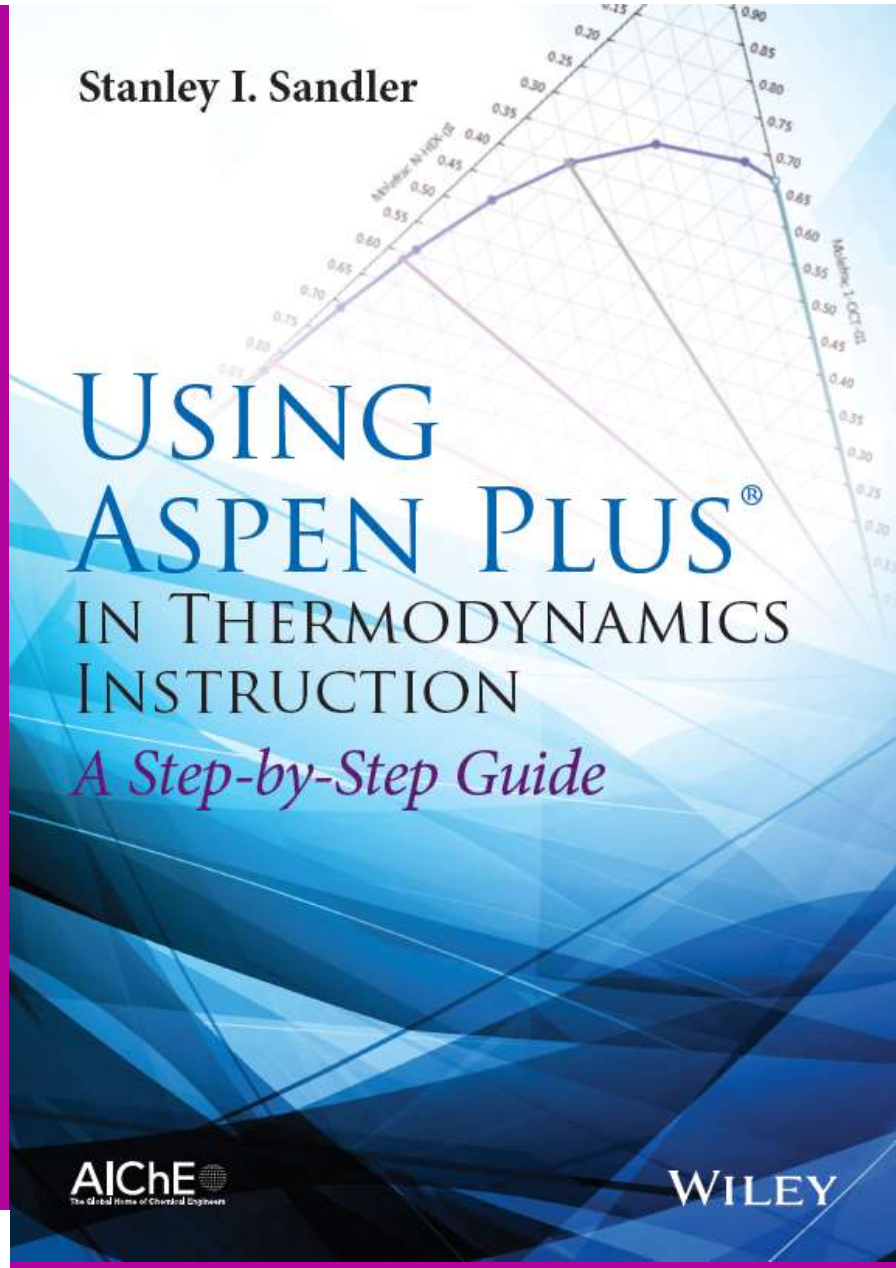
Aalto University
School of Engineering

EEN-E3002 Power Process Simulation

Introduction

Process Simulation on Aspen Plus®



aspentech

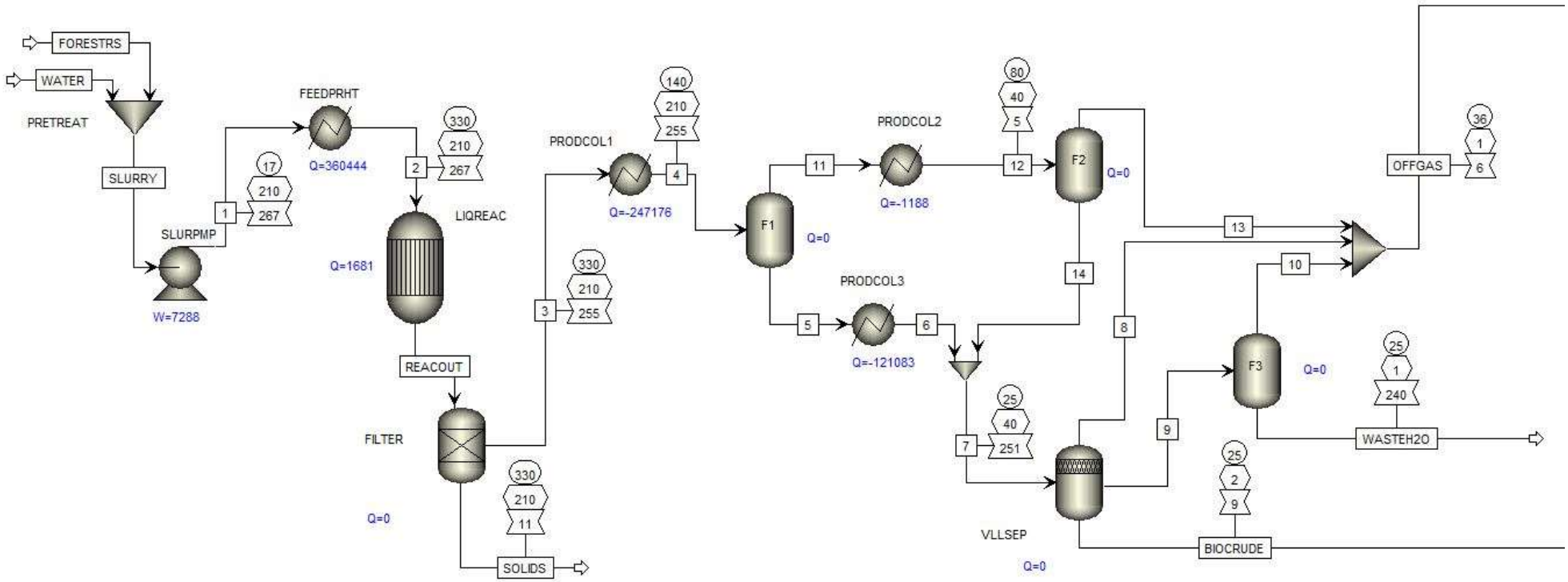
Mika Järvinen

3th March, 2022

What is a process flowsheet?

- A process flowsheet can simply be considered as a computational blue print of a plant or process layout.

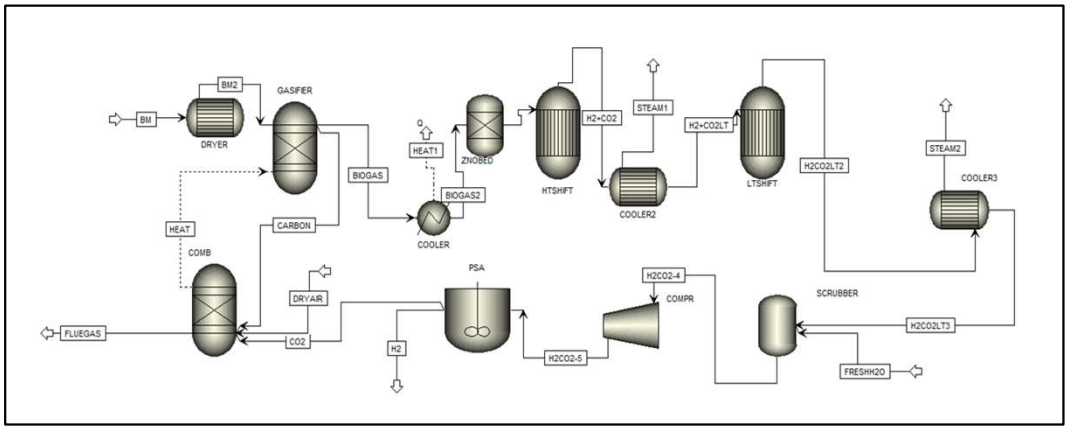
