

May-2024

INTRODUCTION TO ASPEN PLUS COMPUTATIONAL TOOL - APPLICATIONS TO MULTICOMPONENT DISTILLATION AND SOLVENT EXTRACTION PROCESSES

Isabel A.A.C. Esteves
i.esteves@fct.unl.pt

Chemical and Biochemical/Biological Engineering
 Separation Processes
 2023/24

PS - AspenPlus - Isabel Esteves

Planning of practical classes

14 May – 6 June	Introductory notions of ASPEN. Examples of multicomponent distillation and solvent extraction. Practical work on Aspen Plus
10 June	Delivery of the work report (pdf report file AND Aspen files)
17 June	Oral work presentations, with prior delivery (1 day before) of the ppt file

- **Evaluation method:**

- Continuous assessment in class.
- Aspen module corresponds to 30% of the final grade, where a minimum classification of 10 (9.5) in a scale of 0 to 20 is required in this evaluation component.
- Includes a practical work (in teams of 4), with report and oral presentation, of a separation process (multicomponent, azeotropic, extractive distillation or L-L extraction) using ASPEN.

- **Structure of final report and oral presentation of 5 min maximum:**

- Problem posed, objective to solve and framework (Summary / Abstract);
- ASPEN strategy to solve the problem: unitary operation(s) and optimization approaches used to solve the separation problem, highlighting the most relevant parameters/variables according to classes
- Results presented clearly and critically discussed
- Relevant conclusions
- Note: classifications can be different within each group; all group elements must present



Process simulation - WHY and WHAT is it for?

- Prediction of the behavior of a process based on basic engineering relationships (mass and energy balances, chemical and phase equilibria, etc.);
- Design and dimensioning of processes (laboratory and/or industrial) based on thermodynamic data and real operating conditions;
- Parametric analysis and optimization of processes by interactive specification variation (processual diagram; operating conditions; feed compositions, etc.);
- More efficient and economically more profitable processes



WHAT DOES ASPEN STAND FOR?

- **ASPEN** is an acronym of **A**dvanced **S**ystem for **P**rocess **EN**gineering.
- It is based on a flowsheet simulation:
 - Computer software used to quantitatively model a chemical processing plant, which includes the core unit, pre- and post-treatment steps, coupled auxiliar units, instrumentation, etc.
 - Thus, simulation of an entire chemical process, starting from the raw material to the final finished product, is represented by different icons where each icon stands for a unit operation, chemical process, input/output material stream, input/output energy stream, or input/output electric/pneumatic signal.



Aspen Plus can simulate actual plant behavior.

Aspen Plus flowsheet simulation enables us to run many tasks:

- conduct “what if” tests;
- design specification (plant configuration) checks;
- carry out “de-bottlenecking of constricting parts of a process” studies;
- perform sensitivity analyses;
- run optimization investigations.



With this process simulator, we can design better plants and increase profitability in existing plants. It is useful throughout the entire lifecycle of a process, starting from a rough R&D idea and zooming to refined project details (from conceptual, basic or detailed engineering, to finally plant operations and revamps).

Aspen Plus allow us to construct simulation models based on unitary operations capable of predicting the behavior and performance of processes in real operating conditions.

HOW?

What is an **Aspen Plus Process Simulation Model**?

What are the skeletal steps required to have such simulation model?



What is an Aspen Plus Process Simulation Model?

