Aalto University School of Engineering

### EEN-E3002 Power Process Simulation Introduction

### Process Simulation on Aspen Plus®





AIChE

WILEY

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### 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.





### 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." <sup>1</sup>



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### When do we use process modelling?



representation and

realized plant.

optimized version of

more detailed models to address new research questions and specific physical phenomena are developed in an iterative fashion.

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hazards and risk.

### 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

#### **Open source:**

- DWSIM (link)
- COCO (<u>link</u>)

#### Equation-oriented

- gProms
- VMGSim
- Aspen Custom Modeler

ASCEND (<u>link</u>)



## 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 

   ß for future process design and synthesis projects.



### Planned Activities (Aspen Plus® part)

- - 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

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Input Changed	Check Status

### 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

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### RSTOIC stream result sheet

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🖌 🎯 Setup							
Specifications	USD	USD/Year off	MW % of Actual off				
Stream Class	Main Flowsheet × CC (R	Stoic) - Stream Results ×	CC (RStoic) × +				
Solids	Material Heat Load	Vol.% Curves Wt. % C	urves Petroleum Polymers Solids				
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Report Options	Mole Flow kmol/sec			0,124667 0 0,249334			
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🛛 📷 Streams	► H2O	0	0				
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▷ 100 02	Mass Frac						
	► CO2	0	0	0,365771			
⊿ 🔯 CC	CH4	1	0	0			
💽 Setup	H2O	0	0	0,299454			
Convergence	D2	0	1	0,334775			
Dynamic     Block Options	Total Flow kmol/sec	0.124667	0.406265	0.53092			
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Stream Results	Tomostatura C	25	25	2047.95			
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🕞 🔀 Convergence	Liquid Frac	0	0	0			
Flowsheeting Options	Solid Frac	0	0	0			
Model Analysis Tools	Enthalpy J/kmol	-7,452e+07	-3,7253e-09	-1,7498e+07			
Results Summary	Enthalpy J/kg	-4,6451e+06	-1,164e-10	-619340			
Run Status	🕨 🕨 Enthalpy kW	-9290,17	-1,513e-12	-9290,17			
Streams	Entropy J/kmol-K	-80487,6	109,441	104193			
<b>TT</b> (10)	Entropy J/kg-K	-5017,07	3,42017	3687,95			
Properties	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.)





# Thank you for your attention.