- A basic flowsheet includes all input material and energy streams, *boundary (or scope)-specific* unit operations, inter-stage chemical and/or physical conversion mechanisms and finally the product streams.



Aalto University

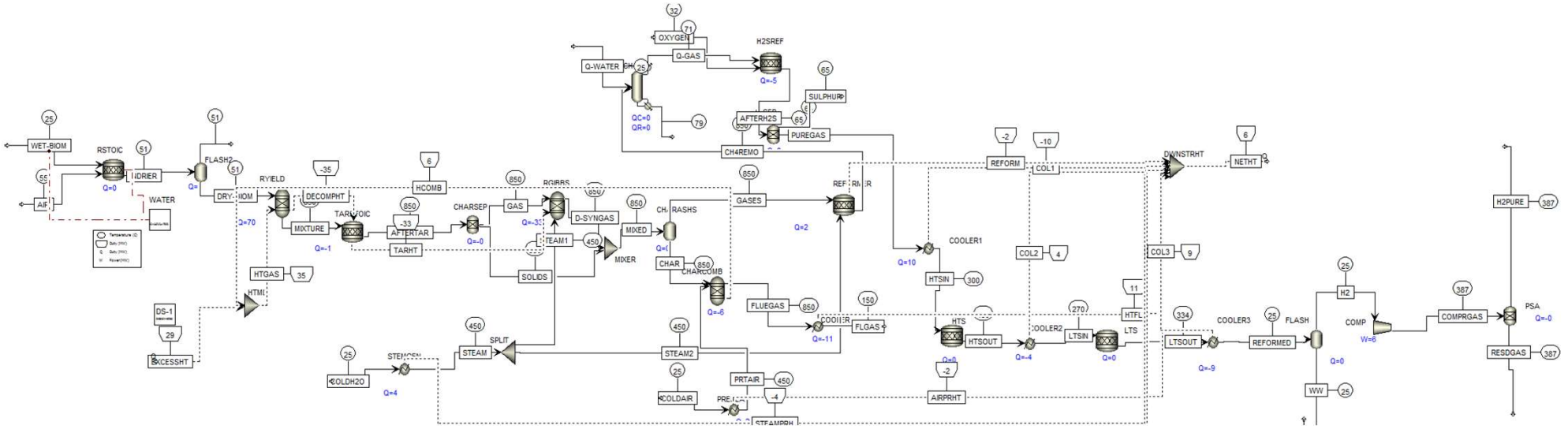
What is a process flowsheet?

An example from a student group project 3 years ago, H_2 gas from biomass



Above block diagram (or process units) is what they started with…

below (mass/heat/chemistry conversion steps) is what they ended at



Why do we do process modelling?