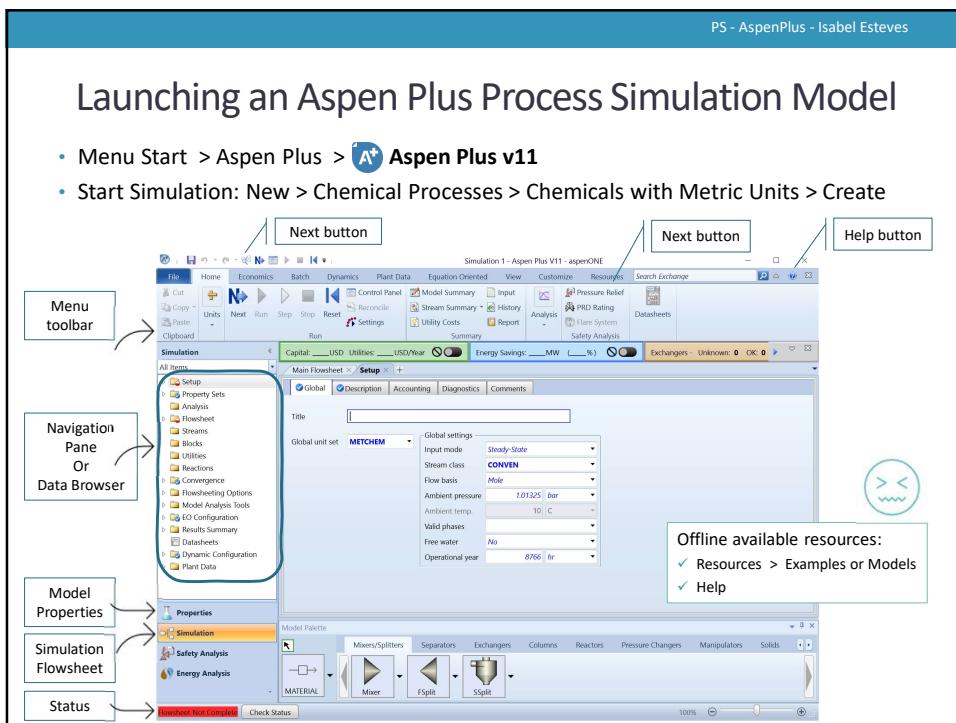
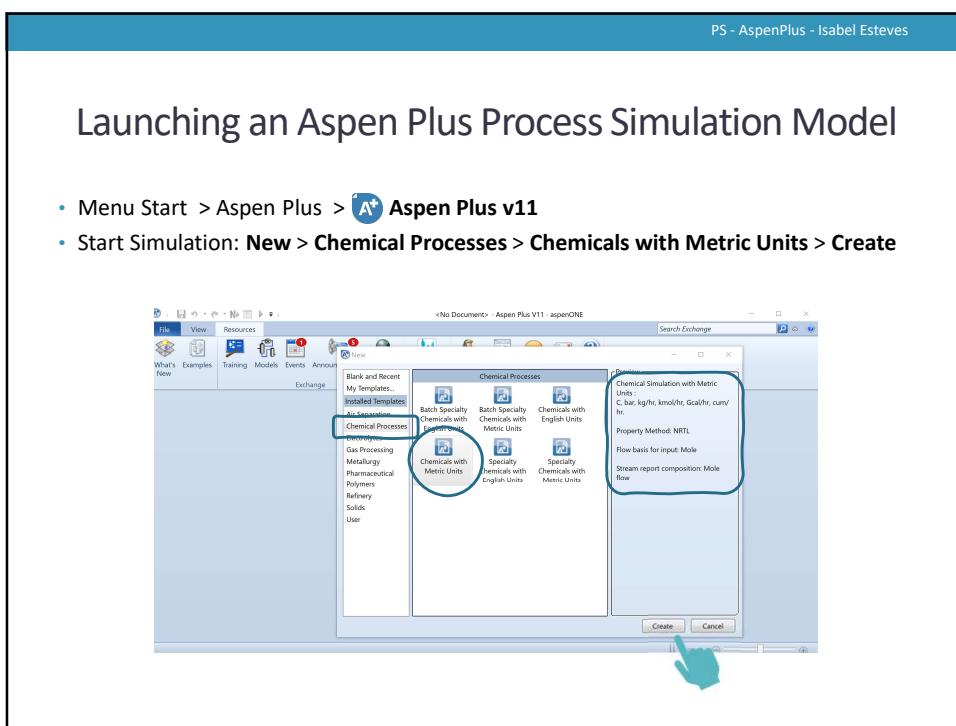
1. Define the process diagram - flowsheet - with the unit operations (blocks) of the process:
 - I. input and output streams in and between each unit operation;
 - II. template models from the ASPEN PLUS library that describe each unit operation.
2. Specifying:
 - I. chemical compounds present in the process (manually by the user or using the program's database);
 - II. thermodynamic models that describe the physical properties of pure compounds and their mixtures;
 - III. flow rates and thermodynamic conditions (temperature and pressure) of all feed streams;
 - IV. operating conditions of the unit operation.

Specifications can be tested to compare the new results with the old (previous) results, and then decide whether to accept or reject new process alternatives.



- Aspen Plus allows you to interactively change:
 - ✓ Flowsheet configuration;
 - ✓ Operating conditions;
 - ✓ Feed compositions;in order to analyze all possibilities of performance of the process.
- In addition, ASPEN PLUS allows estimation of physical properties, generating graphs and results tables, adjusting experimental data to simulation models and optimizing the process.





PS - AspenPlus - Isabel Esteves

This Symbol	On a(n)	Means
	Input form or sheet	Required input complete, or visited and no data required *
	Input form or sheet	Required input incomplete
	Input form	No data entered
	Mixed form	Input and results
	Results form	No results present (calculations have not been run)
	Results form	Results available without Errors or Warnings (OK) **
	Results form or flowsheet	Results available with Warnings **
	Results form or flowsheet	Results available with Errors **
	Results form	Results inconsistent with current input (input changed)
	Input folder	No data entered
	Input folder	Required input incomplete
	Input folder	Required input complete, or visited and no data required *
	Results folder	No results present
	Results folder	Results available – OK **
	Results folder	Results available with Warnings **
	Results folder	Results available with Errors **
	Results folder	Results inconsistent with current input (input changed)
	Folder or form	Object deactivated

Note: Deactivated items still need to be complete. Incomplete deactivated items show this icon, not the incomplete icon.

* The required input complete icons and appear on some forms and folders in the navigation pane where no input is required as soon as you enter the form. You can restore these to the no data entered icons by right-clicking the icon and selecting Delete. In this case, the form or folder will not be deleted, but it will be restored to its original status in a blank simulation.

