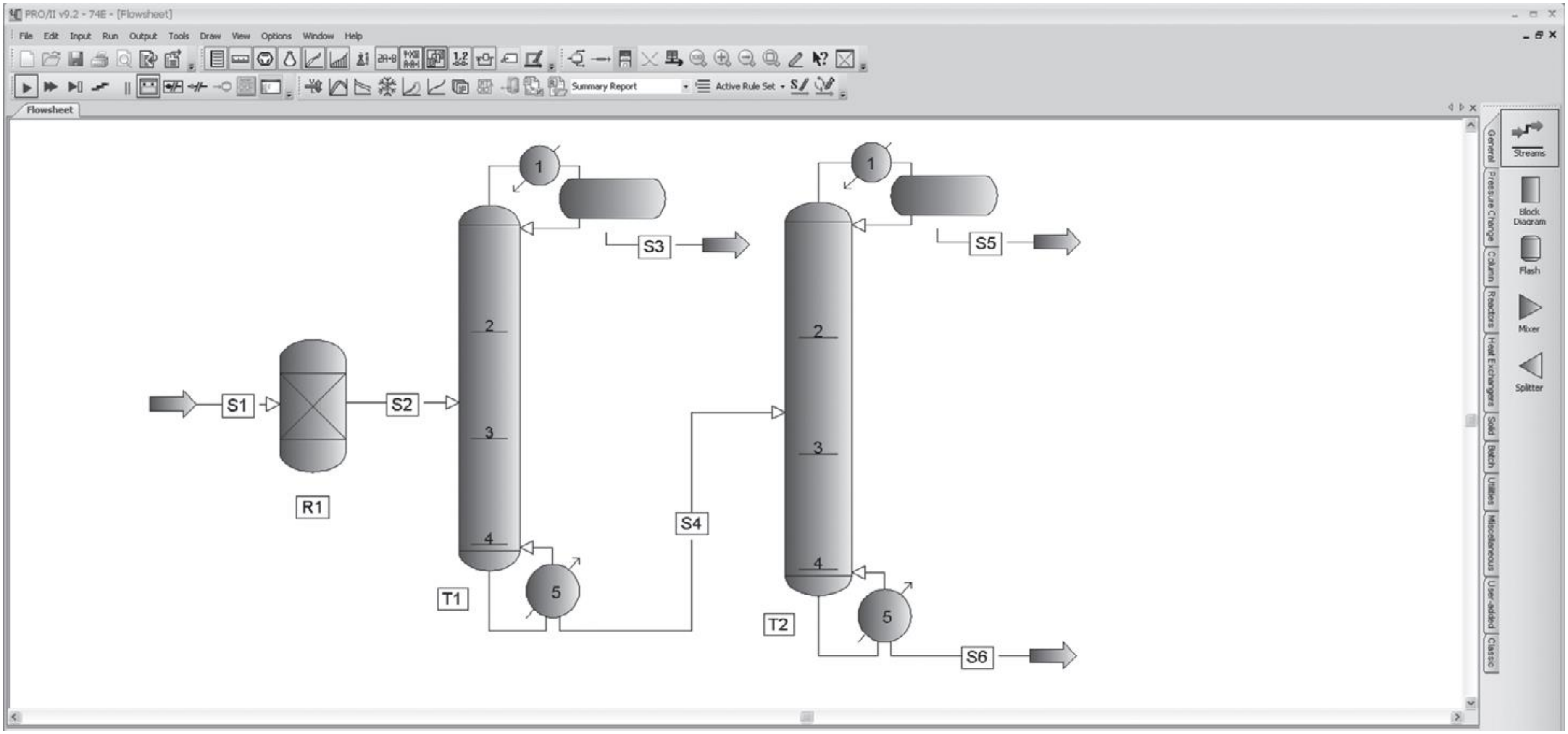
It is not a Process Engineer !

What is a Process Simulator? ASPEN



It is not a Process Engineer !