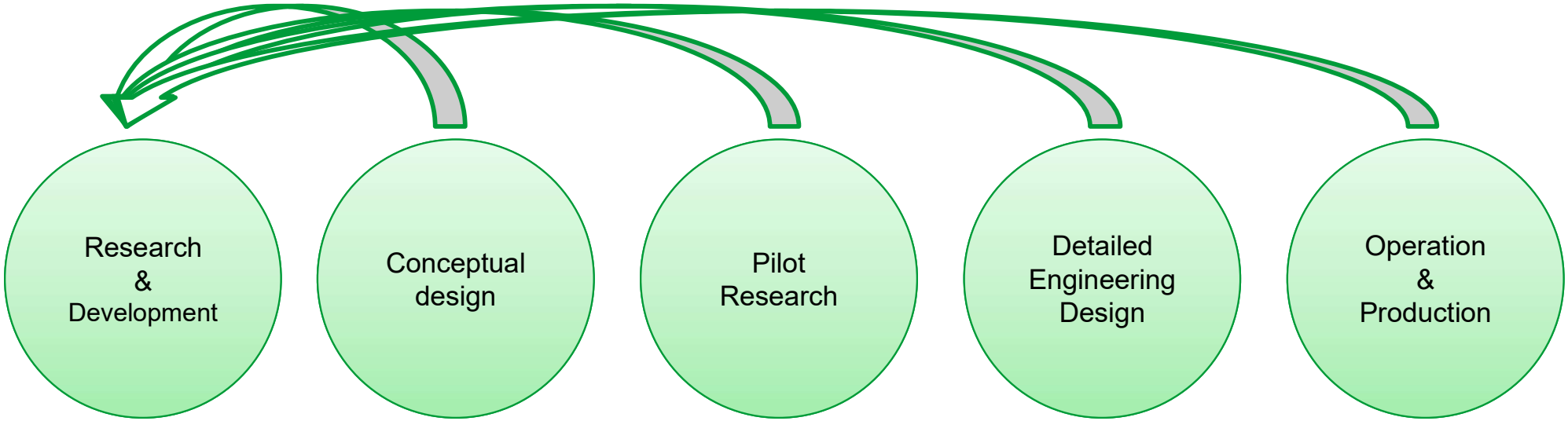
- **Practicality: COST (Time – Materials – Risk)**
- **Advantages of Computer-aided process simulation:**
  - Reduces plant design time as it allows designers to quantitatively assess the performance of various plant configurations.
  - Improve existing operations by answering ”What If” scenarios. (Retrofit studies)
  - Determine optimal process conditions within given constraints.
  - Debottleneck the constraining or limiting sections of a plant (heat, water and material integration studies).
- **Disadvantage of Computer-aided process simulation:**

  “Manual solution of a problem usually forces someone to think deeper on the problem, find novel approaches to solve it, and evaluate and reevaluate the assumptions closer. A drawback of process flowsheet simulators may be cited as the lack of this detailed interaction with the problem. This might act as a double-edged sword.

  On one side it hides the complexities of a problem so you can concentrate on the real issues at hand. On the other side this hiding may also hide some important understanding of the problem as well.” [1]

1 http://www.umich.edu/~elements/

When do we use process modelling?



Initial stages include semi-empirical models for technology **synthesis**, screening and evaluation.

During project life-cycle more detailed models to address new research questions and specific physical phenomena are developed in an iterative fashion.

Simulation models are used to examine production levels with detailed **design** and **analysis** of the main equipment of interest formulated. Reduce future operational hazards and risk.

Process models are used to predict the impact of **scaling (sizing) equipment**. Typically at this stage models are **validated** with pilot experimental determinations.

Last stage before project realization. Process models are combined with mechanical, electrical and control system designs to provide a highly accurate representation and **optimized** version of realized plant.

Performance monitoring, predictive maintenance, troubleshooting, **process retrofit and improvement** studies.

Important Guide

Keep in mind

Your model is as good as the ability to answer the questions set

1- The predefined outer boundary conditions and inner level of complexity.

2- The input information you provided for the model.

3- The interpretation extracted from the model results.

Always validate (justify) your modelling approach.

Steady-state vs Dynamic simulation models?

- Steady state models are characterized with the absence of time-determent variables.
- Steady state models generally constitute continuous processes, Aspen Plus as a software is initially designed for such systems.

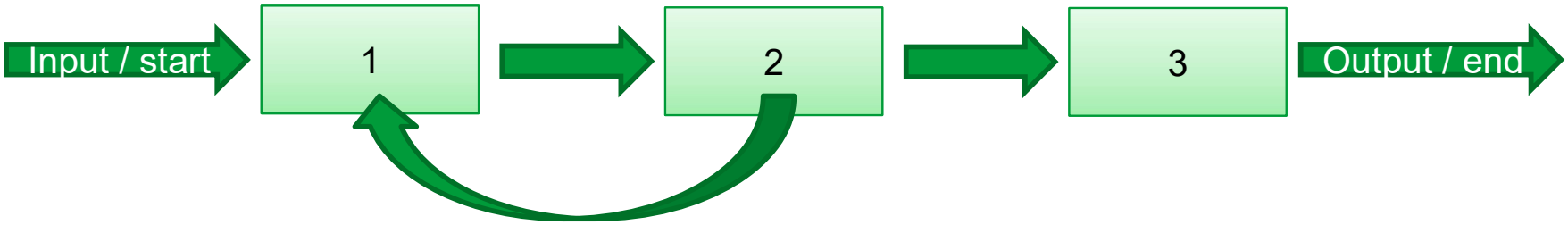
Input – Output + Sources/Sinks = 0

- However, you are able to imitate slowly changing processes with sequential steady states, think if this could be the case.
- For true transient cases, Aspen HYSYS is the required software, Aalto has also license for this.

