Chapter III: Simulation of gas-liquid, liquid-liquid contactors and liquid-solid

III-1- Introduction

Within the realm of chemical engineering, the simulation and comprehension of absorption/stripping phenomena, including those with chemical reactions, and the processes of liquid-liquid and liquid-solid extraction stand as pivotal pillars for numerous industrial applications. This chapter embarks on an exploration of these specific aspects, utilizing the powerful simulation capabilities of Aspen Hysys, a preeminent software tool widely acclaimed in the field of chemical engineering.

Focused primarily on absorption/stripping phenomena, these processes involve the transfer of components between gas and liquid phases, often incorporating chemical reactions. Aspen Hysys serves as an invaluable platform for understanding and optimizing these intricate systems, enabling engineers to delve into the intricacies of mass transfer, phase equilibrium, and the effects of chemical reactions on the overall process dynamics.

Additionally, this chapter encompasses the simulation of liquid-liquid and liquid-solid extraction processes. Liquid-liquid extraction involves the selective transfer of components between two immiscible liquid phases, crucial in industries such as pharmaceuticals, petrochemicals, and environmental engineering. Likewise, liquid-solid extraction plays a vital role in separating target compounds from solid matrices in diverse applications, including pharmaceuticals, food processing, and wastewater treatment.

Aspen Hysys stands out as an exceptional simulation tool that integrates advanced thermodynamic models, mass transfer correlations, and comprehensive unit operation models. Through its capabilities, engineers can accurately model the behavior of these contactors, predict performance under varying conditions, and optimize the design and operational parameters without extensive reliance on costly experimental trials.

Throughout this chapter, the focus remains dedicated to elucidating the methodologies, tools, and features within Aspen Hysys, specifically tailored for

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simulating absorption/stripping processes with and without chemical reactions, as well as liquid-liquid and liquid-solid extraction. From defining initial parameters to integrating complex chemical kinetics and interpreting simulation outcomes, this chapter endeavors to provide engineers and researchers with a thorough guide to harnessing Aspen Hysys' capabilities in these critical separation processes.

In conclusion, the utilization of Aspen Hysys for simulating absorption/stripping processes without and with chemical reactions and liquid-liquid extraction not only facilitates a deeper understanding of these complex systems but also empowers engineers to optimize and innovate within their respective industries. This chapter strives to illuminate the methodologies and strategies essential for leveraging Aspen Hysys in modeling these specific contactors, aiming to equip practitioners with tools for enhanced efficiency and reliability in industrial operations.

III-2- Why Simulation of these columns

The simulation of absorption/stripping phenomena, incorporating chemical reactions, and liquid-liquid extraction processes stands as a critical facet in chemical engineering and industrial applications. Utilizing tools like Aspen Hysys, engineers benefit from comprehensive platforms to model and optimize these intricate separation techniques.

Simulating absorption and stripping columns offers engineers a virtual environment to optimize operating conditions, comprehend complex mass transfer phenomena, and achieve cost-effective design modifications. Aspen Hysys aids in predicting performance variations, considering chemical reactions, and refining phase equilibria, ensuring enhanced efficiency in gas-liquid separation processes.

Similarly, the simulation of liquid-liquid extraction through Aspen Hysys enables engineers to optimize solvent-to-feed ratios, understand interfacial interactions, and design efficient extraction systems. This approach allows for the identification of optimal conditions, leading to improved product purity and higher yields while minimizing solvent usage and energy consumption.

In summary, leveraging Aspen Hysys for simulating absorption/stripping processes with chemical reactions and liquid-liquid extraction empowers engineers to optimize designs, understand complex phenomena, and enhance separation

processes across various industrial sectors.

III-3- Simulation of various Reactors using Aspen Hysys

As mentioned in the previous sections, the next points will give a perfect guide for the users of Aspen Hysys in order to simulate and assess the performances of various mentioned processes

III-3-1- Absorption/Stripping processes

In order to perform these types of simulation, some examples will be taken into consideration, and then numerous steps will be followed in order to resolve them.

- **Example 1:** Separation of SO2 from Air mixture using Absorption column, in which the parameter are as follows:

Solvent (Water, T=20°C, m=60.05 kg/s, p=2 bar)

Flue gas (Mixture "Air: 97mol%, SO2: 3mol%", T=20°C, m=1.717 kg/s, p=2 bar)

Absorber parameters: 20 stages, Top pressure:1.2 bar, Bottom pressure: 1.5 bar

In order to solve this example, there are numerous steps that should be followed using Aspen Hysys, they can be presented as points as follows:

- **Launch Aspen HYSYS:** Open the Aspen HYSYS software on your computer.

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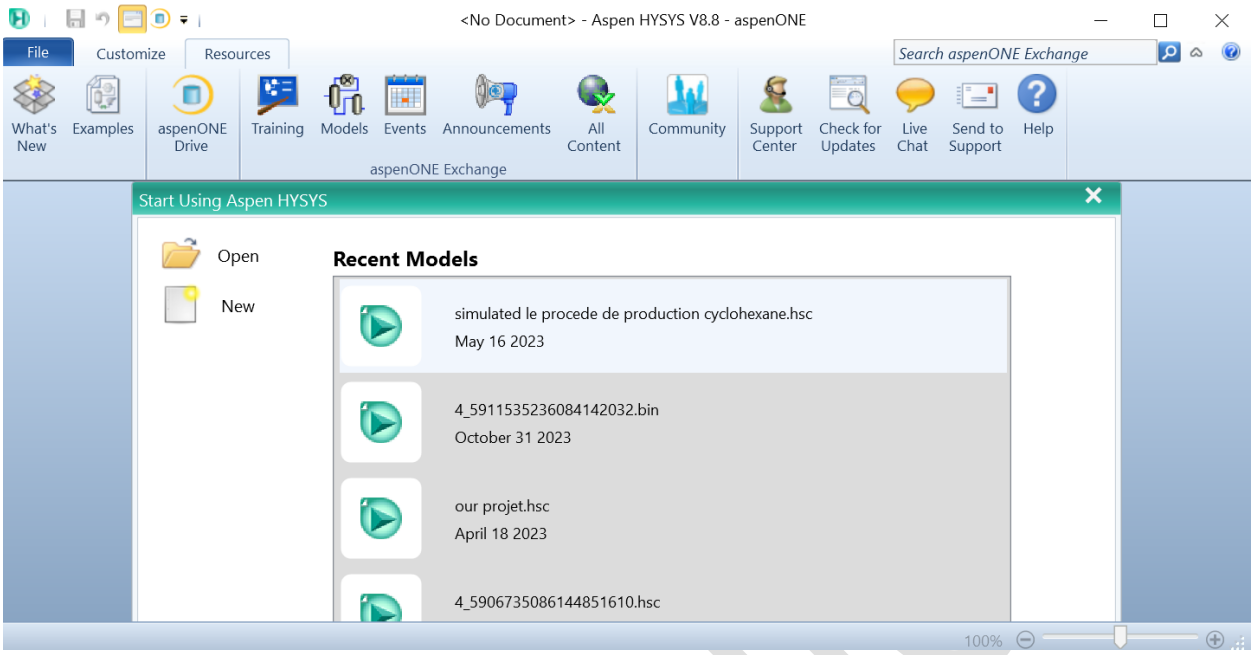

Figure 1. Launch Aspen HYSYS

- **Create a New Project:** Start a new project (case) or open an existing one if you have it. Projects help you organize and save your simulation work.

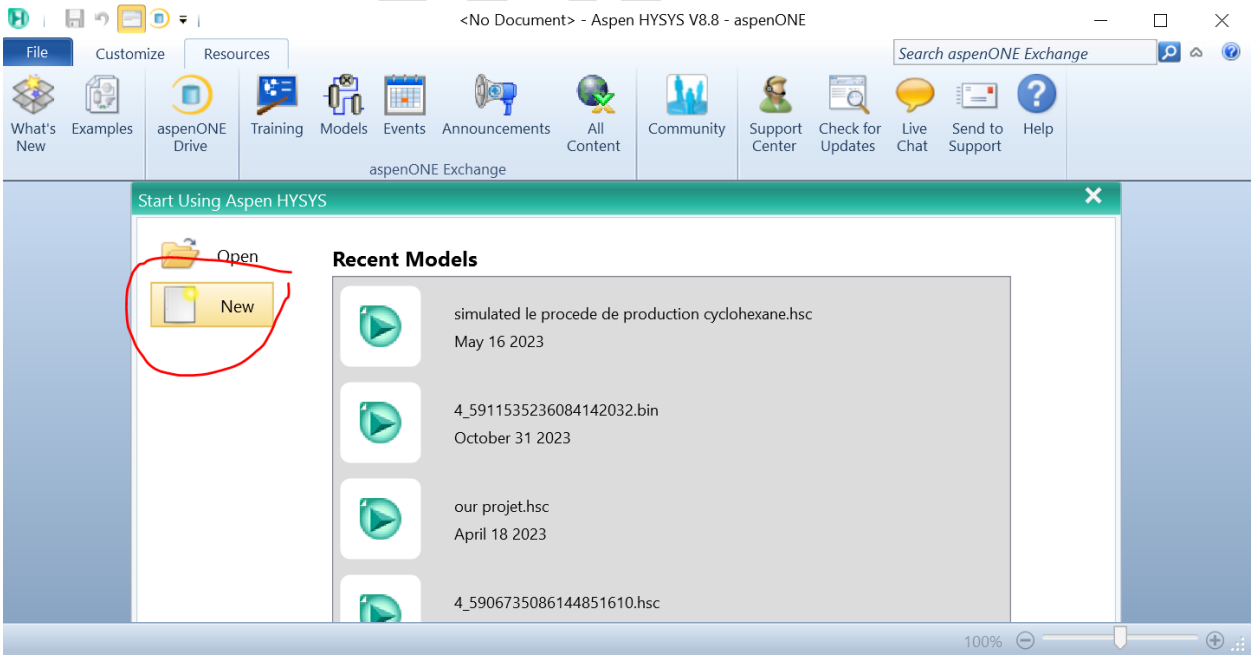

Figure 2. Open a new case

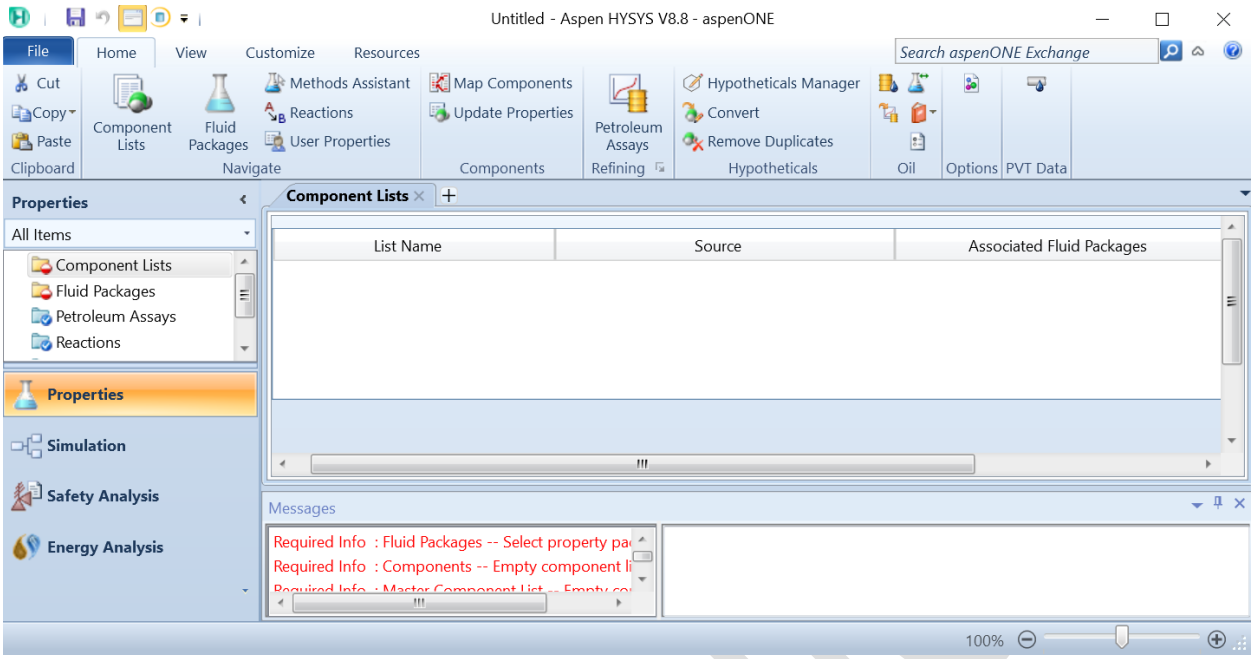

Figure 3. Appeared window after opening a new case or project

- **Define Component list and Fluid Package:** Specify the chemical substances that will take place in the reactor. Also you have to choose the suitable fluid package in order to perform the different associated calculations.