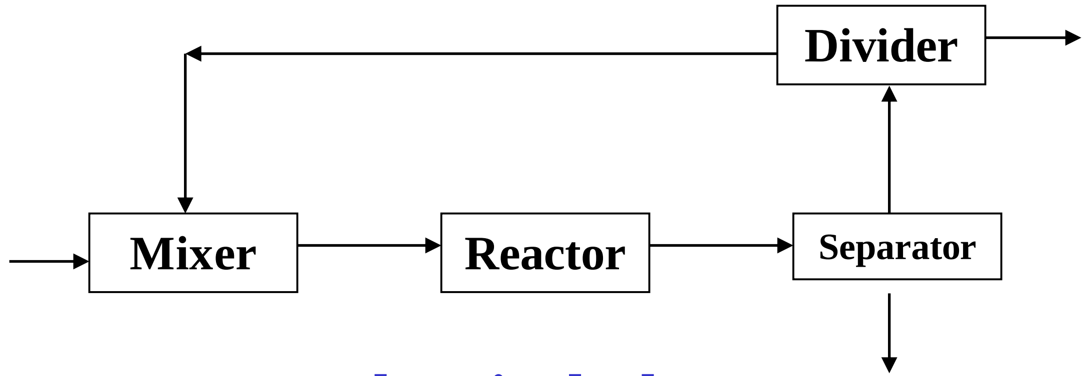
What is a Process Simulator? PROII



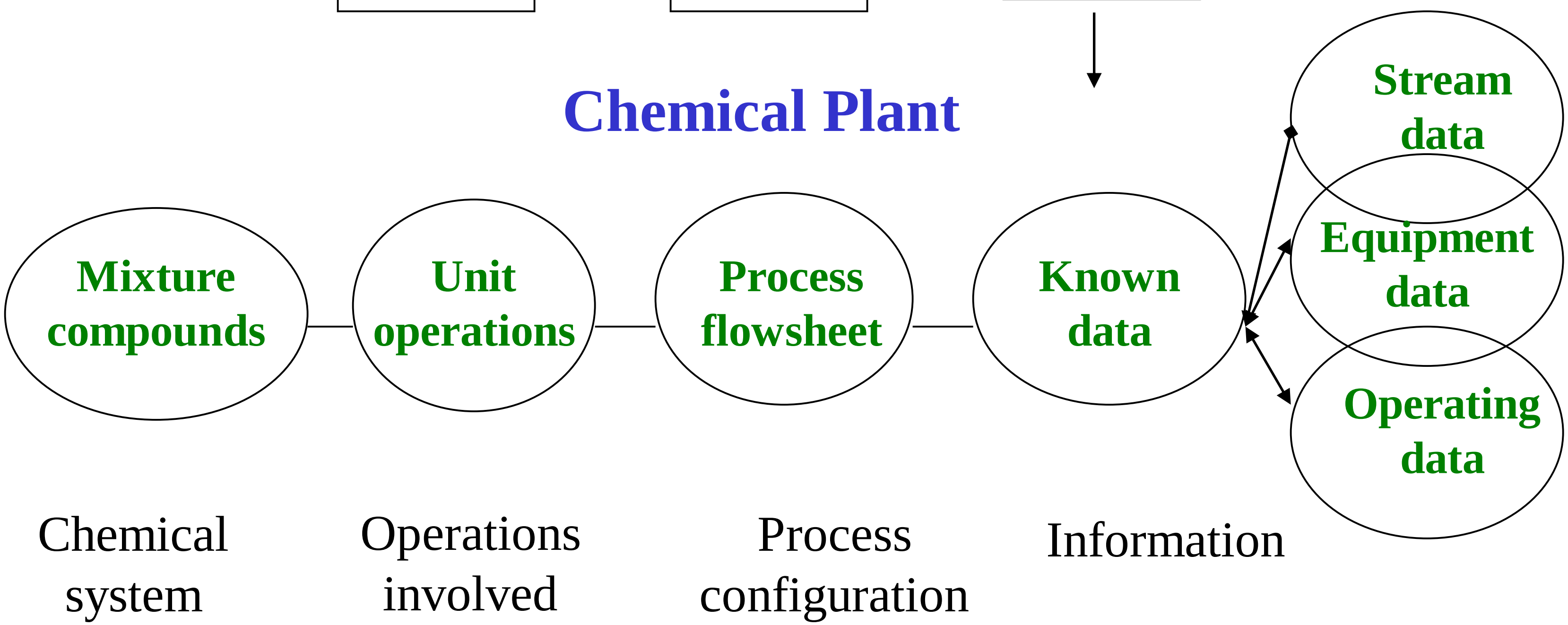
It is not a Process Engineer !