In addition to these symbols, if you place the mouse pointer over one of the forms or folders in the navigation pane, a tooltip will appear showing the status in text. This status includes additional information which may not be conveyed by the icon, such as EO synchronization status and reconciled status. Also, inactive blocks (see Activating and Deactivating Blocks) are shown with their names struck through.

ASPEN PLUS - Status Indicators in Menu Data Browser

PS - AspenPlus - Isabel Esteves

Mandatory to follow

- Only fill the options needed to perform your problem with the input given to solve it.
 - Be curious and research, but do not click in all the options available in each panel of the Aspen tool.
 - Usually clicking in will help you to fill what you need.

PS - AspenPlus - Isabel Esteves

ASPEN PLUS - Application to Multicomponent Distillation

- Feed:**
 - Propane/isobutane of molar fraction: 40/60 %
 - binary mixture as the simplest case-study to explore the effect of the variation of operating variables on the distillation results;*
 - trial-and-error simulations are assumed;*
- Operating Conditions:**
 - T = 322 K ; P = 14.2 bar ; feed flow rate = 100 kmol/hr
- Distillation Column:**
 - RadFrac, total condenser
 - Reflux ratio = 2
 - N_T = 32; N_F = 16
 - P_C = 14 bar; $\Delta P = 0.1$ psi per stage
- Objective:**
molar fraction of propane in distillate = 97%

Engenharia de Processos de Separação, E. G. Azevedo, A.M. Alves (2009)

ASPEN PLUS - Application to Multicomponent Distillation PS - AspenPlus - Isabel Esteves

Entering Components in Aspen Plus Process Simulation Model

- In PROPERTIES panel**

Components > Specifications (propane – C3H8, isobutane)
Methods > Global (UNIFAC, packages for predictive property methods to generate VLE data)

ASPEN PLUS - Application to Multicomponent Distillation PS - AspenPlus - Isabel Esteves

Specifying the Property Method in Aspen Plus Process Simulation Model

- A property method is a set of models used to calculate thermodynamic, kinetic, and transport properties. If the components selected do not work with Aspen Plus methods, then such methods can be modified by the user.
- The thermodynamic method, a subset of the property method, can be broadly classified as:
 - an activity coefficient-based method (polar compounds at low pressures < 10 bar and away from the critical region; highly nonideal liquid mixtures);
 - an equation of state method (in the critical region and when there are no polar components; hydrocarbon systems with light gases such as CO₂, N₂, and H₂S).

Guidelines for choosing a Property Method!

Examples of activity coefficient-based models are "NRTL" (Non-Random-Two-Liquid), "UNIFAC" (UNiversal Functional Activity Coefficient), and "UNIQUAC" (UNiversal QUAsichemical Activity Coefficient). "UNIFAC" is based on group contributions rather than molecular contributions and is very predictive.

Note PS - AspenPlus - Isabel Esteves

WHY IS THE THERMODYNAMIC METHOD SO IMPORTANT?

Aspen has 4 main types of *Property Methods*:

Ideal, Equation of State, Activity Coefficient, and Special Systems

- Ideal Methods rely on using ideal system equations to calculate the equilibrium distribution ratio (K), which is then used to determine the equilibrium conditions.
- The Equation of State Property Methods use the various equations of state that are learned about in chemical engineering thermodynamics, to calculate the equilibrium distribution ratio. Most familiar methods: PENG-ROB (Peng-Robinson) and RK-SOAVE (also SRK, Redlich-Kwong-Soave).
- The Activity Coefficient group uses various relationships to calculate the liquid phase activity coefficient and then calculate the vapor fugacity using a second relationship. Most common methods: NRTL (Non-Random Two Liquid), UNIFAC, Van Laar and WILSON.

See software Help engine to learn more!

Note

PS - AspenPlus - Isabel Esteves



Why should you use proper Physical Property Models for the system of interest?

More rigorous property models are needed for more accurate predictions for the system of interest.

Example Property Prediction Task:
Predict the molar volume of ethane at the two conditions:

- Condition 1: $p = 1 \text{ atm}$; $T = 573.15 \text{ K}$ (300°C)
- Condition 2: $p = 20 \text{ atm}$; $T = 298.15 \text{ K}$ (25°C)

Is the **Ideal Gas Law** a reasonable assumption ($R = 82.1 \text{ cm}^3 \text{ atm mol}^{-1} \text{ K}^{-1}$)? Use Aspen to predict the volume for the two conditions above using an appropriate Equation of State (EoS) model.

Using the Ideal Gas Law,

$$\frac{V}{n} = \frac{RT}{p}$$

Condition 1 : $V = 47055.6 \text{ ml/mol}$
 Condition 2: $V = 1223.9 \text{ ml/mol}$

Using the **PENG-ROB** EoS (recommended for hydrocarbon processing applications such as gas processing, refinery, and petrochemical processes)

Condition 1: $V = 47611.9 \text{ ml/mol}$
 Condition 2: $V = 1010.7 \text{ ml/mol}$

Conclusion:
 Similar results for Cond.1; but for Cond.2, Ideal Gas Law overestimates V by 21%.
 High-pressure and low-temperatures make intermolecular interactions not negligible; so a more rigorous model is needed.