Architecture of process simulators

1) Sequential: (modular)

Step-wise approach, where the overall system is broken into smaller units (process step) and calculated each at a time, depending on the direction of resources, from input to output.



In case of recycle, iteration is performed

Initiation (guessed) value is compared to calculated variable until error is below tolerance – **Model Converges.**

2) Equation oriented: (non-modular)

All unknown variables are combined into one large matrix of non-linear algebraic equations and simultaneously solved.

3) Combination of both.

Architecture of process simulators

1) Black box: (empirical)

Purely mathematic solving capabilities. Statistical analysis of available process data to obtain correlations (normally without a physical meaning) and test the validity of each to narrow down a list of applicable equations to solve the model.

2) White box: (mechanistic)

More accurate and deterministic approach, however requires extensive information available.

The model is built based on available fundamental thermo-physical principles like

- Mass and Energy balance.
- Equilibrium relationships.
- Rate correlations (chemical reactions and mass/heat transfer).

For complex chemical systems you will not have all determinstic data available for a White box approach so process simulaters combine both in (so called Grey box models).

Architecture of process simulators

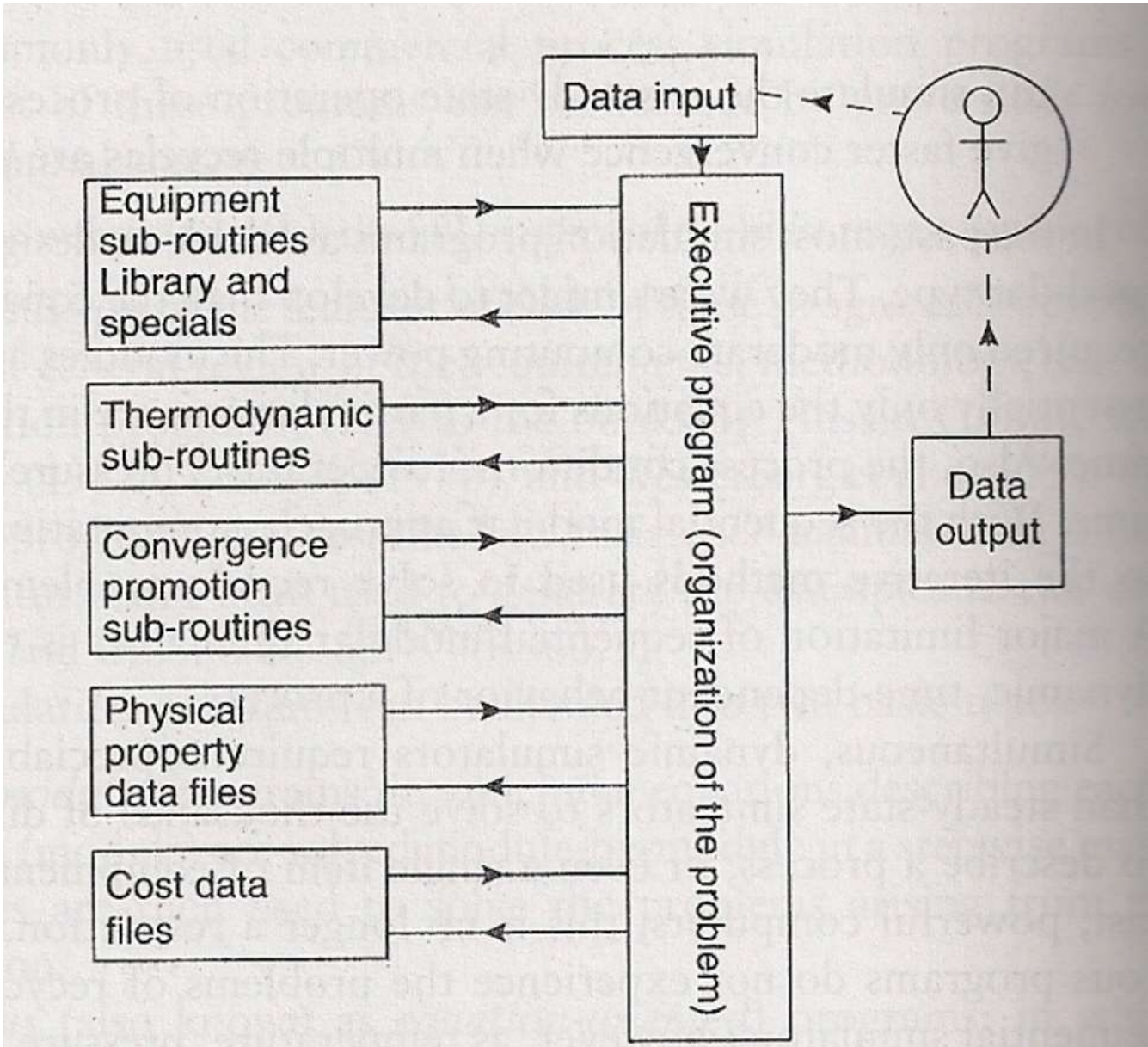


Figure 4.4. A typical simulation program.