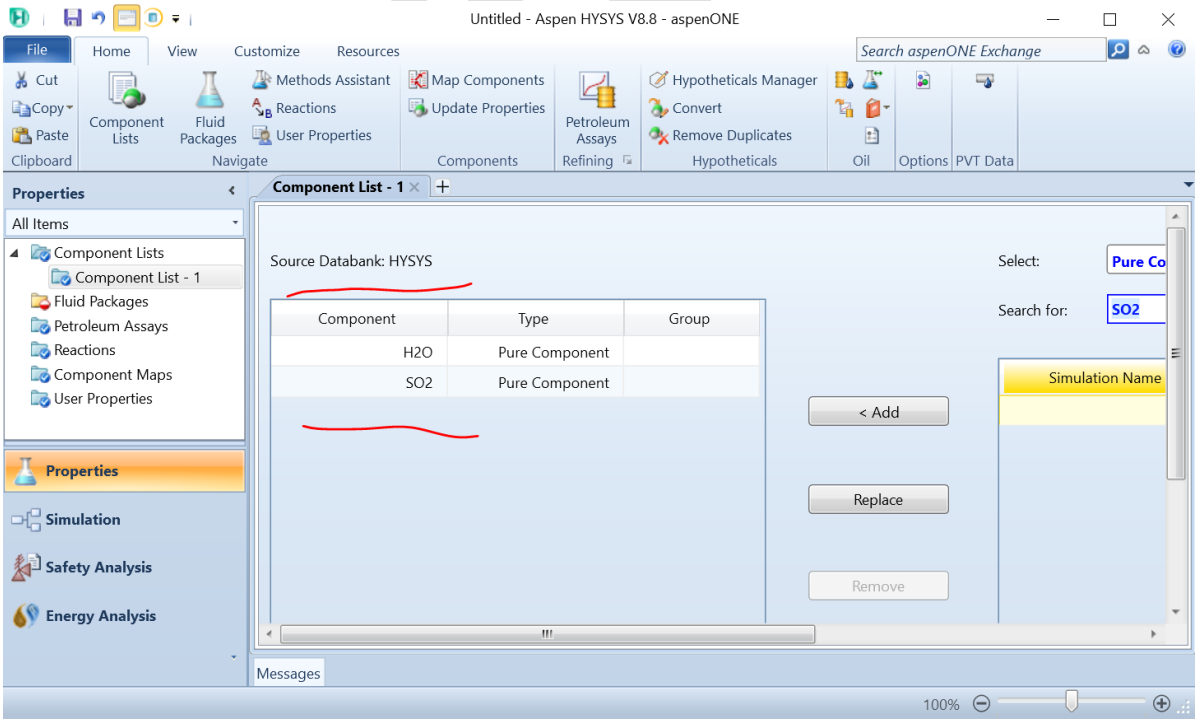

Figure 4. Adding the component list

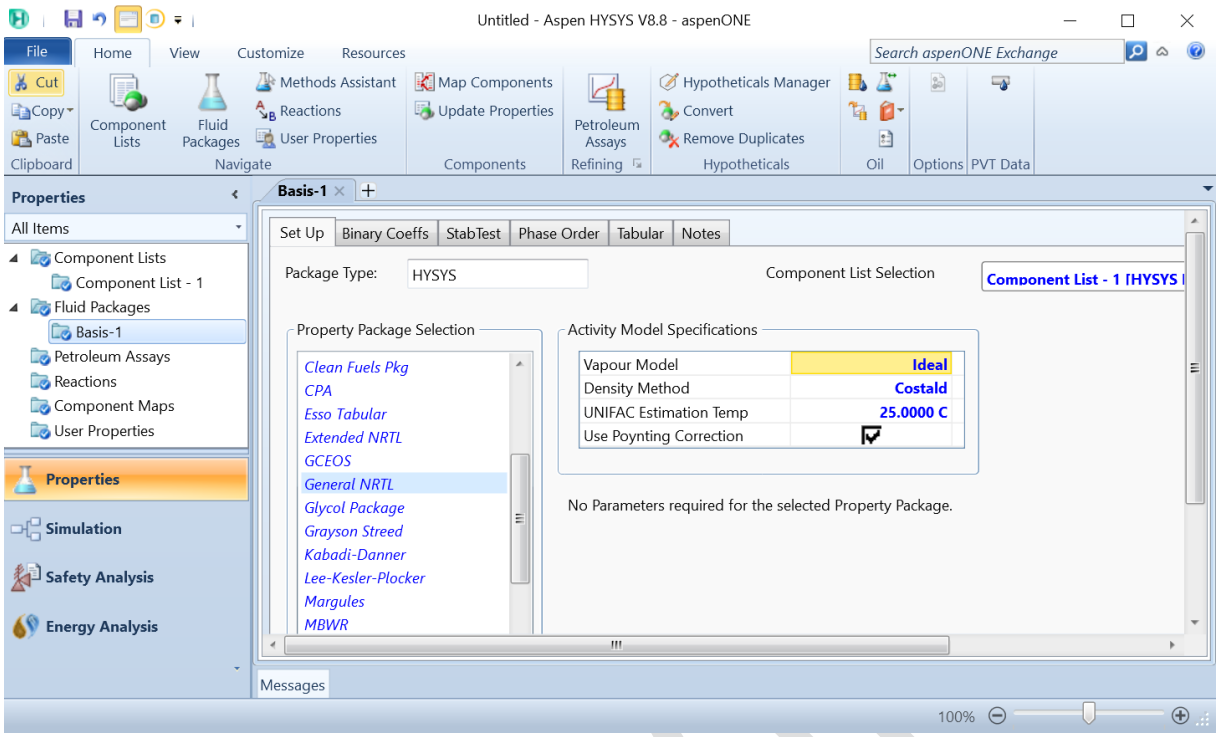

Figure 5. Choose the fluid package

- **Go to simulation environment:** by clicking on the simulation icon on the down left.

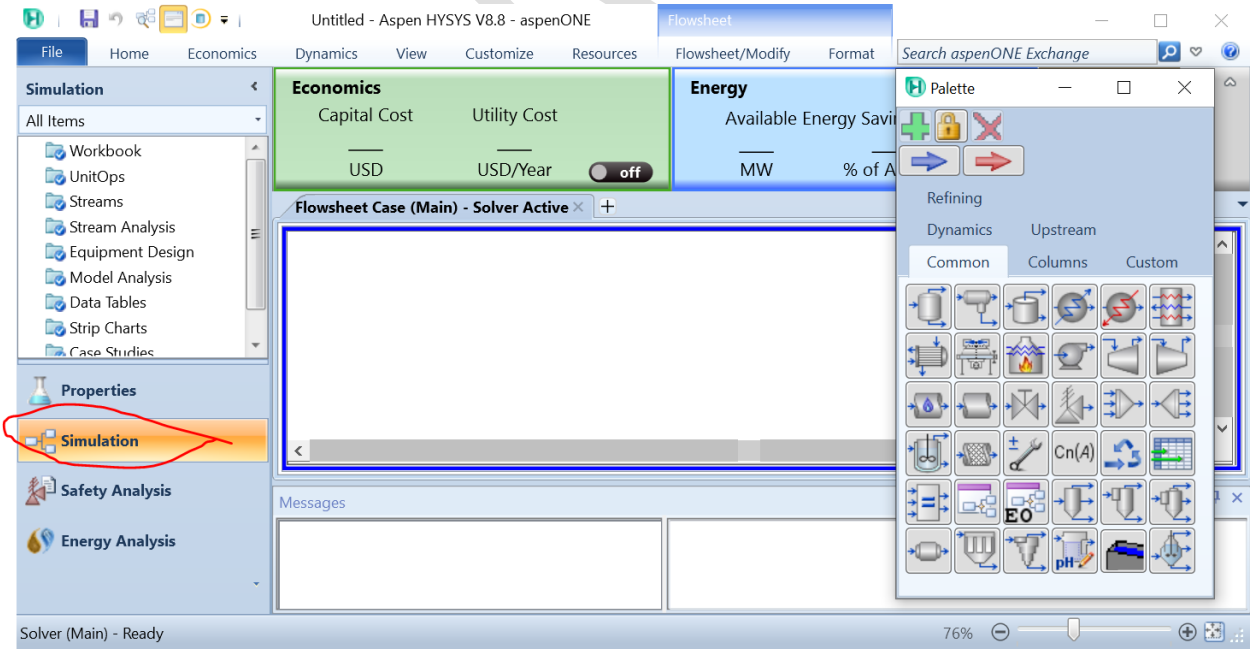

Figure 6. clicking on Simulation Icon

- **Add Absorber:** from the Palette, add an absorber by selecting the absorber you want to simulate.