ASPEN PLUS - Application to Multicomponent Distillation

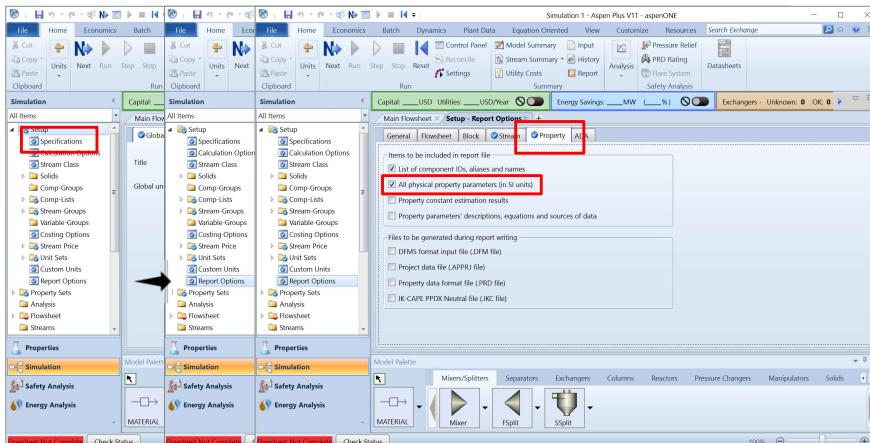
PS - AspenPlus - Isabel Esteves



Starting the Flowsheet

- SIMULATION panel**
- In Setup folder:

Specifications > Title (optional) and Report Options: Stream > Fraction basis in Mole, and Property > All physical property parameters in SI units (optional)



PS - AspenPlus - Isabel Esteves

GOOD FLOWSHEETING PRACTICE

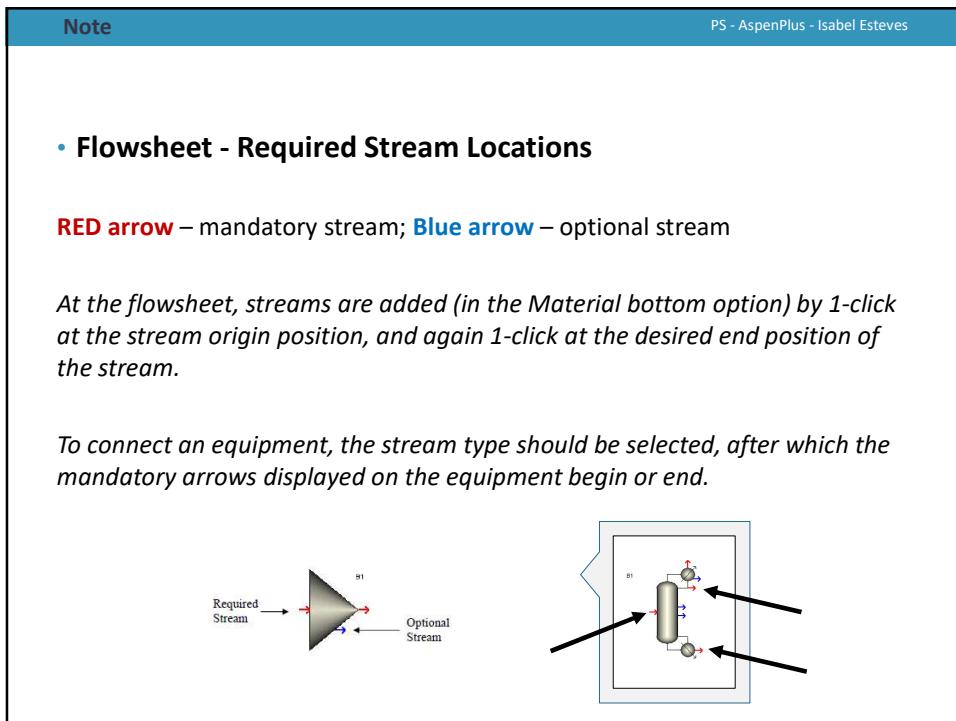
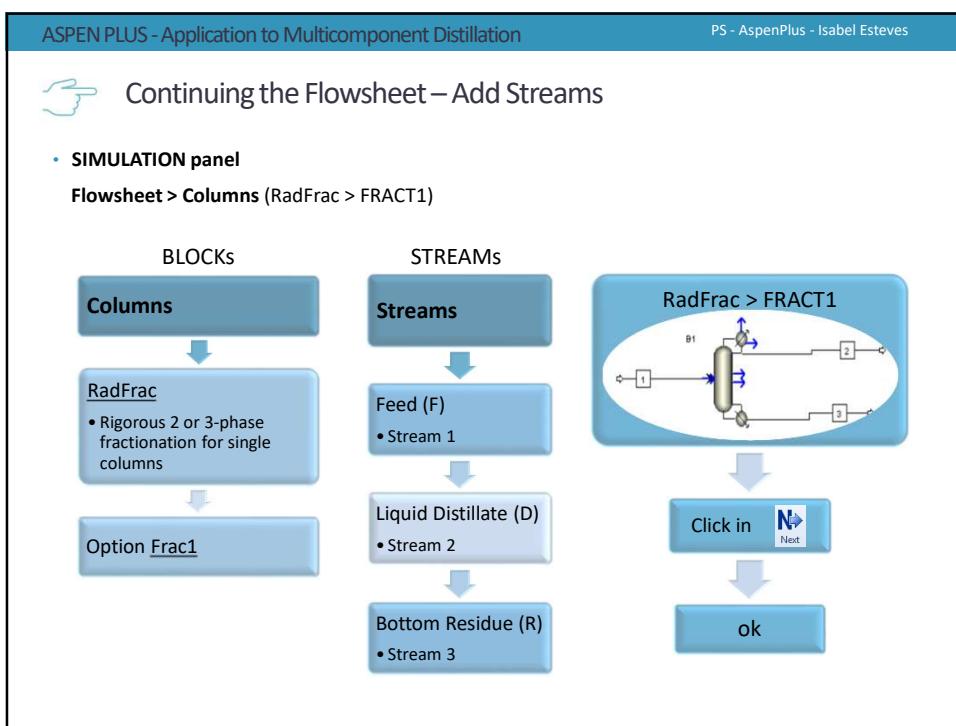
- Start small and simple and then slowly grow up.
- To build large flowsheets, you should start with a few blocks at a time. In this way, you will have a better chance to troubleshoot errors if they occur.
 - Ensure that flowsheet inputs are reasonable.
- After carrying out the simulation using Aspen Plus, check that results are consistent and realistic.
 - Try it repeatedly without fear to fail.
 - Use ASPEN PLUS built-in Help.