Simulation Problem Definition -

What information do we need?

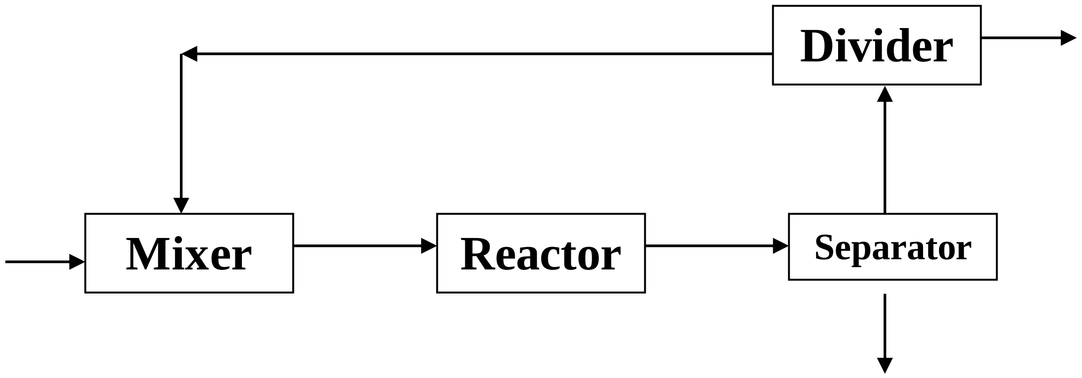


Chemical Plant



Simulation Problem Definition -

What do we need to select (depends on simulation model)?



Chemical Plant

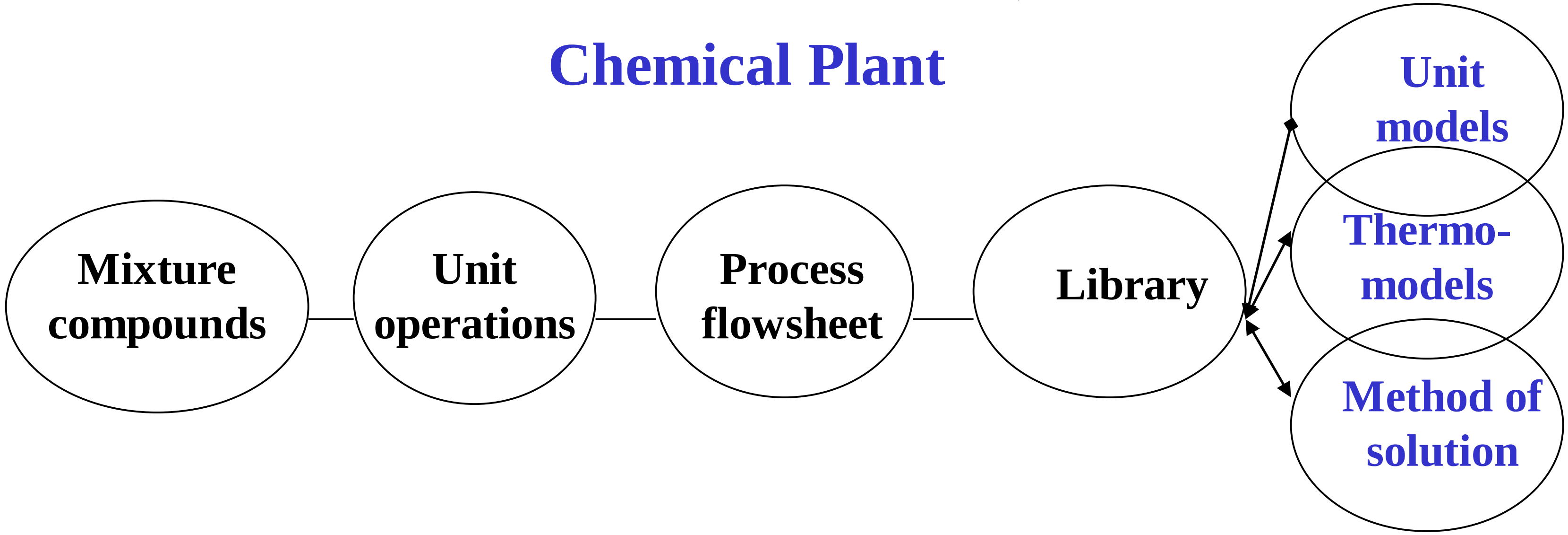


Table 7.1 Simple Modules of Unit Operations (Mass Balances Only)