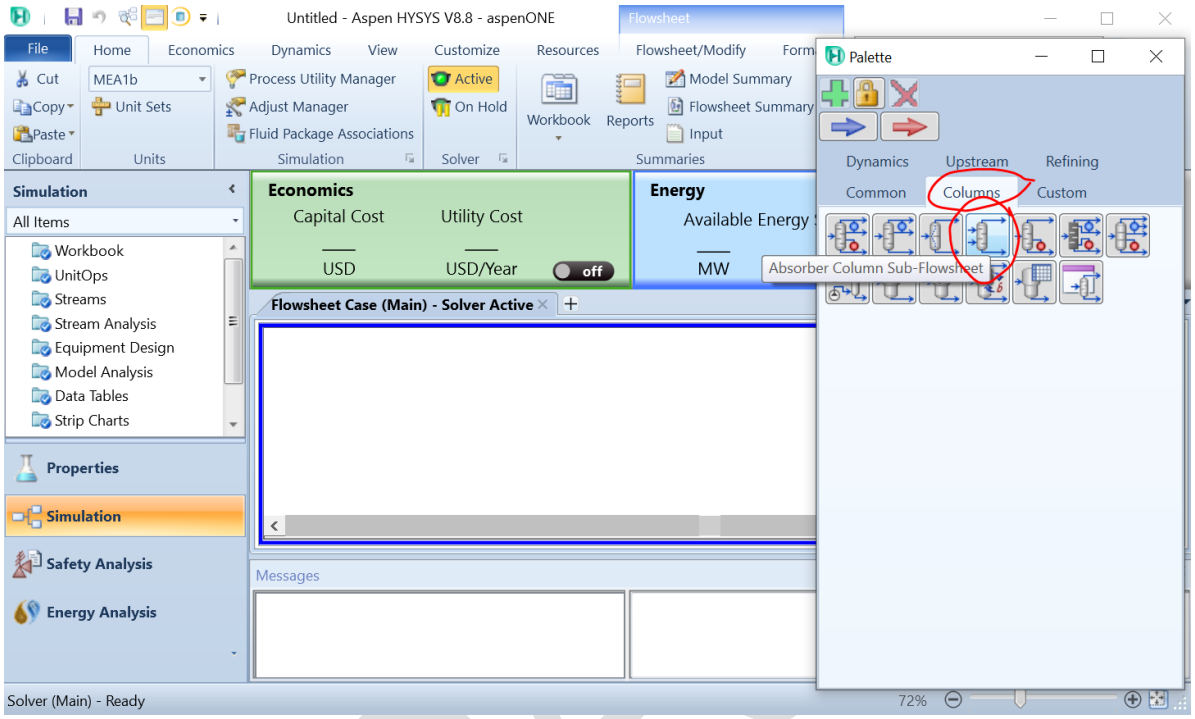

Figure7. Absorber from the palette

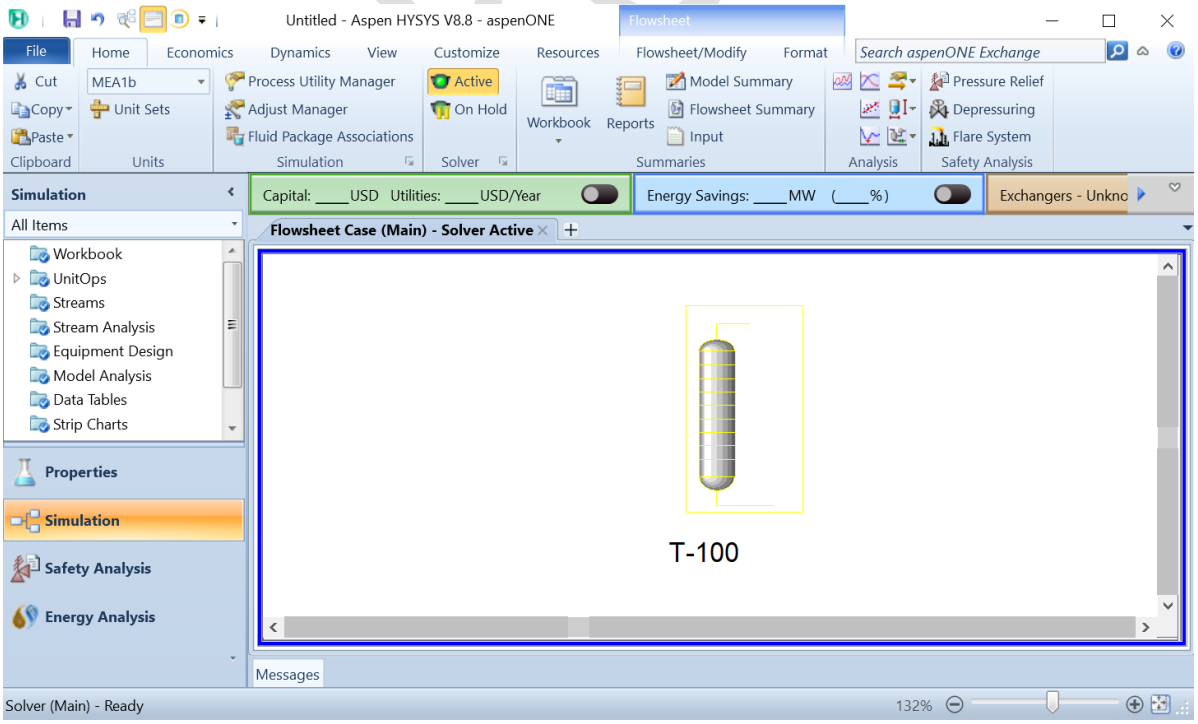

Figure 8. Add the absorber to the PFD

- **Set Operating Conditions:** Define the operating conditions of the absorber, such as temperature, pressure, and flow rates. These conditions significantly impact the reaction rate and product formation.