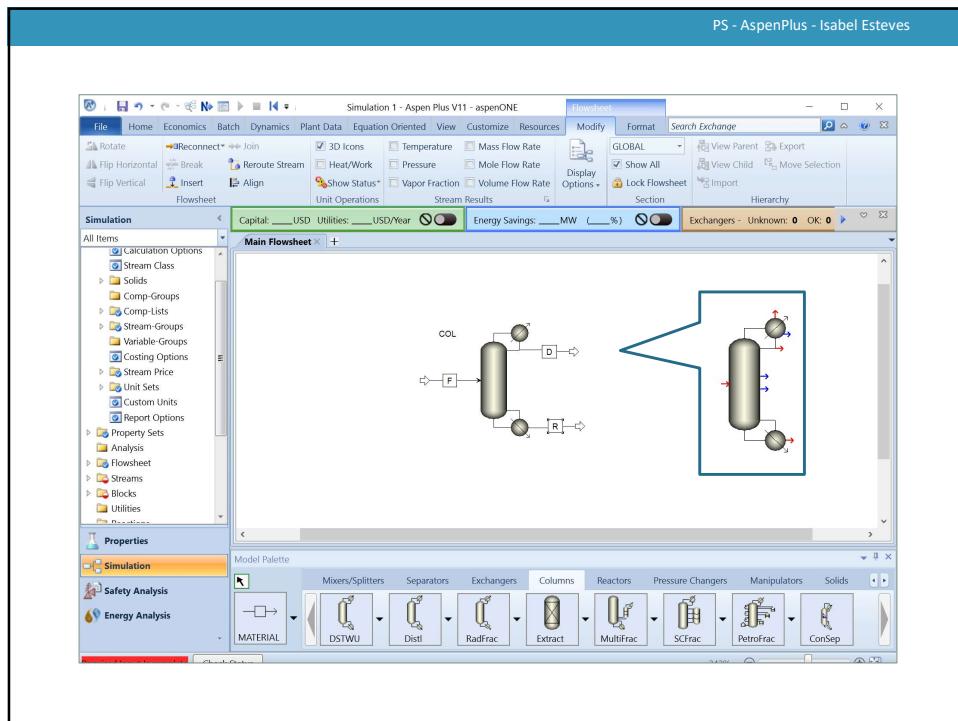
ASPEN PLUS - Application to Multicomponent Distillation PS - AspenPlus - Isabel Esteves

Starting the Flowsheet – Add Block

- **SIMULATION panel**

Flowsheet > Columns (RadFrac > FRACT1)





ASPEN PLUS - Application to Multicomponent Distillation PS - AspenPlus - Isabel Esteves