Unit Module	ASPEN PLUS	PRO/II	UniSim®Design
DIVIDER	FSplit (feed stream, split fraction)	Splitter (feed stream, split fraction)	TEE (feed stream, split fraction)
MIXER	MIXER (feed streams)	MIXER (feed streams)	MIXER (feed streams)
REACTOR (Stoichiometric reactor)	RStoic (feed stream, reaction, conversion)	Conversion reactor (feed stream, reaction, conversion)	Conversion reactor (feed stream, reaction, conversion)
SEPARATOR	Sep (feed stream, separation fractions)	Stream calculator (feed stream, separation fractions)	Component splitter (feed stream, separation fractions)

Users need to make decisions; Available options in simulators for unit models from simulator model library

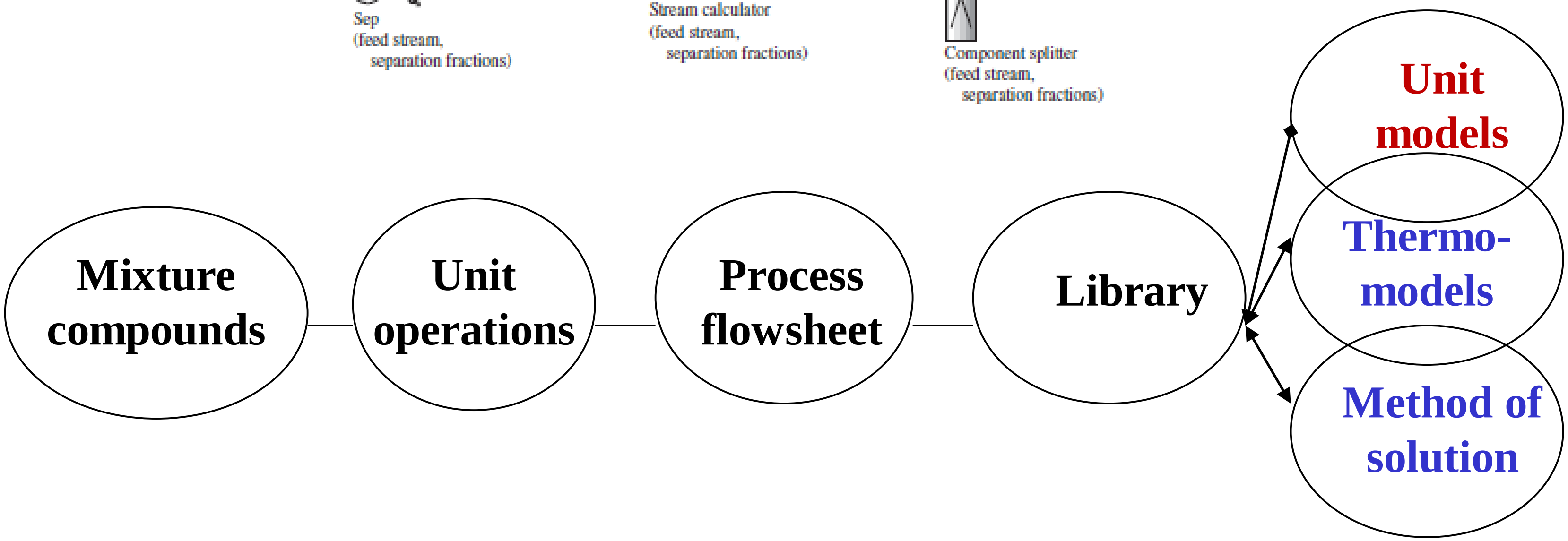


Table 7.2 Rigorous Models of Unit Operations

Unit Module	ASPEN PLUS	PRO/II	UniSim®Design
Simple (one stream) heater or cooler (temperature changer)	Heater (thermal and phase state changer; models heater, cooler, condenser, and so forth; specify feed stream, temperature, pressure)	