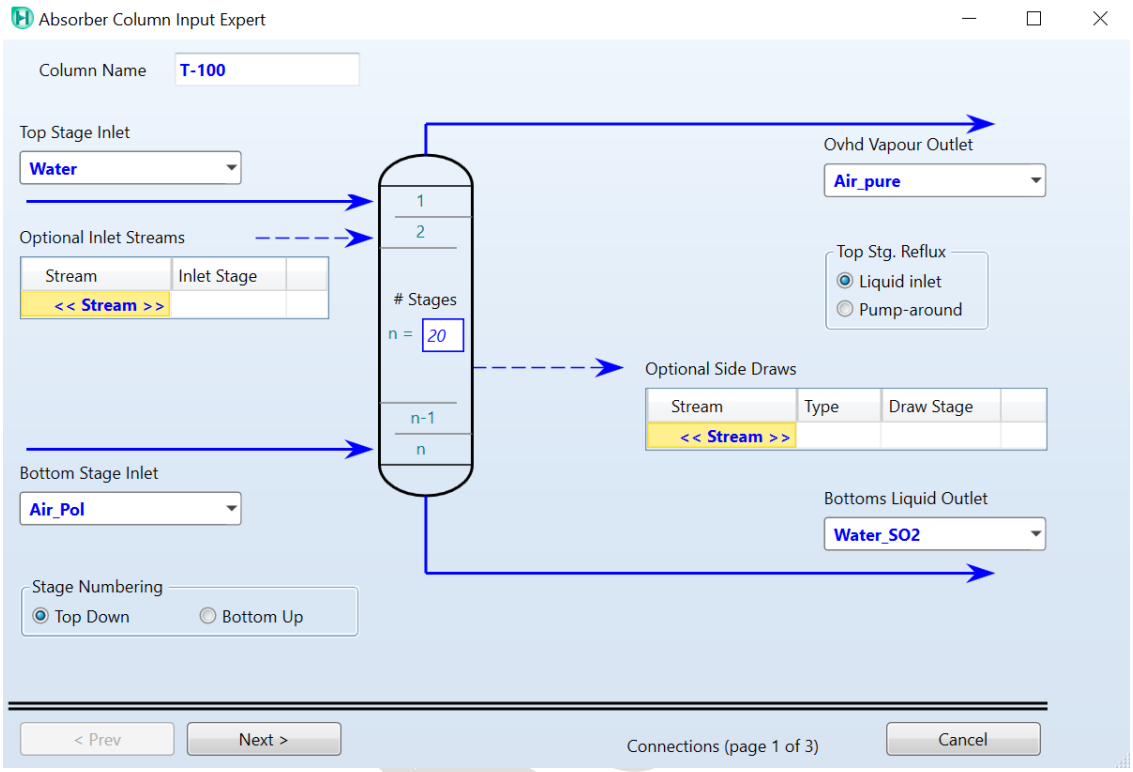

Figure 9. Setting the streams in the absorber

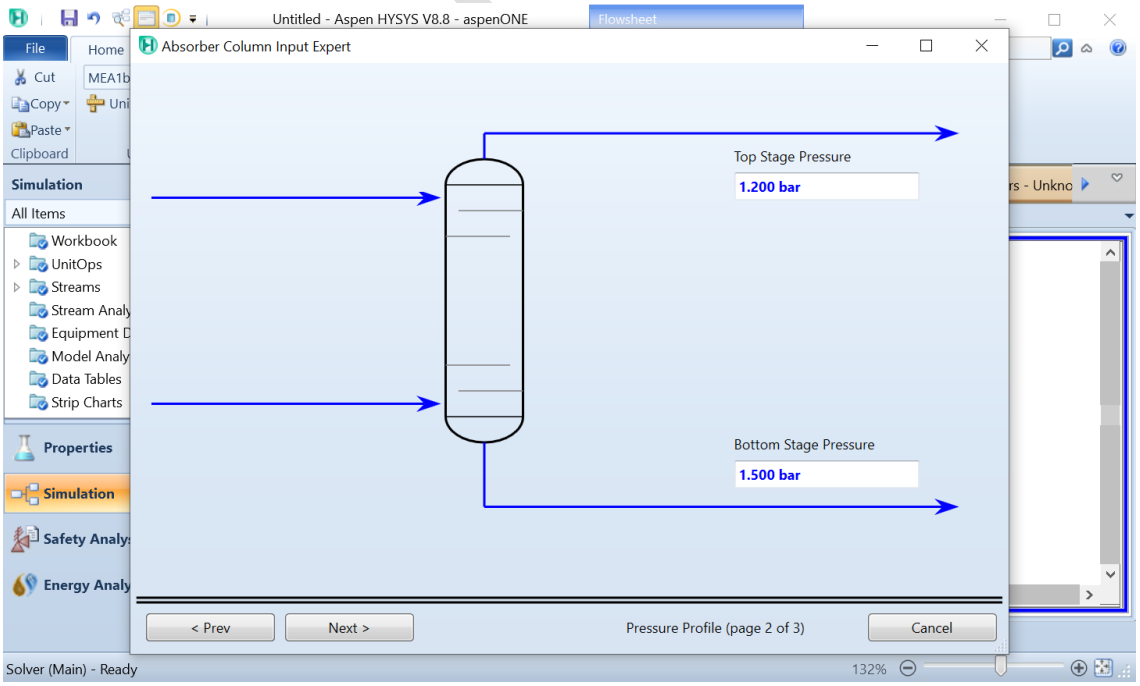

Figure 10. Setting the parameters of the absorber

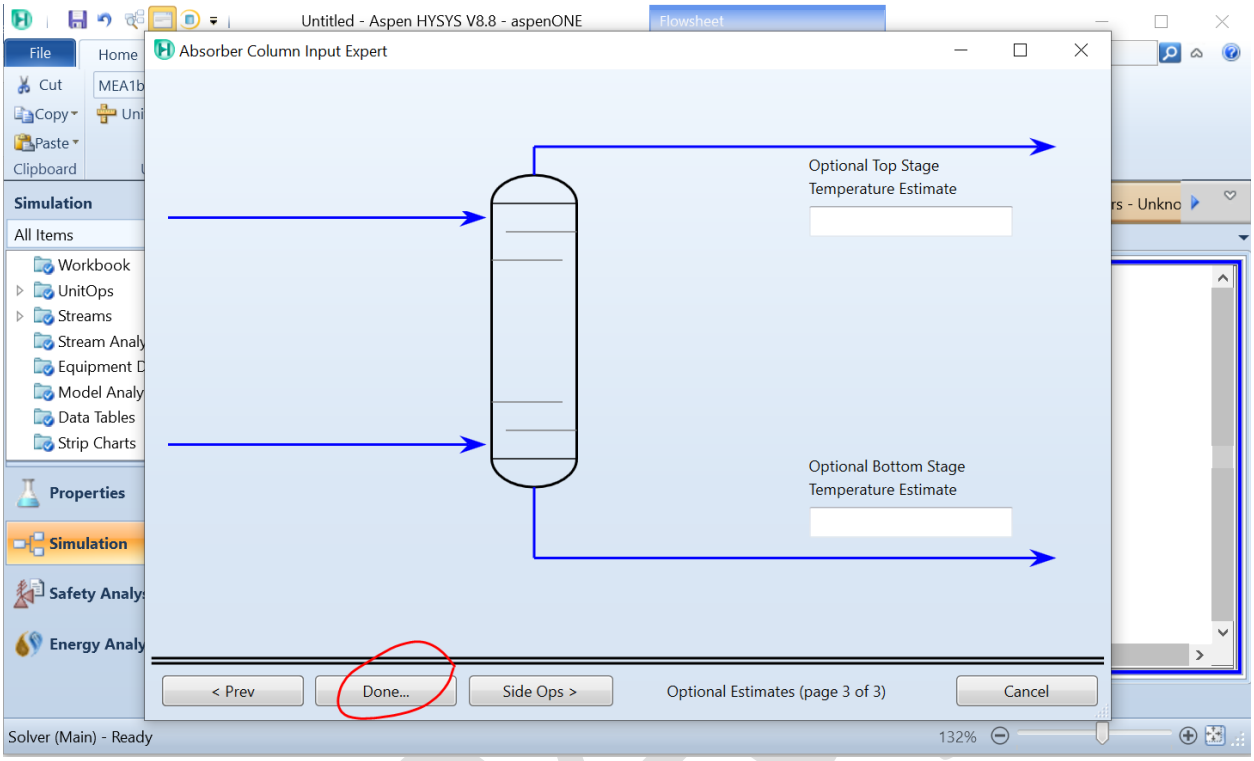

Figure 11. Complete absorber settings

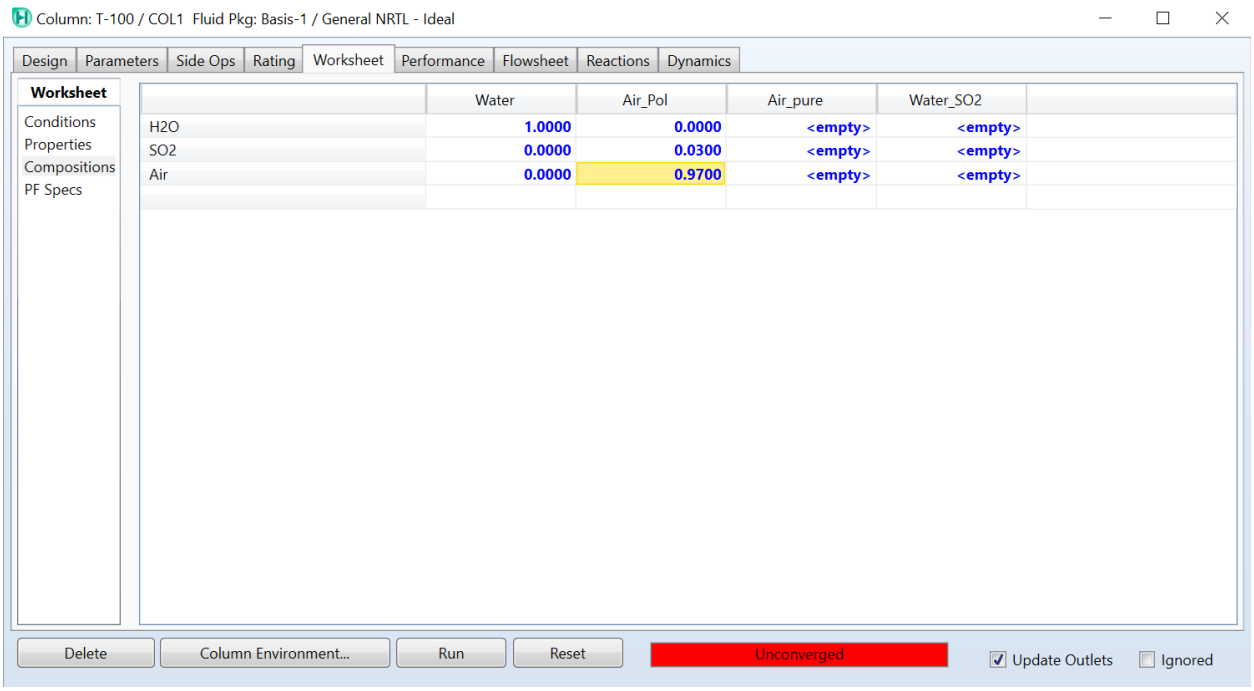

Figure 12. entering the different conditions 1

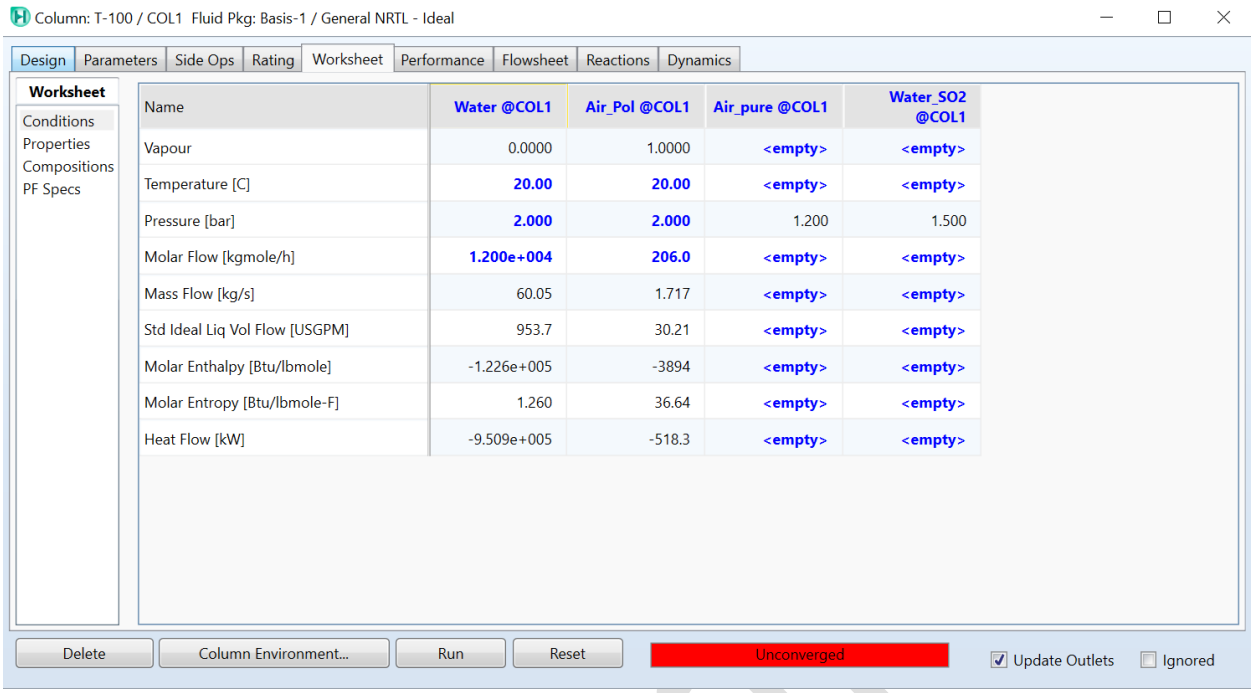

Figure 13. entering the different conditions 2

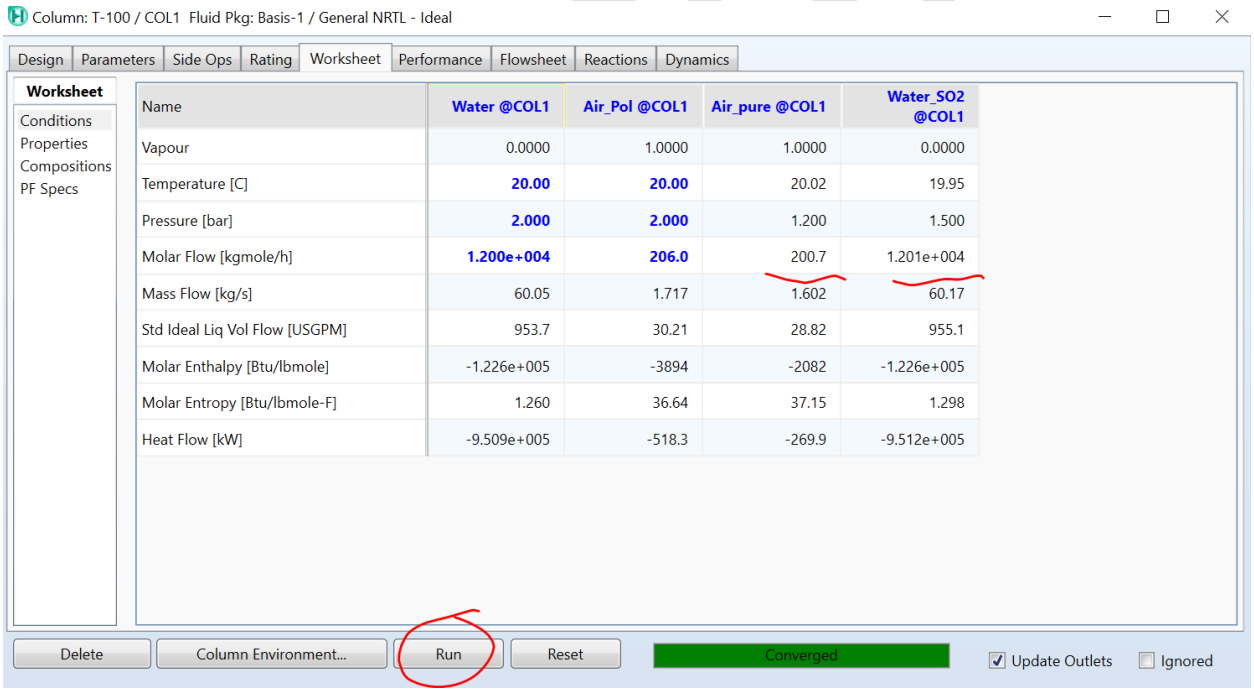

Figure 14. Click on run and the column will be converged

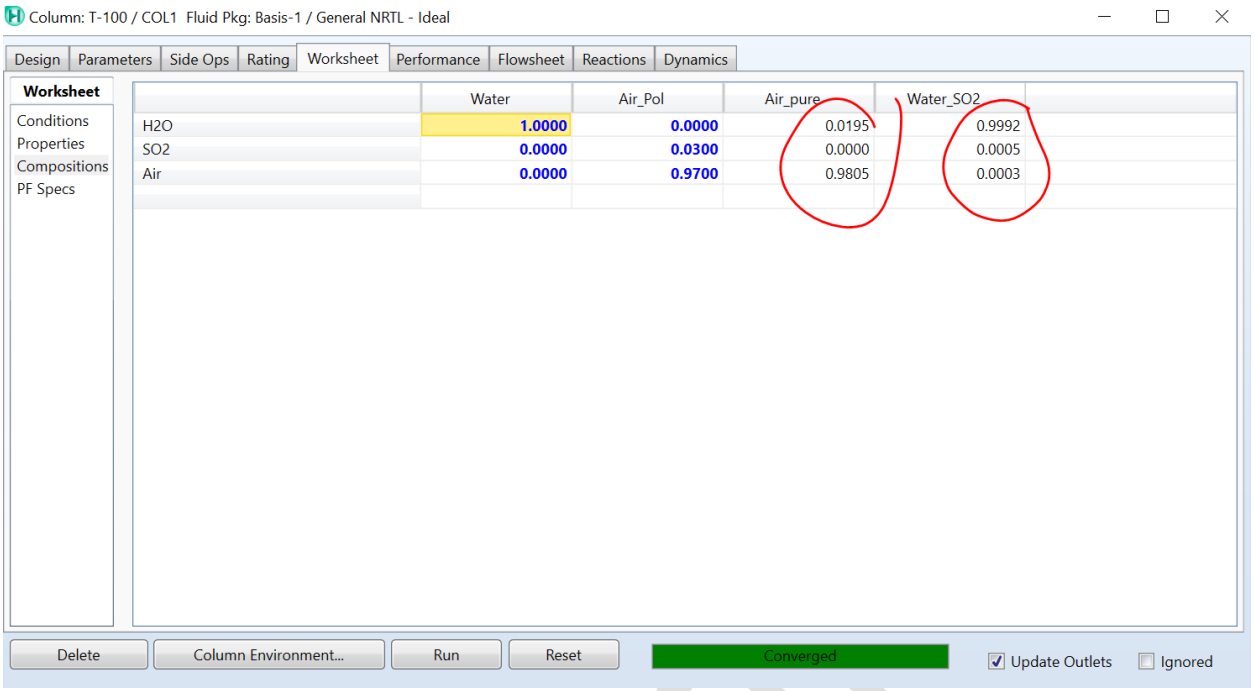

Figure 15. the obtained results 1

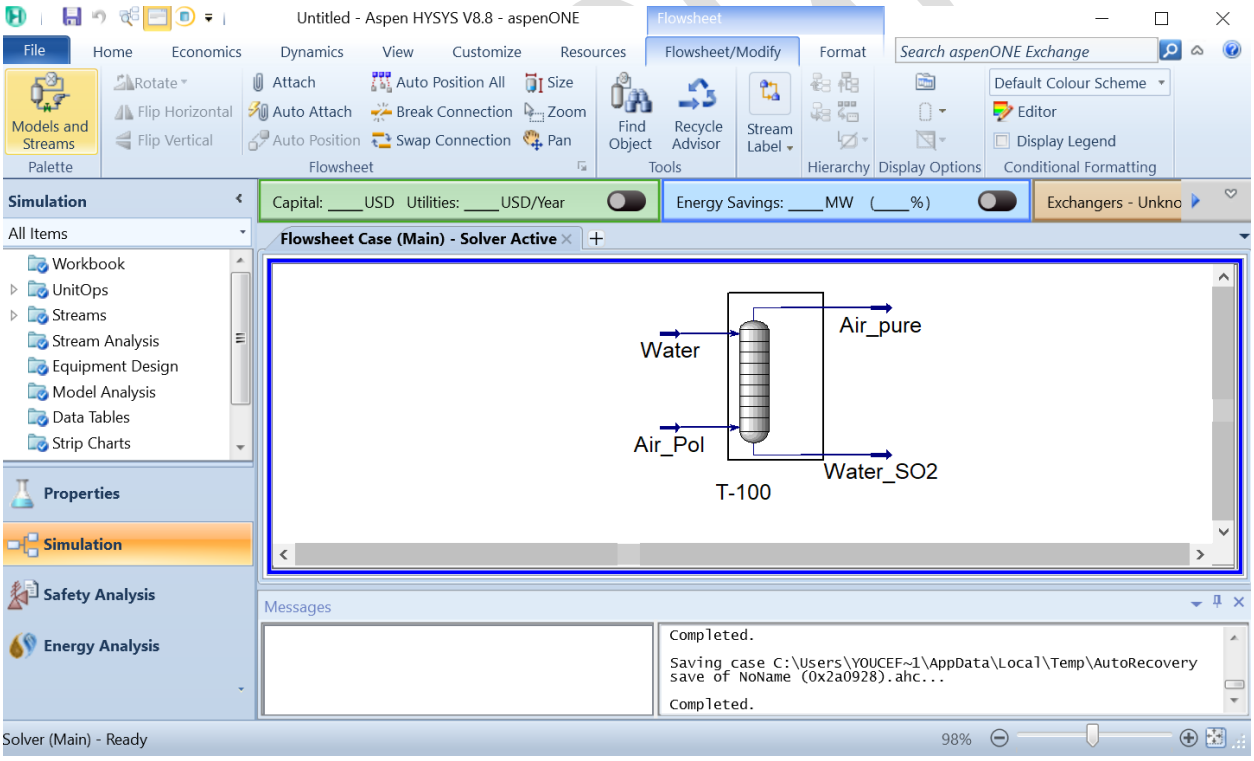

Figure 16. the obtained results 2

These steps provide a general guideline for simulating the absorber column in Aspen HYSYS. However, the specific details and nuances can vary depending on

the type of solvent and the complexity of the process involved. It's essential to consult Aspen HYSYS documentation and resources for more in-depth guidance on using the software effectively.