Continuing the Flowsheet – Add Feed

- Feed (F) Specifications

In Properties > Components

- ✓ Propane
- ✓ Isobutane

In Properties > Methods

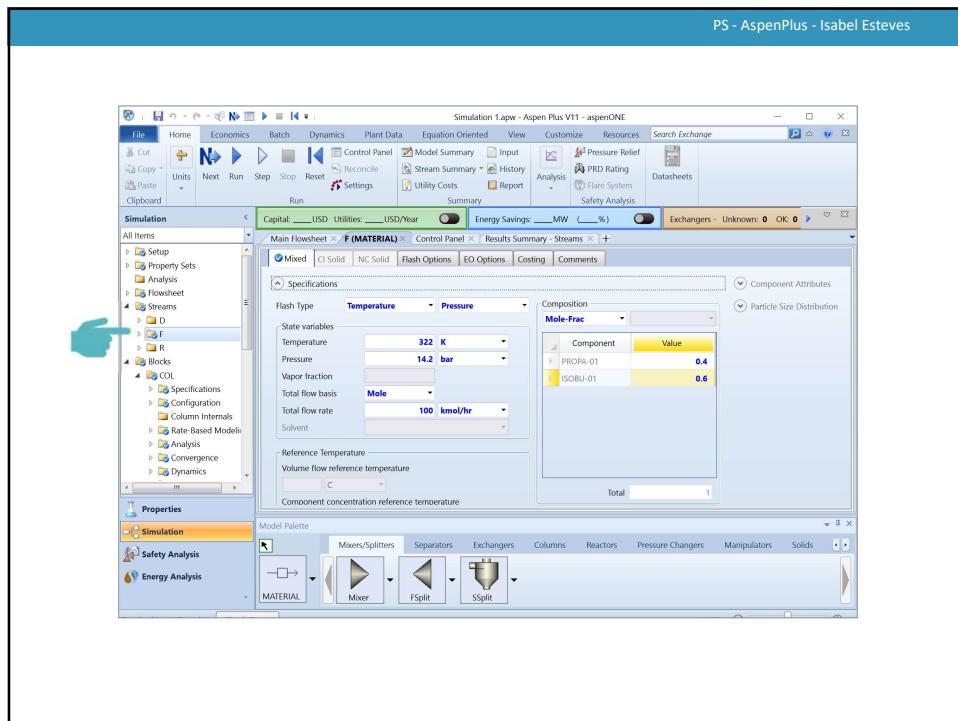
- ✓ Base Method: UNIFAC (packages for predictive property methods to generate VLE data)

In Simulation > Streams > F > Input

- Temperature 322 K
- Pressure 14.2 bar
- Total mole-flow 100 kmol/hr
- Mole-fraction propane 0.4
- Mole-fraction isobutane 0.6

Attention to units!

Attention to the point or comma on your computer!



ASPEN PLUS - Application to Multicomponent Distillation PS - AspenPlus - Isabel Esteves

Continuing the Flowsheet – Add Block Specs

- **Column Specifications (B1/COL)**

Blocks > B1 (or COL) > Setup > Configuration

- Number of stages 32 (in Aspen N_r includes Condenser and Boiler)
- Condenser Total
- Distillate Rate 40 kmol/hr
- Reflux ratio 2
- Do not change Reboiler, Valid phases, Convergence

Blocks > B1 (or COL) > Setup > Streams

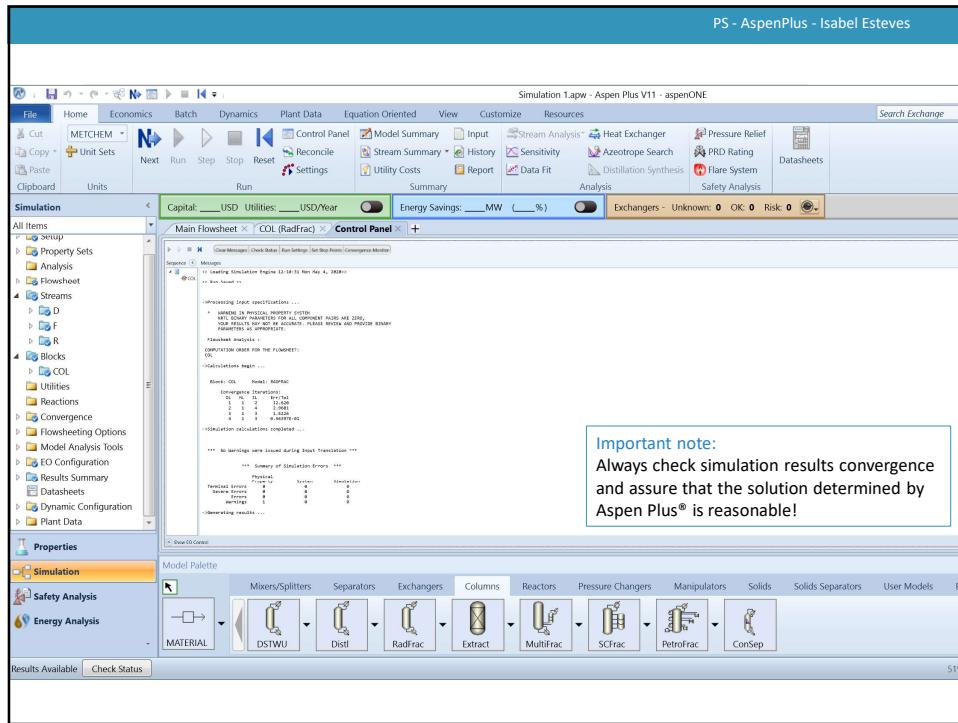
- In the RadFrac model, there are N stages. Stage 1 is the top stage (the condenser); stage N is the bottom stage (the boiler).
- Feed: stage 16