Simple heat exchanger (thermal and phase state changer; models heater, cooler, condenser, and so forth; specify feed stream, temperature, pressure)	Cooler Heater LNG exchanger (feed stream, duty, outlet temperature
Shell-and-tube heat exchanger	HeatX (two stream heat exchanger; models cocurrent and countercurrent shell-and-tube heat exchanger; process fluid, specify service fluid, exchanger specification)	Rigorous heat exchanger (two stream heat exchanger; models cocurrent and countercurrent shell-and-tube heat exchanger; specify process fluid, service fluid, exchanger specification)	Heat exchanger (tube side inlet and outlet, shell side inlet and outlet)
Pump (pressure changer)	Pump (feed stream, discharge pressure, duty)	Pump (feed stream, discharge pressure, duty)	Pump (feed stream, discharge pressure, duty)

Users need to make decisions; Available options in simulators for unit models from simulator model library

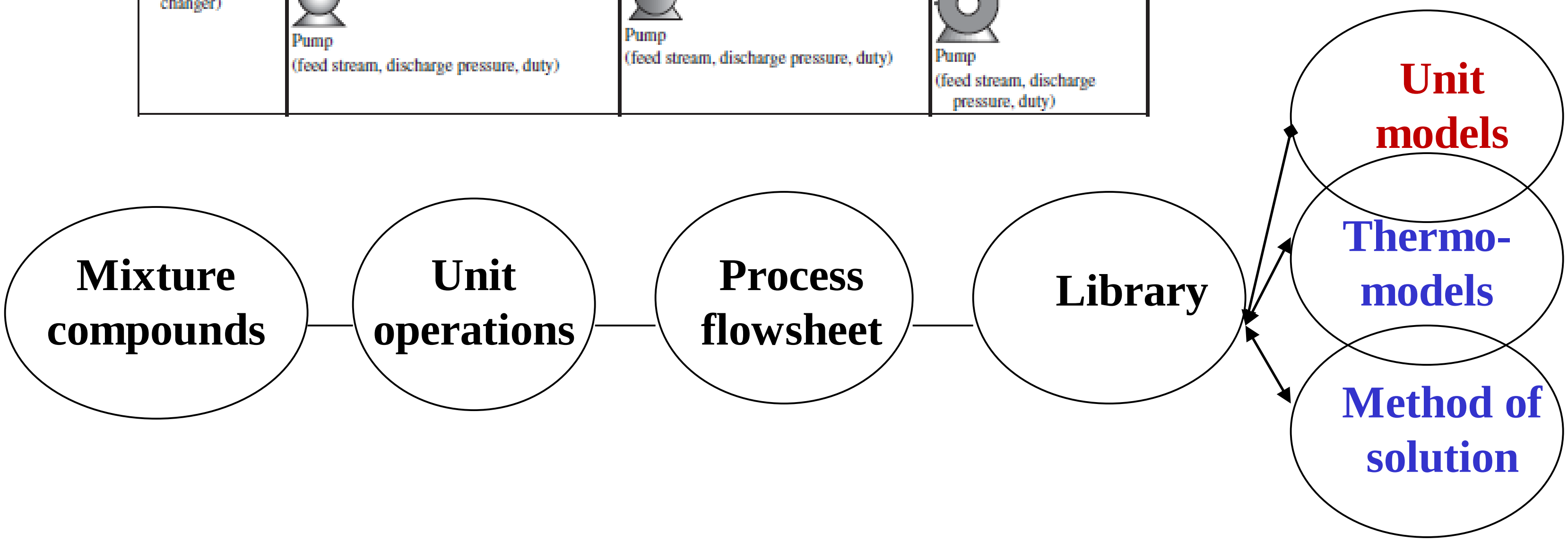
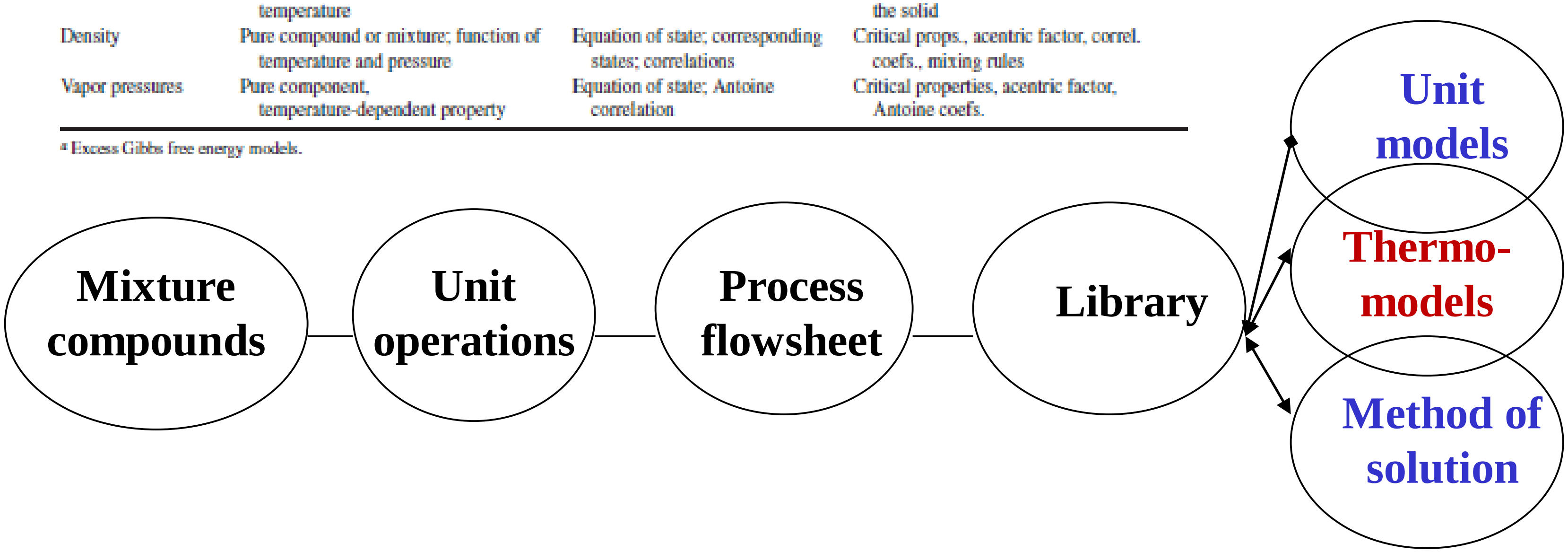