Towler and Sinnott , "Chemical Engineering Design : Principles , Practice, Economics of Plant and Process Design" , Elsevier (2008)

Examples of process simulation tools

Commercial steady-state process simulators:

Sequential

- **Aspen Plus**
- Aspen Hysys
- ChemCheet
- PRO II
- UniSim
- Many others

Equation-oriented

- gProms
- VMGSim
- Aspen Custom Modeler

Open source:

- DWSIM (link)
- COCO (link)
- ASCEND (link)

Aalto University

Based on: A. Carrero, N. Quirante, J. Javaloyes, 2016

Intended learning outcomes of the course (Aspen Plus®)

- Understand the governing principles of process modelling/flowsheeting. (Today's lecture)
- Build a steady-state model and simulate a pre-designed power production processes on Aspen Plus®.
- Utilizing the software to formulate material and energy balances in order to evaluate different feedstock, energy conversion technologies and operational design conditions for power production.
- Acquire the necessary skills and the know-how of basic flowsheeting tools in Aspen Plus ® for future process design and synthesis projects.

Planned Activities (Aspen Plus® part)

- **Introduction to Aspen Plus ®** & process modelling. (Today's lecture)
  - Reading assignment – No submission needed.
- **Learning Exercise 1 (Wednesday 9.3):** Familiarize with Aspen Plus® interface, building a simplified Rankine cycle model and equilibrium combustion process.

  – Submission deadline Wednesday 16.3 at 14:00.
- **Learning Exercise 2 (Wednesday 16.3):** Building a model for a solid fuel combustion .

  – Submission deadline Wednesday 23.3 at 14:00.
- **Period V project:**
  - CHP case study, different process values for different groups.
  - Instructions will be shared on MyCourses.

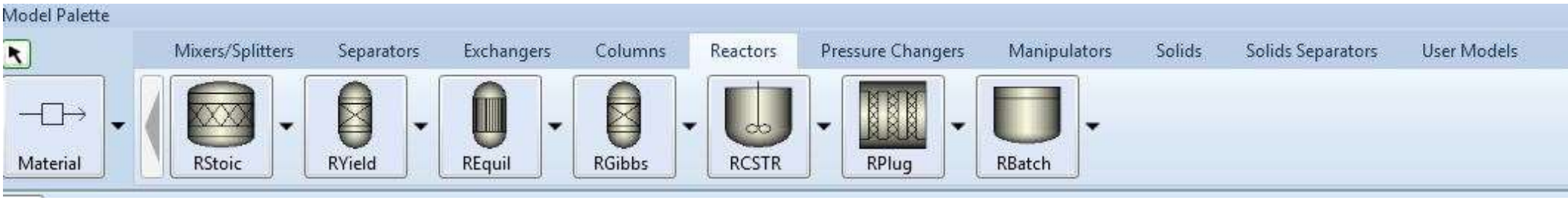
Practicalities (Aspen Plus® part)

- **You need to use vdi.aalto.fi interface to access Aspen Plus from home. Please see instructions from course MC home page.**
- **Additional literature** will be shared during the course on relevant topics as extra reading.
- **Books**
  - Chavez, Ivan. *Process Analysis and Simulation in Chemical Engineering*, Springer International Publishing, 2016.
  - Sandler, Stanley I. *Using Aspen plus in thermodynamics instructions : a step by step guide*. the American Institute of Chemical Engineers and John Wiley & Sons, 2015.

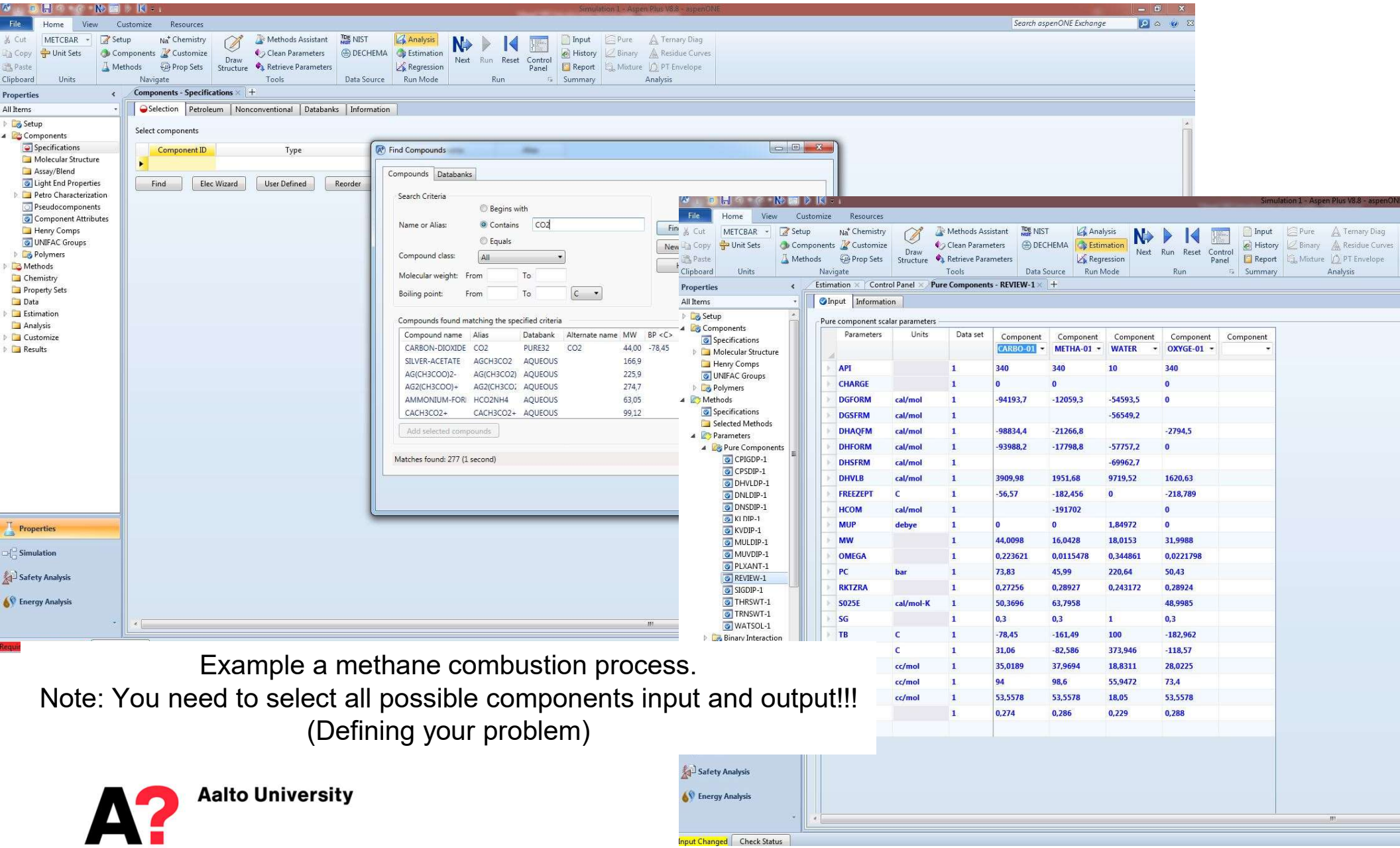
VERY IMPORTANT: You only have the right to use Aspen Plus® in work related to the activities of this course. If you want to apply to another personal project, please consult the instructors.