Blocks > B1 (or COL) > Setup > Pressure

- Top-stage / Condenser pressure 14 bar
- Pressure drop for the rest of the column (per stage) 0.1 psi

Run

- Status messages on execution
- No errors > "All blocks have been executed"
- Warnings are not errors; simulation runs



Analysing the Results

- Simulation results: Results Summary > Streams (results table)

Stream	Flow Rate (kg/h)	Temperature (°C)	Pressure (kPa)	Concentration (%)
SG-1	1000	20	101325	50.00
SG-2	500	40	101325	50.00
SG-3	500	60	101325	50.00
SG-4	500	80	101325	50.00
SG-5	500	100	101325	50.00
SG-6	500	120	101325	50.00
SG-7	500	140	101325	50.00
SG-8	500	160	101325	50.00
SG-9	500	180	101325	50.00
SG-10	500	200	101325	50.00
SG-11	500	220	101325	50.00
SG-12	500	240	101325	50.00
SG-13	500	260	101325	50.00
SG-14	500	280	101325	50.00
SG-15	500	300	101325	50.00
SG-16	500	320	101325	50.00
SG-17	500	340	101325	50.00
SG-18	500	360	101325	50.00
SG-19	500	380	101325	50.00
SG-20	500	400	101325	50.00
SG-21	500	420	101325	50.00
SG-22	500	440	101325	50.00
SG-23	500	460	101325	50.00
SG-24	500	480	101325	50.00
SG-25	500	500	101325	50.00
SG-26	500	520	101325	50.00
SG-27	500	540	101325	50.00
SG-28	500	560	101325	50.00
SG-29	500	580	101325	50.00
SG-30	500	600	101325	50.00
SG-31	500	620	101325	50.00
SG-32	500	640	101325	50.00
SG-33	500	660	101325	50.00
SG-34	500	680	101325	50.00
SG-35	500	700	101325	50.00
SG-36	500	720	101325	50.00
SG-37	500	740	101325	50.00
SG-38	500	760	101325	50.00
SG-39	500	780	101325	50.00
SG-40	500	800	101325	50.00
SG-41	500	820	101325	50.00
SG-42	500	840	101325	50.00
SG-43	500	860	101325	50.00
SG-44	500	880	101325	50.00
SG-45	500	900	101325	50.00
SG-46	500	920	101325	50.00
SG-47	500	940	101325	50.00
SG-48	500	960	101325	50.00
SG-49	500	980	101325	50.00
SG-50	500	1000	101325	50.00

ASPEN PLUS - Application to Multicomponent Distillation PS - AspenPlus - Isabel Esteves

Analysing the Results

- Simulation results > Results Summary > Models

Parameter	Value
Calculated distillate rate (kmol/hr)	40
Condenser / top stage temperature (IC)	45.0725
Condenser / top stage pressure (Tst)	14
Condenser / top stage heat duty (kcal/hr)	-0.400979
Condenser / top stage subcooling duty	0
Condenser / top stage reflux rate (kmol/hr)	80
Condenser / top stage free water reflux ratio	2
Reboiler pressure (Pst)	14.2137
Reboiler heat duty (kcal/hr)	76.0000
Reboiler heat duty (kcal/kJ)	0.46650

Explore fearless the simulation results:

- L/D, F, N_P, N_T
- Compositions of streams D and R
- Temperatures of D and R
- L and V minimums and maximums
- Energy consumptions in condenser and boiler

Attention to units!

ASPEN PLUS - Application to Multicomponent Distillation PS - AspenPlus - Isabel Esteves