❖ **Example 2:** A sour water consisted of 97 mol% of H2O and 2 mol% of Ammonia and 1 mol% of H2S is produced from a crude tower should be stripped, the stream is at 103 °C, and 2.8 bar, with a flowrate of 1 kg/s, the required results is a pure water in which the quantity of Ammonia that doesn't achieve 0.005 mol%, while water recovery at least 99.99 mol%.
The stripper has 8 stages in which the stream entered from the 2nd stage.
The condenser pressure is assumed to be 2 bar, while reboiler pressure is assumed to be 2.1 bar.

In order to solve this example, there are numerous steps that should be followed using Aspen Hysys, they can be presented as points as follows:

➢ **Launch Aspen HYSYS:** Open the Aspen HYSYS software on your computer.

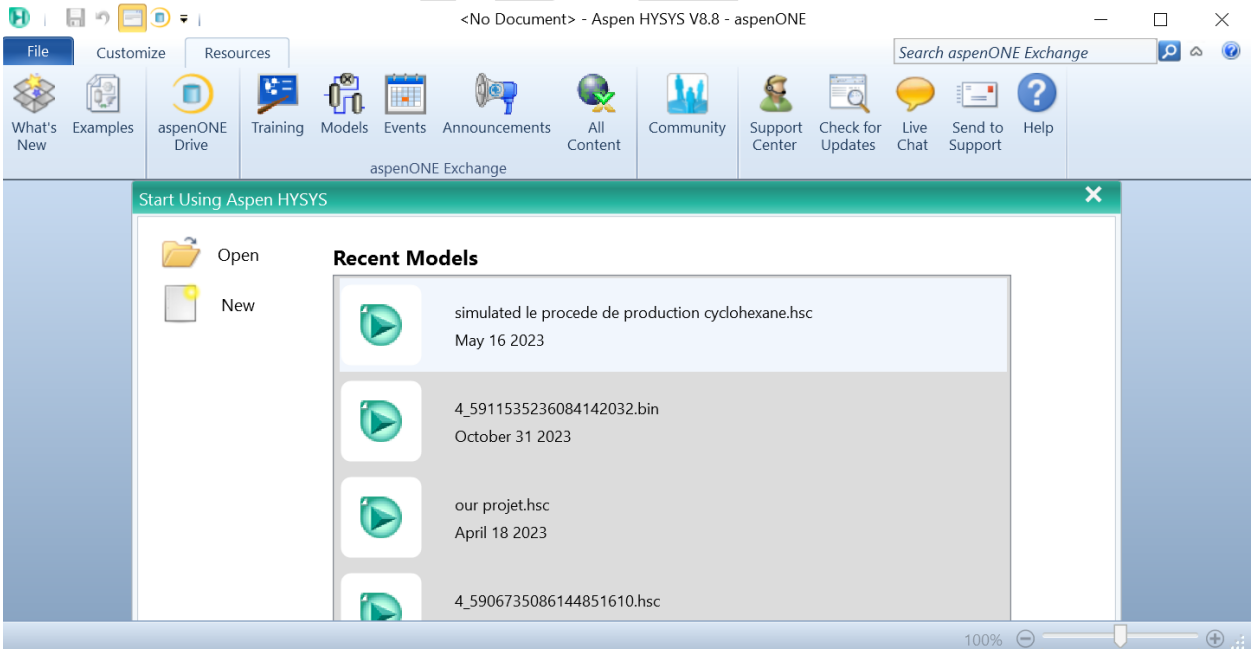

Figure 17. Launch Aspen HYSYS

- **Create a New Project:** Start a new project (case) or open an existing one if you have it. Projects help you organize and save your simulation work.