Introduction to Aspen Plus®

- In 1970s the researchers at MIT Energy Laboratory developed a prototype for process simulation. They called it Advanced System for Process Engineering (ASPEN). This software was later commercialized in 1980s by the foundation of a company named AspenTech.
- Aspen plus® has wide range of components (materials) available for simulation and are known as **conventional compounds**, also **non-conventional compounds** could be defined based on their elemental analysis. Other features available are modelling **solids**, petroleum **pseudo compounds** and **electrolytes** (aqueous salts).
- Aspen plus® V8.8 has built in library for unit operations (conservation equations) for mixer/splitters, separators, heat exchangers, pressure changers, **reactors**, distillation columns, manipulators, solids handling and custom user models.



Selecting flowsheet species



Example a methane combustion process.

Note: You need to select all possible components input and output!!!

(Defining your problem)

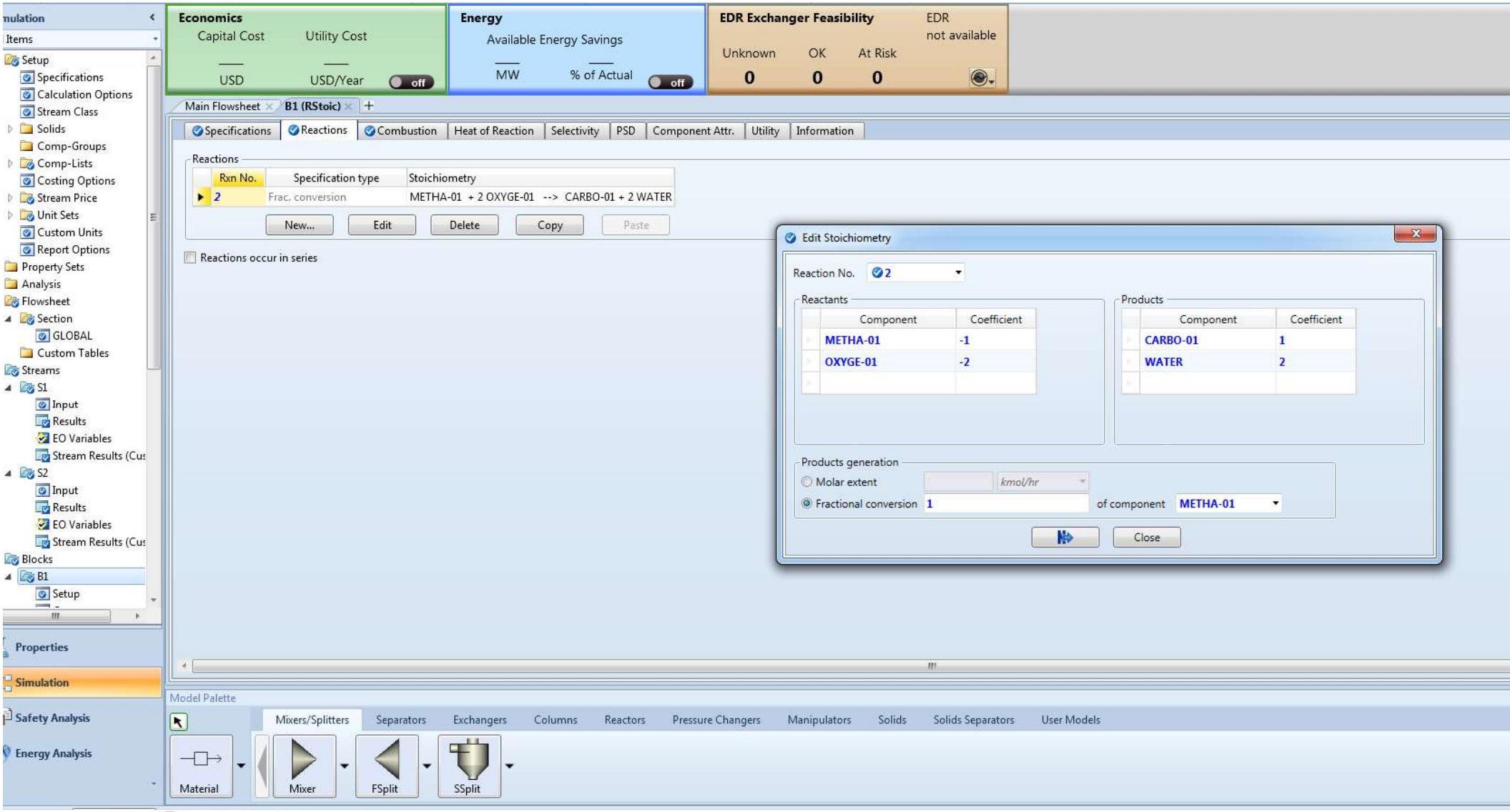
Aalto University

Example of Unit library in Aspen Plus®

Reactors

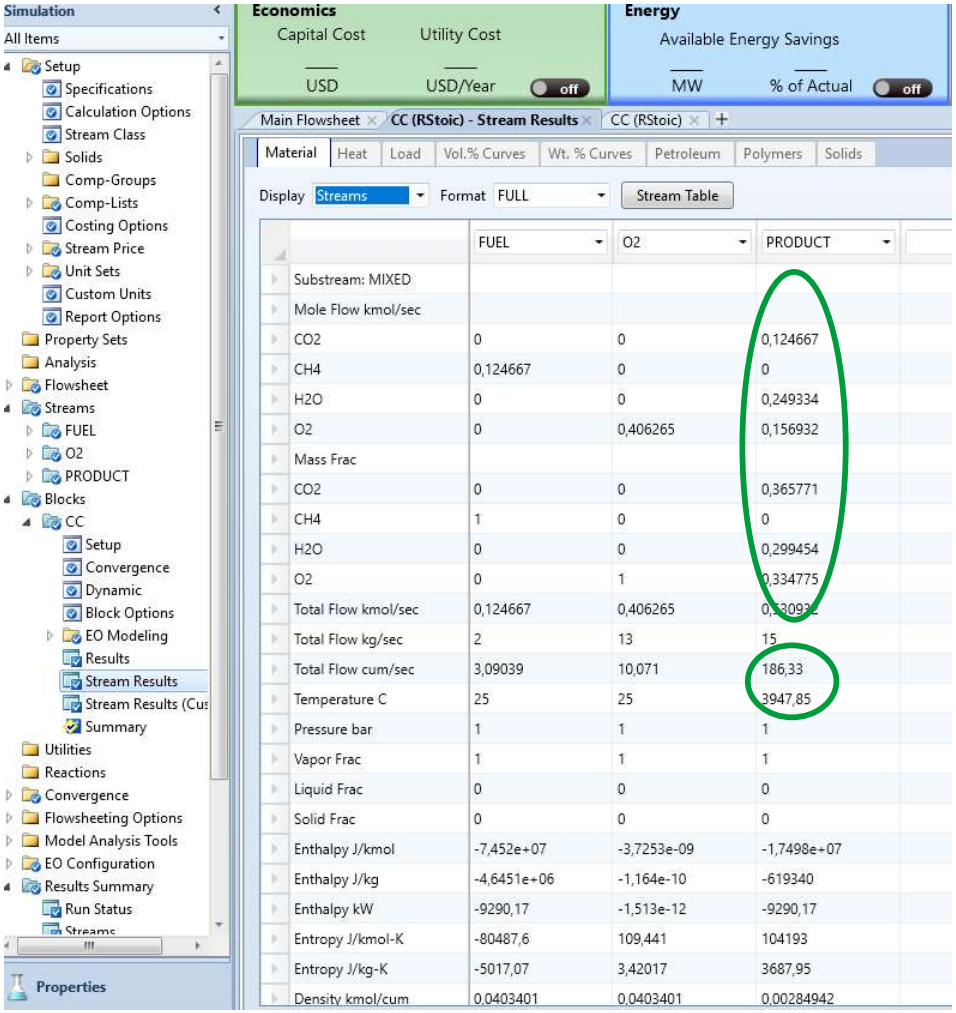
Model	Description	Purpose	Use
RStoic	Stoichiometric reactor	Stoichiometric reactor with specified reaction extent or conversion	Reactors where the kinetics are unknown or unimportant but stoichiometry and extent are known
RYield	Yield reactor	Reactor with specified yield	Reactors where the stoichiometry and kinetics are unknown or unimportant but yield distribution is known
REquil	Equilibrium reactor	Chemical and phase equilibrium by stoichiometric calculations	Single- and two-phase chemical equilibrium and simultaneous phase equilibrium
RGibbs	Equilibrium reactor	Chemical and phase equilibrium by Gibbs energy minimization	Chemical and/or simultaneous phase and chemical equilibrium. Includes solid phase equilibrium.
RCSTR	Continuous stirred tank reactor	Continuous stirred tank reactor	One, two, or three-phase stirred tank reactors with kinetics reactions in the vapor or liquid
RPlug	Plug flow reactor	Plug flow reactor	One, two, or three-phase plug flow reactors with kinetic reactions in any phase. Plug flow reactions with external coolant.
RBatch	Batch reactor	Batch or semi-batch reactor	Batch and semi-batch reactors where the reaction kinetics are known