Table 7.3 Partial List of Thermophysical Properties

Property	Property Type	Model/Algorithm	Parameters
Activity coefficient	Liquid-phase component in a mixture	GE-models[a] (Wilson, NRTL, UNIQUAC, UNIFAC)	Size and volume parameters (molecules or groups); interaction parameters
Fugacity coefficient	Liquid- or vapor-phase component property in a mixture	Equations of state (cubic); PC-SAFT	Cubic EOS (critical properties, acentric factor, binary interaction parameters); PC-SAFT parameters
Vapor–liquid saturation point	Mixture phase equilibrium property	ΔG minimization (γ-ϕ approach or ϕ-ϕ approach)	EOS and GE-model parameters, composition of one coexisting phase plus temperature or pressure
VLE phase diagram	Multiple calculations of VL saturation points	ΔG minimization (γ-ϕ approach or ϕ-ϕ approach)	
LLE phase diagram	Multiple calculations of LL saturation points	ΔG minimization (γ-γ approach); not Wilson GE-model	GE-model parameters
VLLE phase diagrams	Two liquid phases in equilibrium with a vapor phase—ternary or more compounds	ΔG minimization (γ-ϕ approach or ϕ-ϕ approach); not Wilson GE-model	
SLE saturation	Composition of solid in equilibrium with a liquid mixture as a function of temperature	ΔG minimization (γ-approach); solid phase assumed pure	GE-model parameters plus heat of fusion and melting temperature of the solid
Density	Pure compound or mixture; function of temperature and pressure	Equation of state; corresponding states; correlations	Critical props., acentric factor, correl. coefs., mixing rules
Vapor pressures	Pure component, temperature-dependent property	Equation of state; Antoine correlation	Critical properties, acentric factor, Antoine coefs.

[a] Excess Gibbs free energy models.