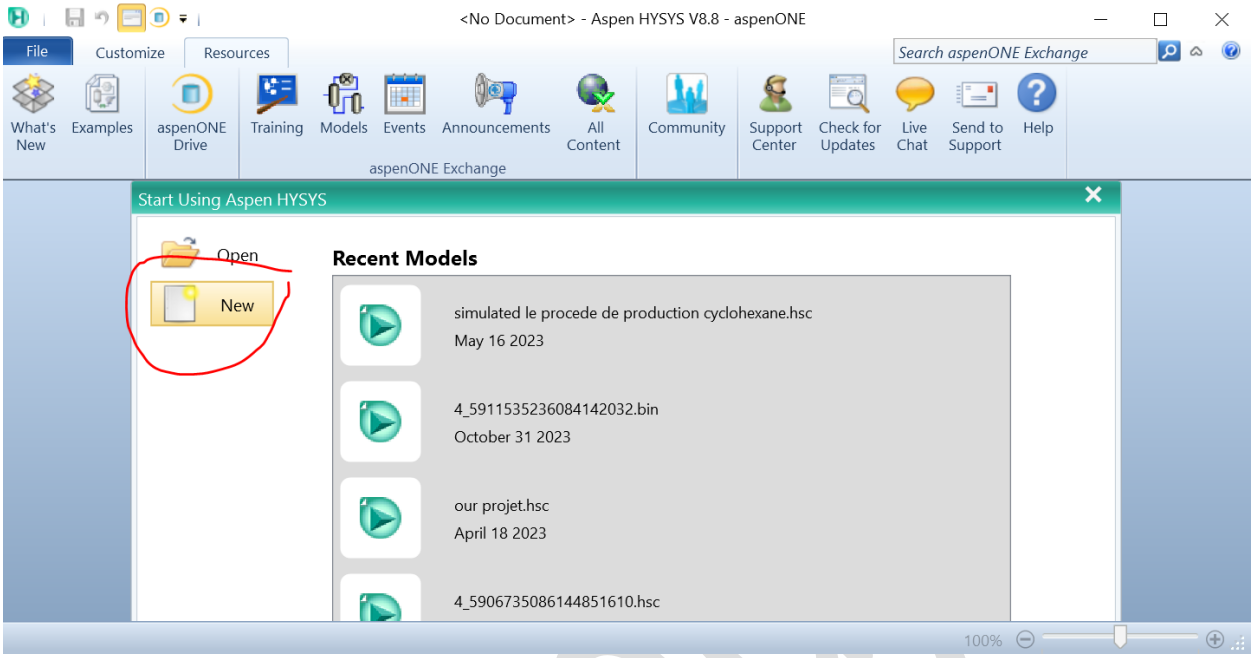

Figure 18. Open a new case

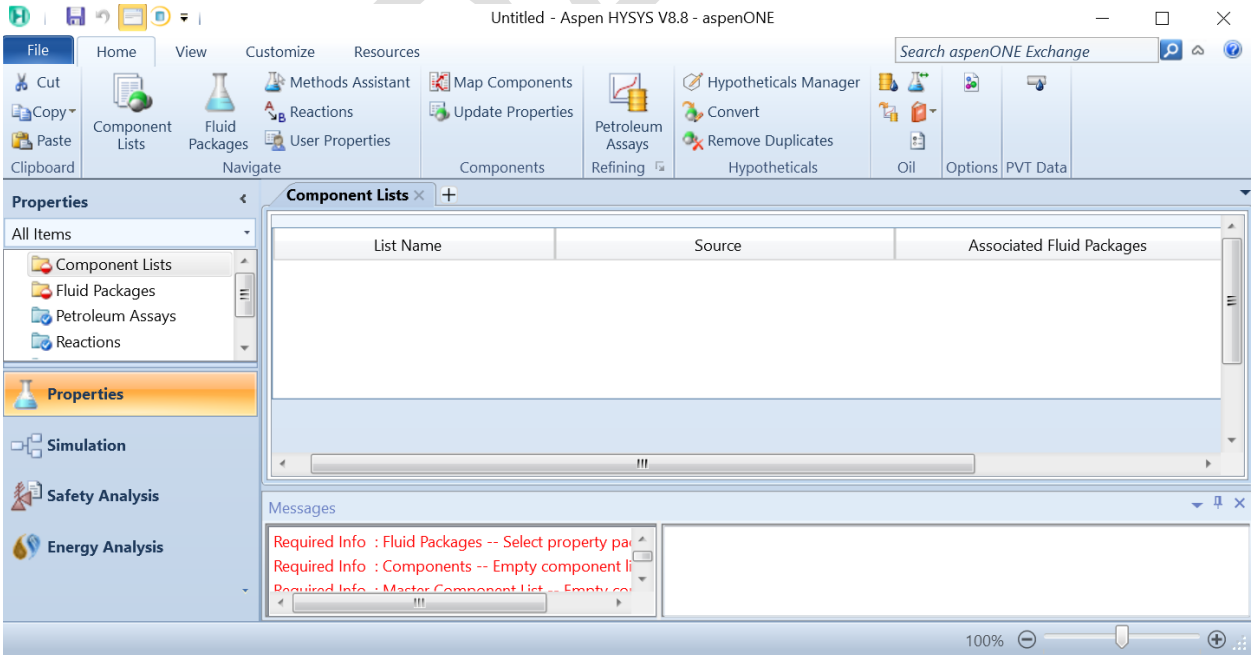

Figure 19. Appeared window after opening a new case or project

- **Define Component list and Fluid Package:** Specify the chemical substances that will take place in the reactor. Also you have to choose the

suitable fluid package in order to perform the different associated calculations.

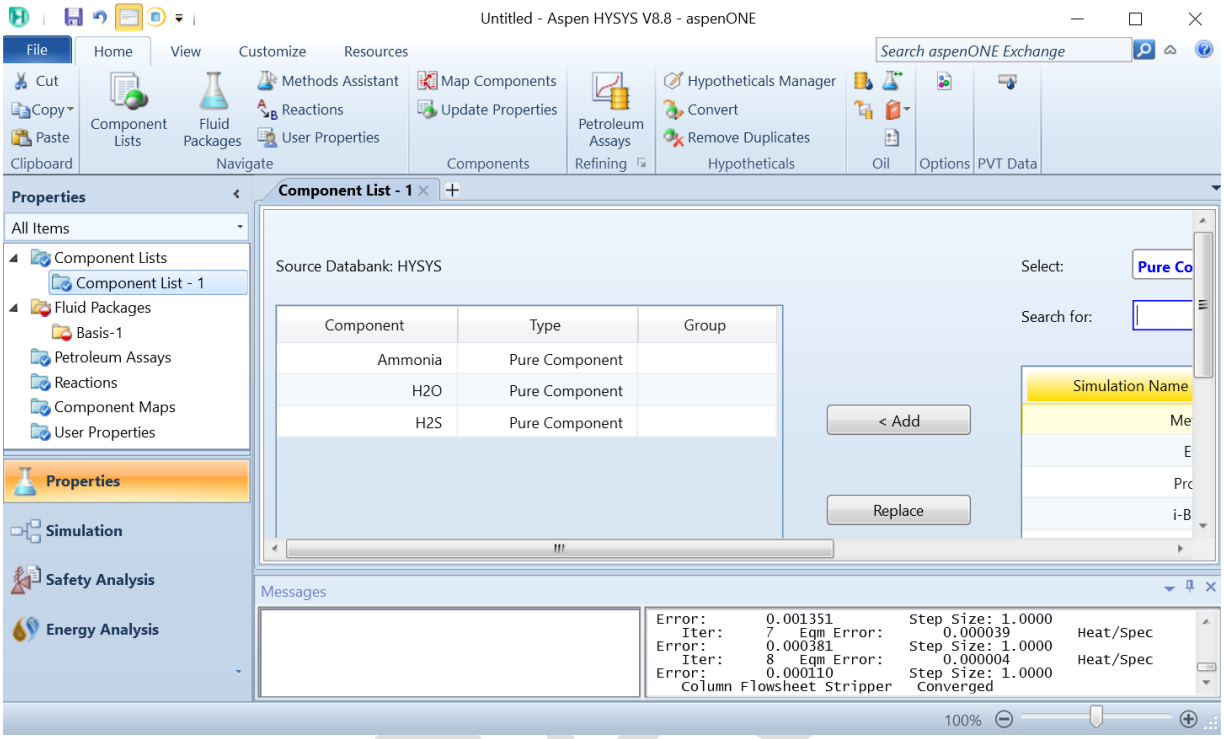

Figure 20. Adding the component list

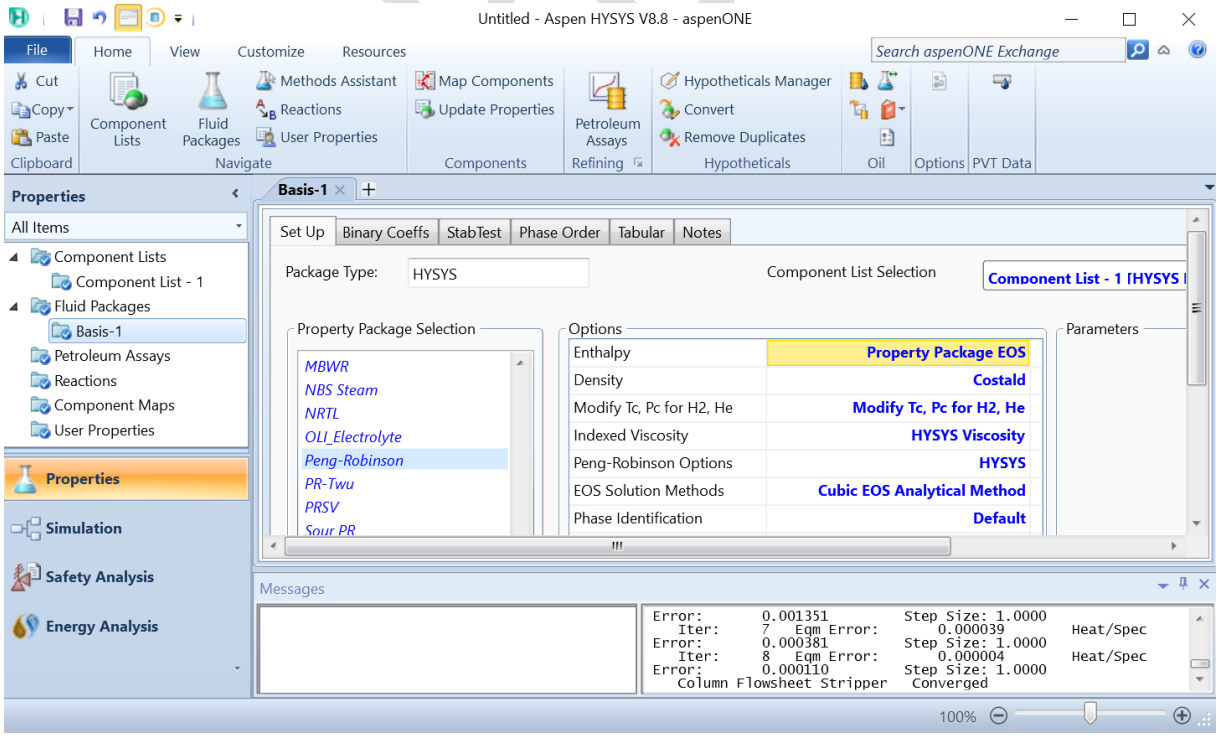

Figure 21. Choose the fluid package

- **Go to simulation environment:** by clicking on the simulation icon on the down left.

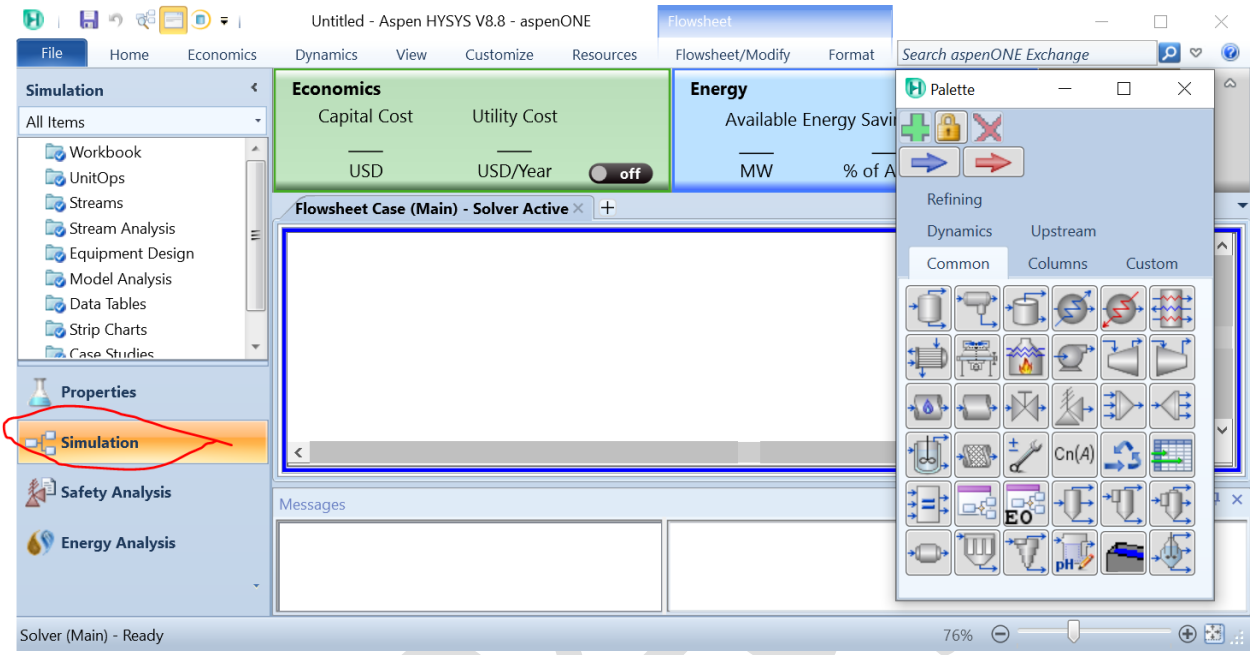

Figure 22. clicking on Simulation Icon

- **Add Stripper:** from the Palette, add a stripper by selecting the distillation column.