Analysing the Results

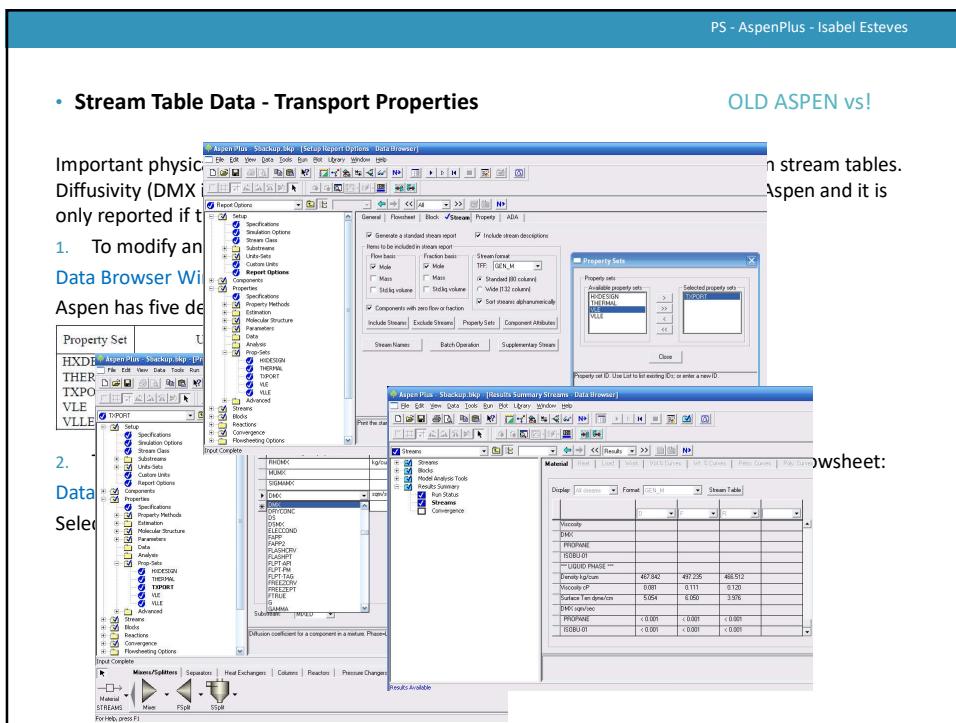
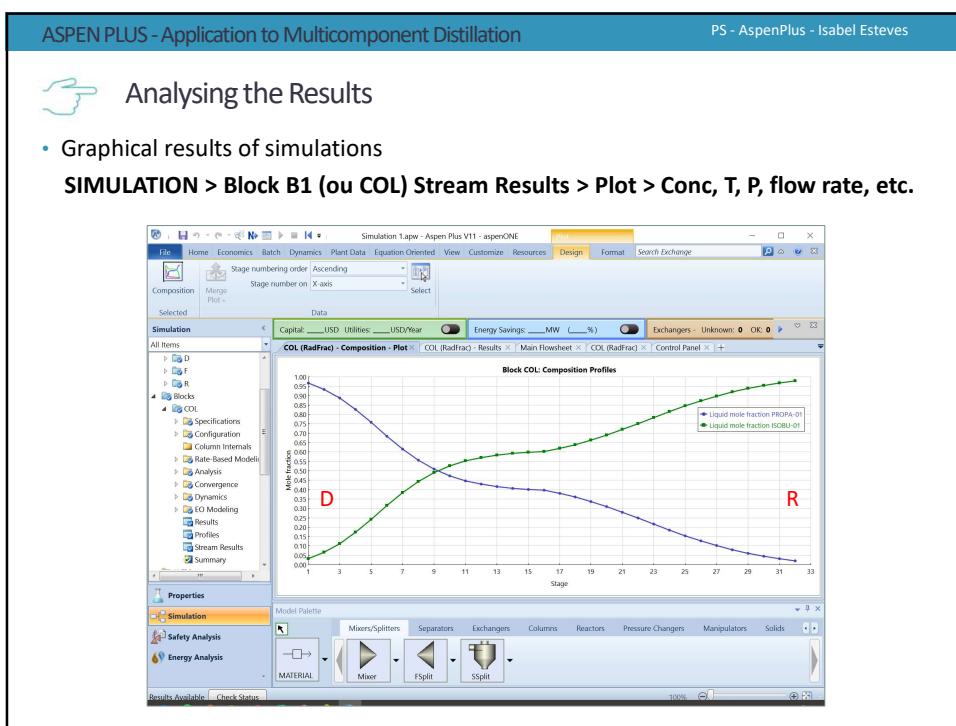
- Simulation Results

Streams Compositions

• Objective initially set:
Molar fraction of propane
in the distillate of 0.97

↓
L/V = 3 ?

Stream	D	F	R
PROPA-01	0.967299	0.4	0.0218006
ISOB-01	0.0327012	0.6	0.978199



ASPEN PLUS - Application to Multicomponent Distillation PS - AspenPlus - Isabel Esteves

Saving the Work!

- Save AspenPlus simulation and close. Results will be saved in a *.apw file. Do not delete de extra Aspen files created in the working folder and store them as part of the exercise. Files *.apw are not compatible across different versions of Aspen Plus.

File > Save As Aspen Plus Document (Aula1.apw)

File > Exit

PS - AspenPlus - Isabel Esteves

Important to follow when working in ASPEN PLUS

- Save AspenPlus simulation file before each run when you are changing parameters to solve a problem. Do it with distinct names (a,b,... or v1,v2, etc.)
- When you do several simulations, the file will store them internally. So, the final results can be affected by those of previous simulations. For more complicated exercises, you should always reset the file content by clicking and then perform the next simulation.

General procedure to solve an exercise/report:

1. Read and identify well the problem proposed.
2. Recognize well the problem inputs and their units.
3. Do a comprehensive presentation of your results.
4. Analyze and be critic of your own results beyond the obvious.
5. Search bibliography related to theory and AspenPlus to analyze well your results.
6. Explore the potential of ASPEN PLUS without fear to fail.

May-2024

INTRODUCTION TO **ASPEN PLUS COMPUTATIONAL TOOL**- APPLICATIONS TO MULTICOMPONENT DISTILLATION AND SOLVENT EXTRACTION PROCESSES

Isabel A.A.C. Esteves

i.esteves@fct.unl.pt

Chemical and Biochemical/Biological Engineering

Separation Processes

2023/24