RSTOIC as a reactor



Aalto University

RSTOIC stream result sheet



	FUEL	O2	PRODUCT
Substream: MIXED			
Mole Flow kmol/sec			
CO2	0	0	0,124667
CH4	0,124667	0	0
H2O	0	0	0,249334
O2	0	0,406265	0,156932
Mass Frac			
CO2	0	0	0,365771
CH4	1	0	0
H2O	0	0	0,299454
O2	0	1	0,334775
Total Flow kmol/sec	0,124667	0,406265	0,530932
Total Flow kg/sec	2	13	15
Total Flow cum/sec	3,09039	10,071	186,33
Temperature C	25	25	3947,85
Pressure bar	1	1	1
Vapor Frac	1	1	1
Liquid Frac	0	0	0
Solid Frac	0	0	0
Enthalpy J/kmol	-7,452e+07	-3,7253e-09	-1,7498e+07
Enthalpy J/kg	-4,6451e+06	-1,164e-10	-619340
Enthalpy kW	-9290,17	-1,513e-12	-9290,17
Entropy J/kmol-K	-80487,6	109,441	104193
Entropy J/kg-K	-5017,07	3,42017	3687,95
Density kmol/cum	0,0403401	0,0403401	0,00284942

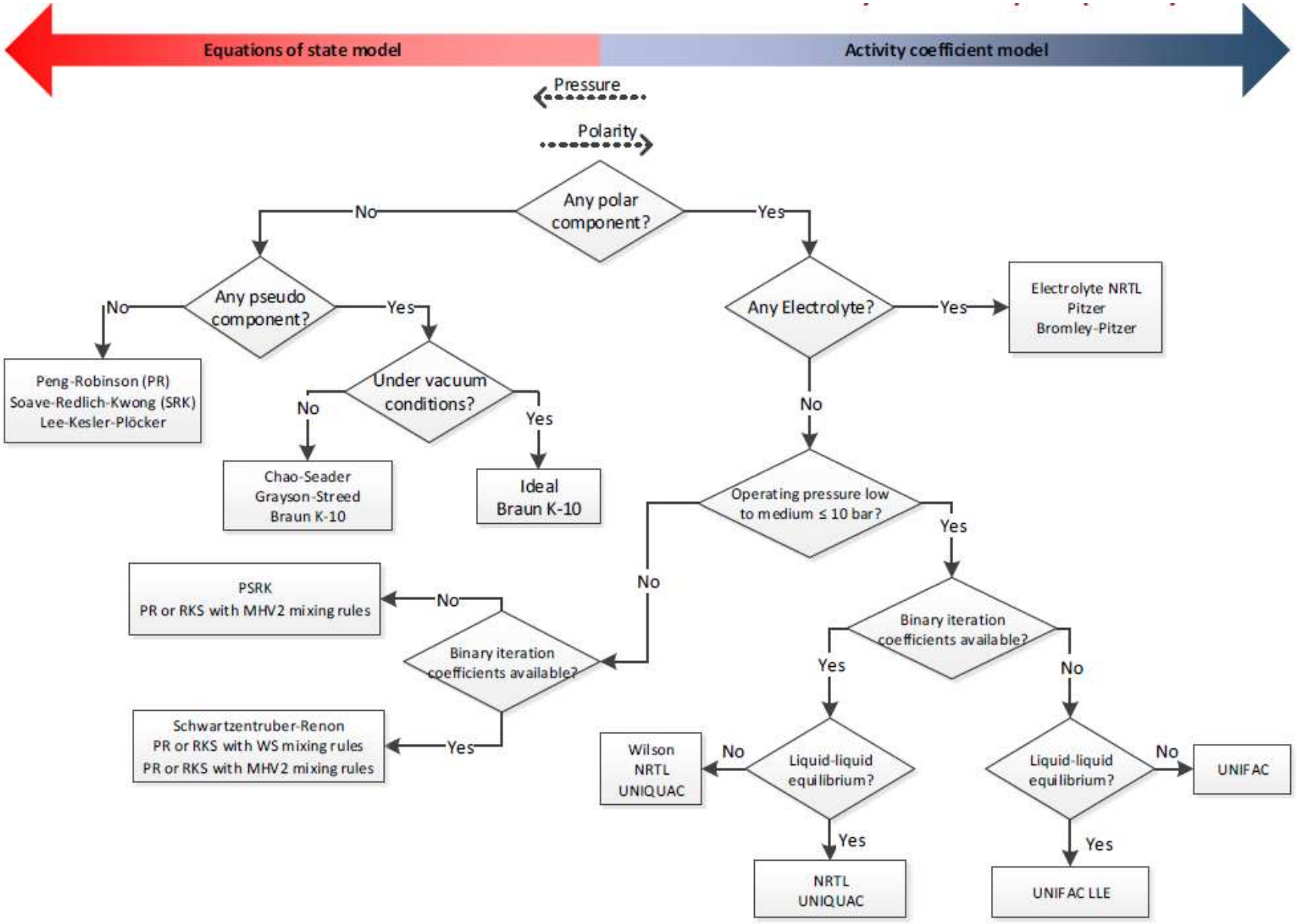
Reactor describing a stoichiometric reaction with 100% conversion

Physical property calculation in Aspen Plus®

90% of computation power goes into the retrieval (for pure) and prediction (for mixture) of the flowsheet components physical properties.

- The key thermodynamic property calculations performed in a process simulation is phase equilibrium.
- The general hypothesis: fugacity in vapor phase is equal to that in liquid phase at equilibria. (no more change in the system)
- In an ideal system, fugacity = vapor pressure of such component. However real mixtures exhibit significant non-ideal behavior.
- Non-ideality of a mixture of compounds is a function of the molecular interactions between such compounds.
- A simplified designation could be that Non-ideality is measured either with equation of states (EOS) for gases/vapor phases and activity coefficients for liquids.

Property package decision tree



Assignment (No submissions)

Warm up for the learning exercises by reading the chapter: Introduction to Aspen Plus® from the book “Teach Yourself the Basics of Aspen Plus” (2016), Second Edition. Ralph Schefflan. (Available in MyCourses.)

Aalto University

Thank you for your attention.