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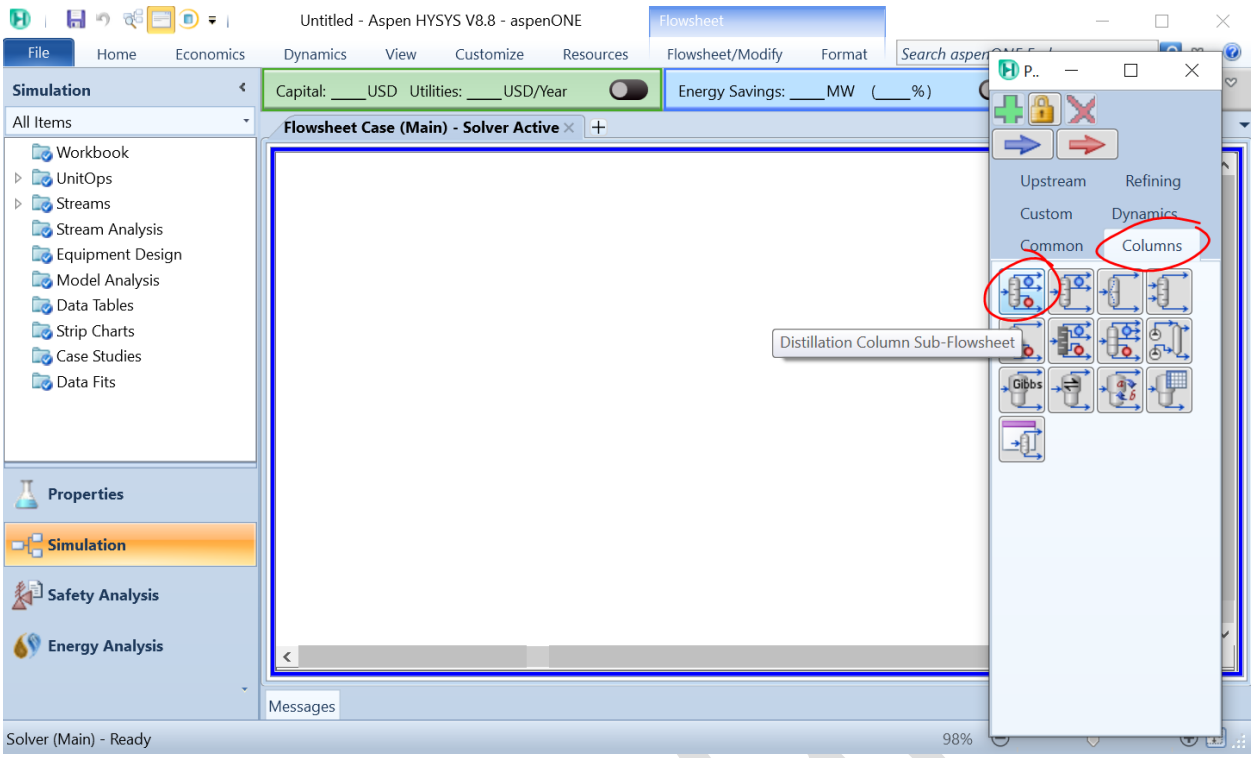

Figure 23. Stripper from the palette

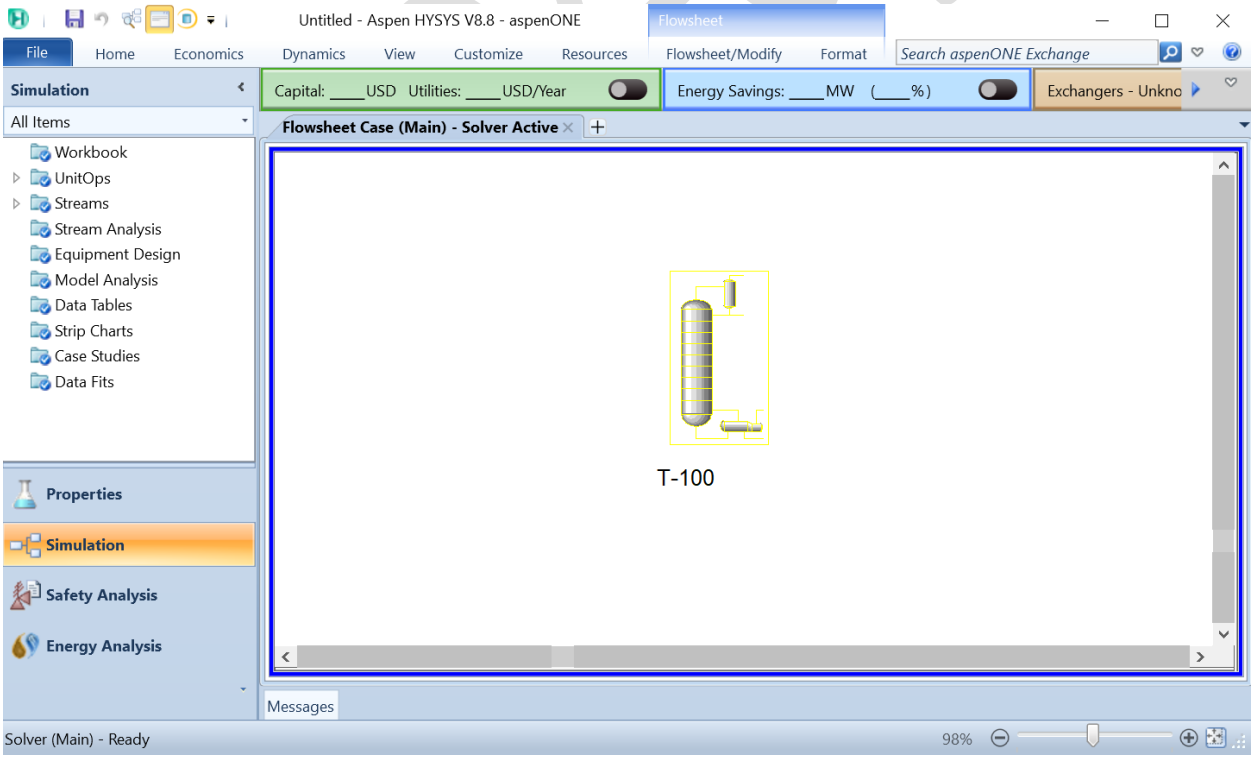

Figure 24. Add the stripper to the PFD

- **Set Operating Conditions:** Define the operating conditions of the stripper,

number of stages, fluxes, temperature, pressure, and flow rates. These conditions significantly impact the process.