Available options in simulators for thermo-models: these models play a very important role

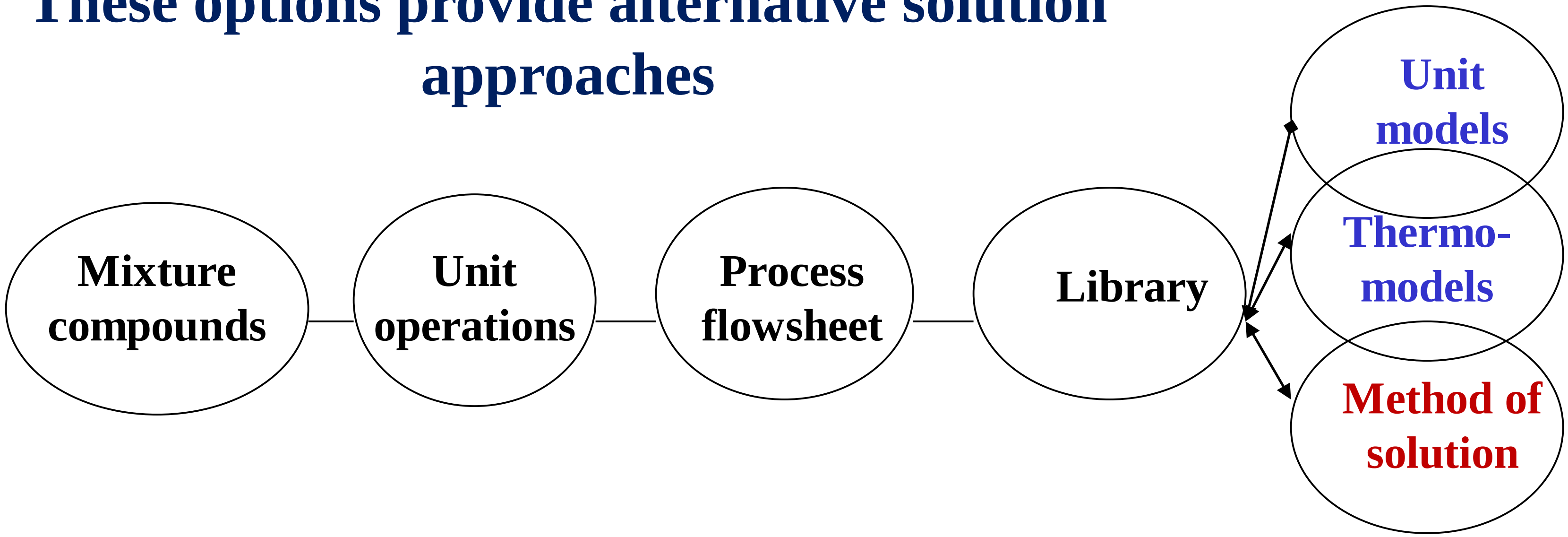


Steady state simulation

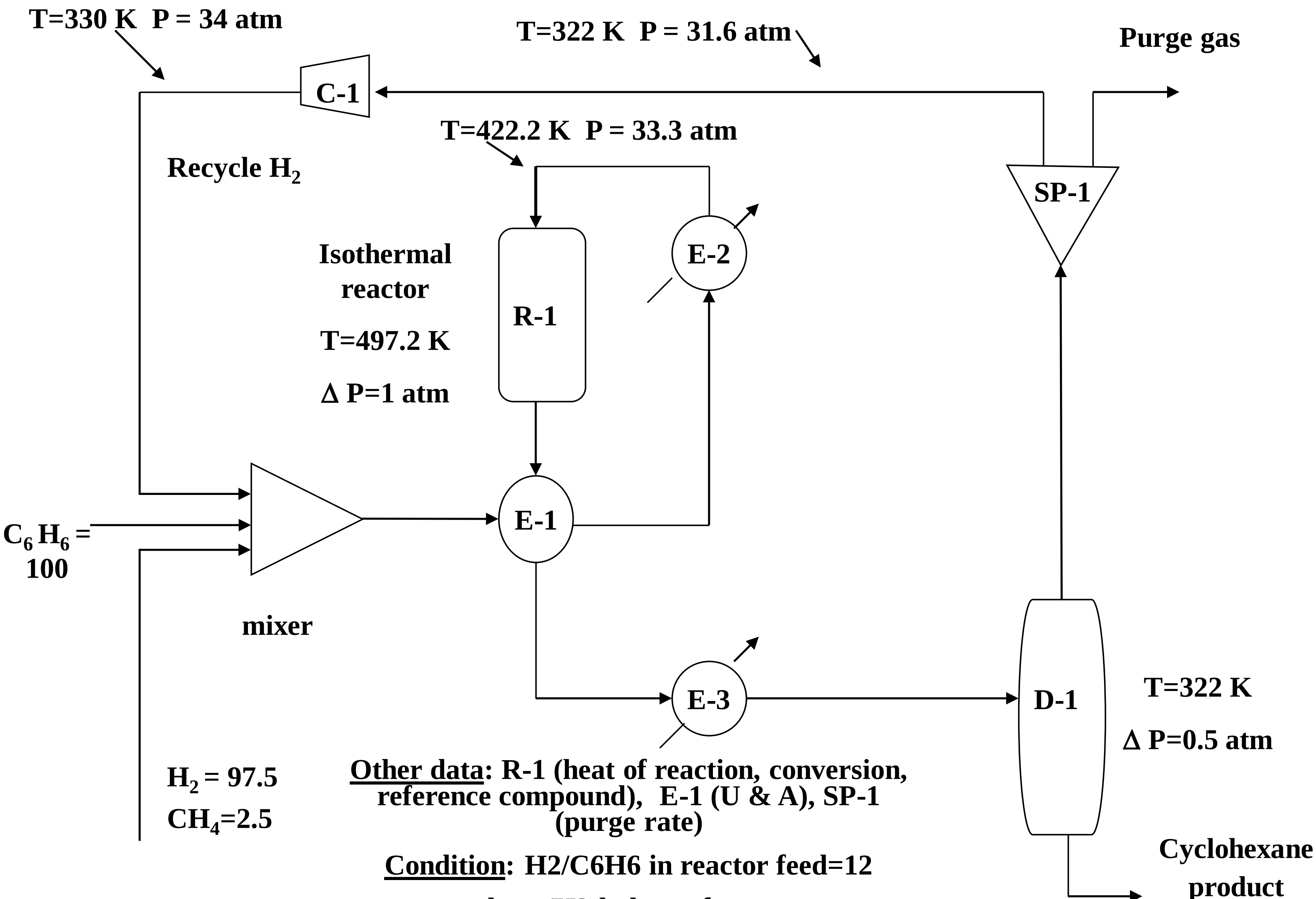
- Convergence technique
- Convergence criteria
- Number of iterations

Available options in simulators for methods of solution

These options provide alternative solution approaches



Flowsheet for cyclohexane production



__Other data__: R-1 (heat of reaction, conversion, reference compound), E-1 (U & A), SP-1 (purge rate)

__Condition__: H2/C6H6 in reactor feed=12

methane/H2 balance for purge

A Simple Example : problem formulation

***Consider*: A benzene feed stream & a hydrogen feed stream with methane as an impurity !**

***We know*:**

benzene + hydrogen = cyclohexane
reaction takes place in vapor phase & there is 99.9 % conversion of benzene; reactor operates at 497.2 K

***We would like to obtain*: pure cyclohexane**

Which simulation problem do we have ?
Which phase equilibirum model to use?
What type of models do we have?
Which method of solution to employ?

A Simple Example

***Consider*: A benzene feed stream & a hydrogen feed stream with methane as an impurity !**

***We know*: benzene + hydrogen = cyclohexane**

reaction takes place in vapor phase & there is 99.9 % conversion of benzene; reactor operates at 497.2K

***We would like to obtain*: pure cyclohexane**

we need, a mixer, a reactor, a separator, a divider, plus utility units (pumps, compressors, & heat exchangers) - we have a flowsheet!

Which simulation problem do we have ?

A Simple Example

***Consider*: A benzene feed stream & a hydrogen feed stream with methane as an impurity !**

***We know*: benzene + hydrogen = cyclohexane**

reaction takes place in vapor phase & there is 99.9 % conversion of benzene; reactor operates at 497.2 K

***We would like to obtain*: pure cyclohexane**

we need, a mixer, a reactor, a separator, a divider, plus utility units (pumps, compressors, & heat exchangers) - we have a flowsheet!

We have the found the equipment parameters and the design of reactor, purge, distillation column, heat exchangers, & compressors

Which simulation problem do we have ?

Today: lecture 1a: process simulation & prerequisites – afternoon tutorial: introduction to simulators