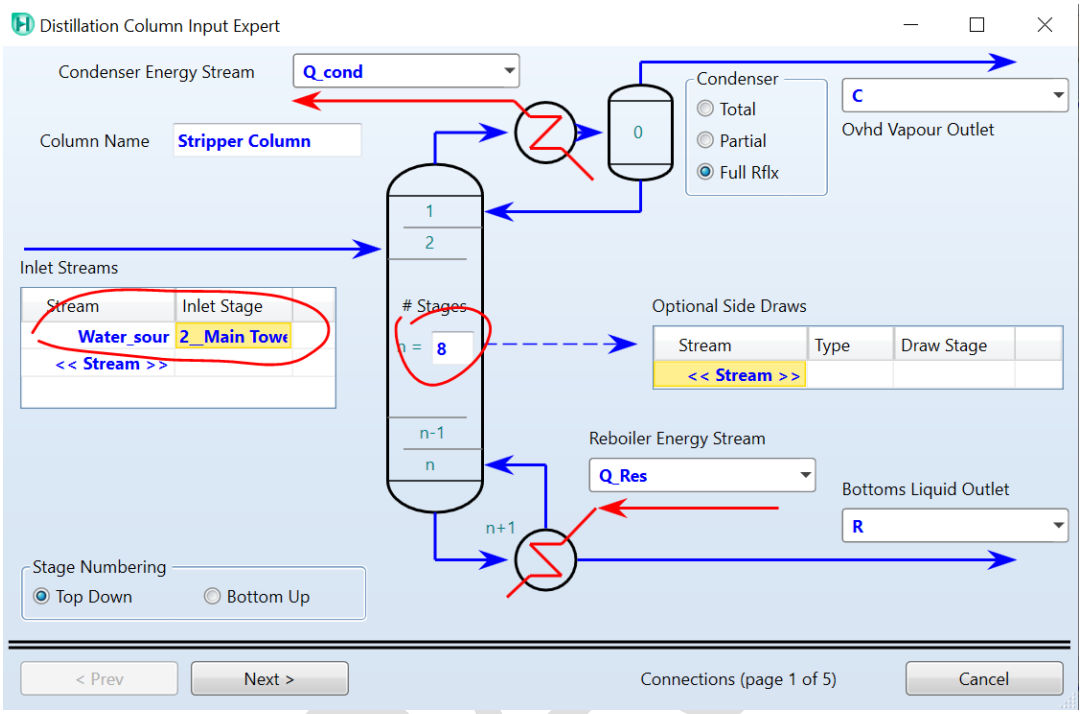

Figure 25. Setting the streams in the stripper

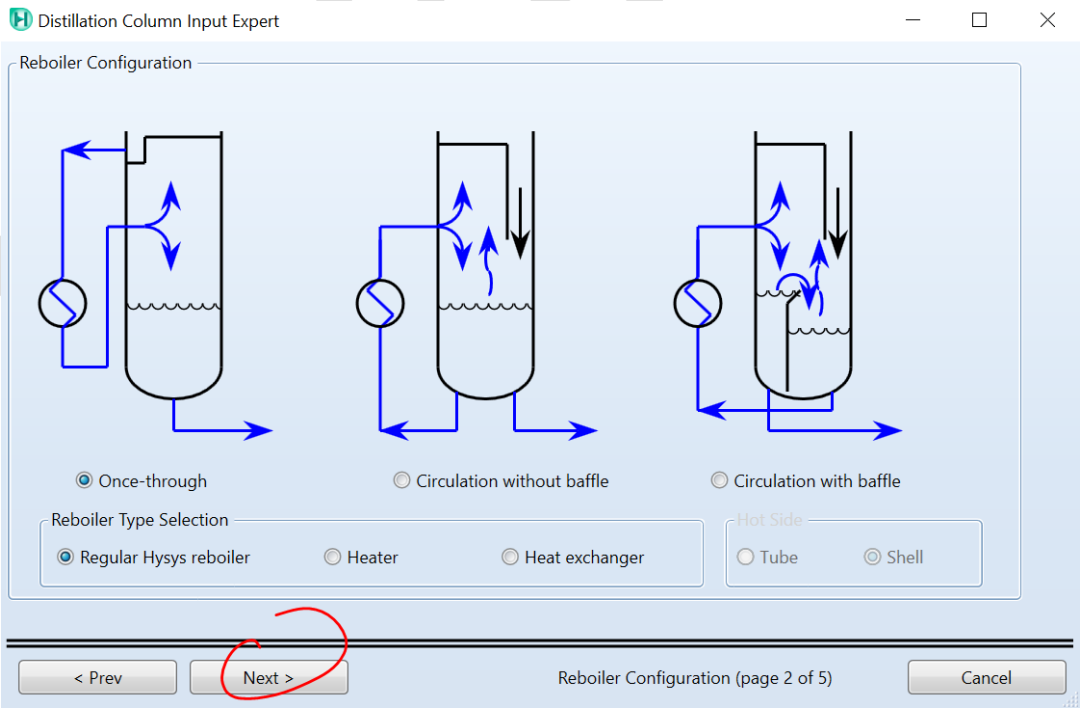

Figure 26. Setting the parameters of the stripper 1

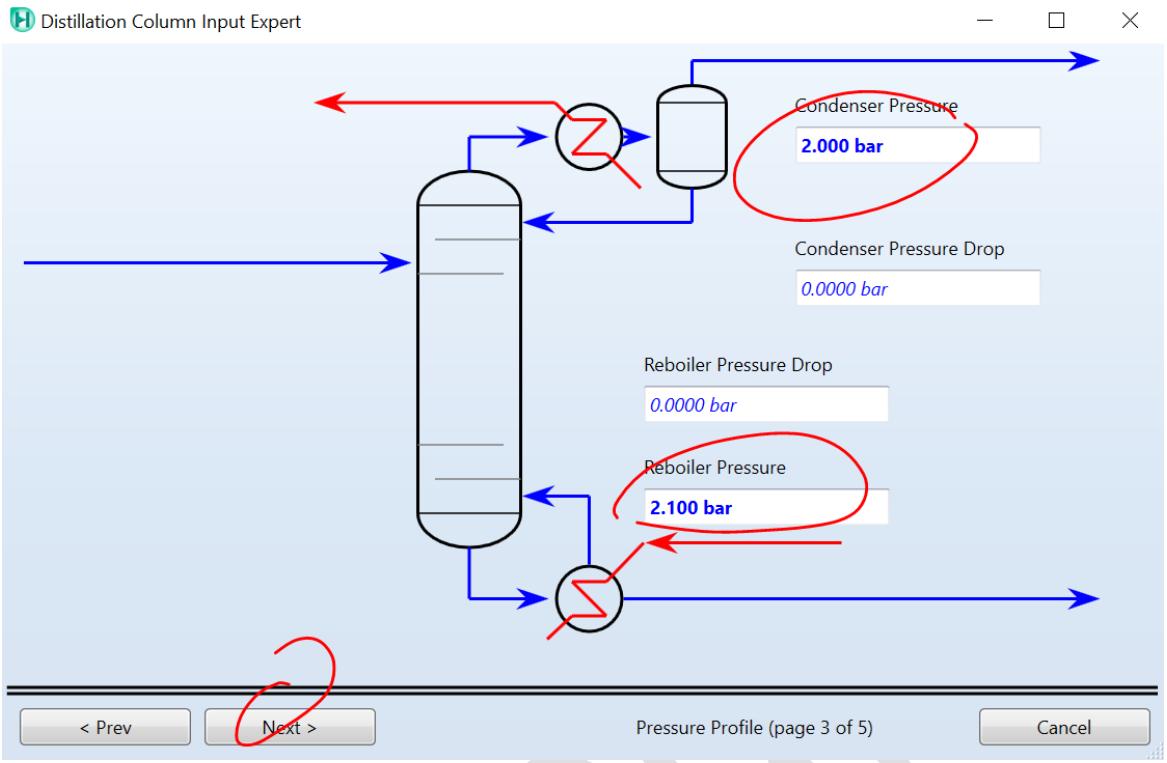

Figure 27. Setting the parameters of the stripper 2

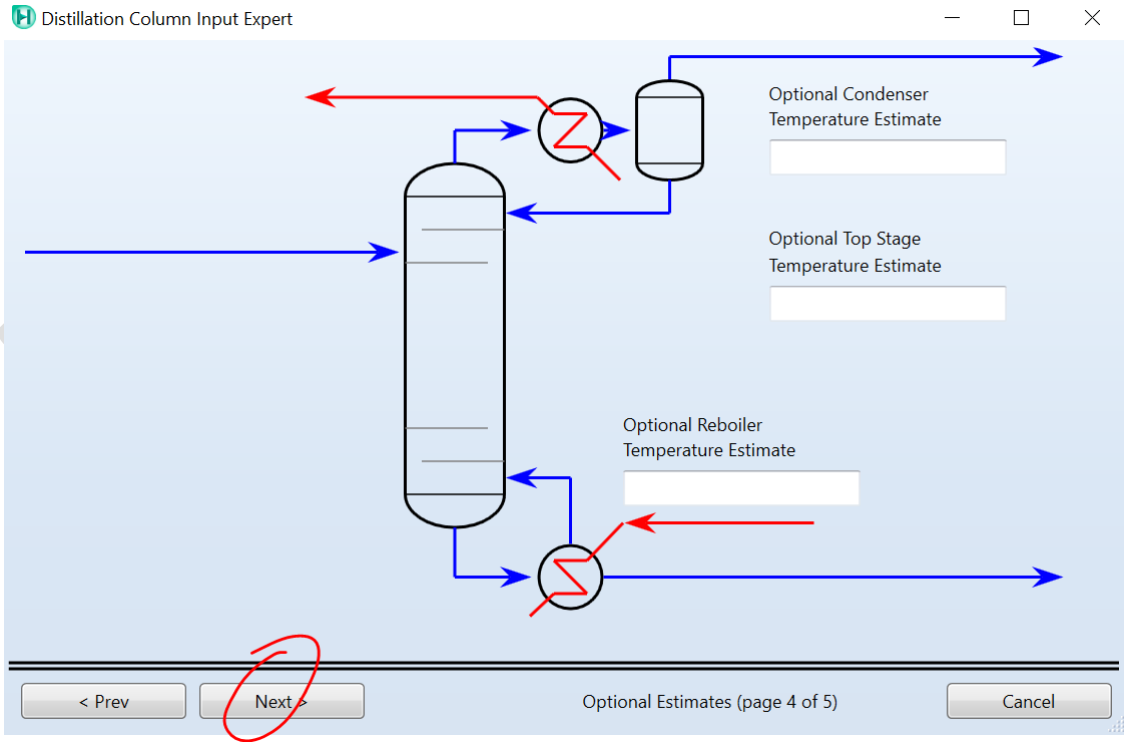

Figure 28. Setting the parameters of the stripper 3

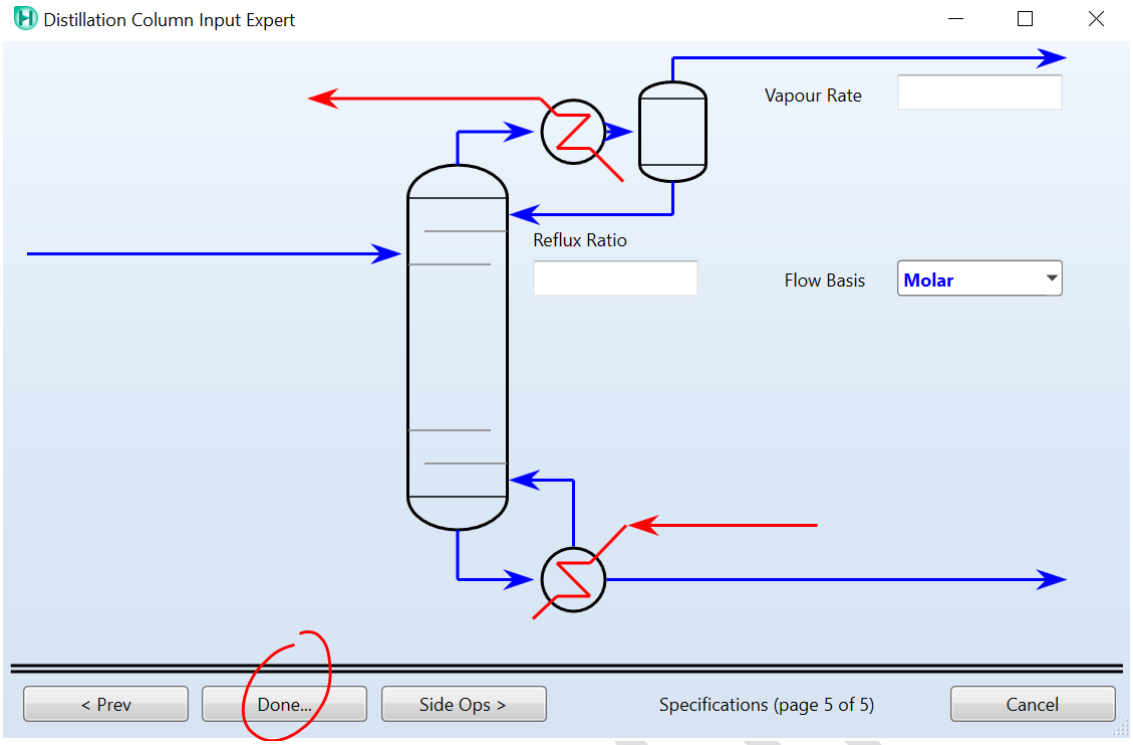

Figure 29. Complete stripper settings

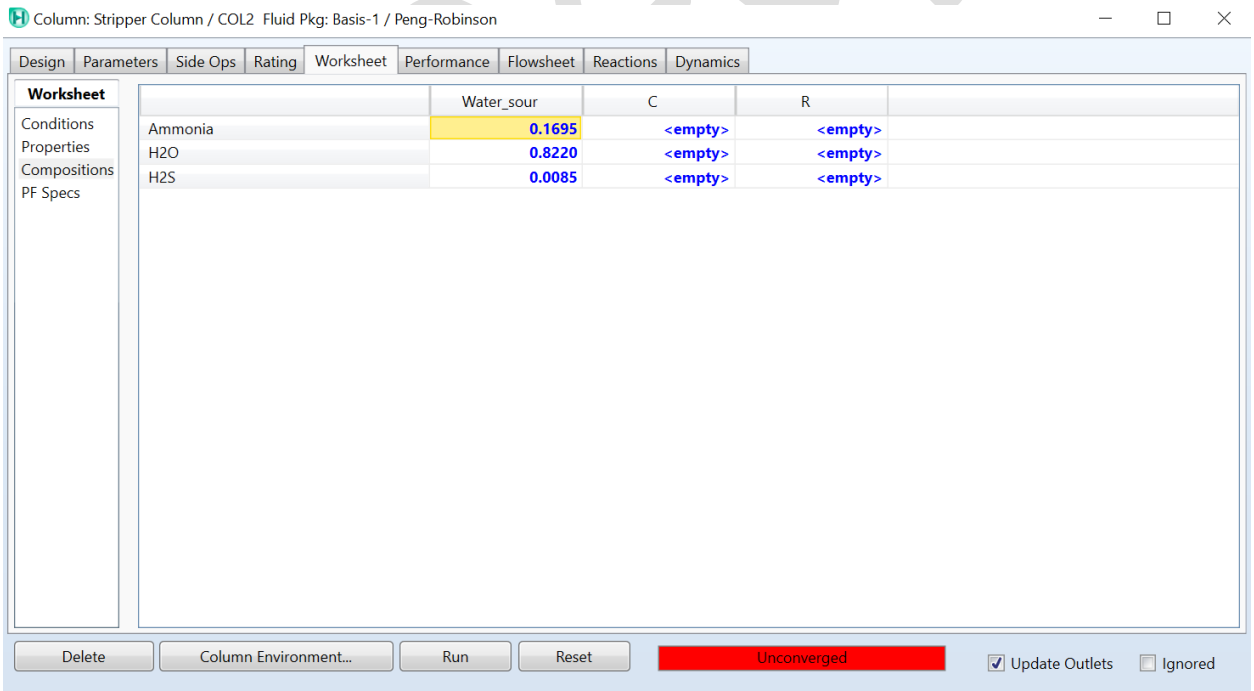

Figure 30. entering the different conditions 1

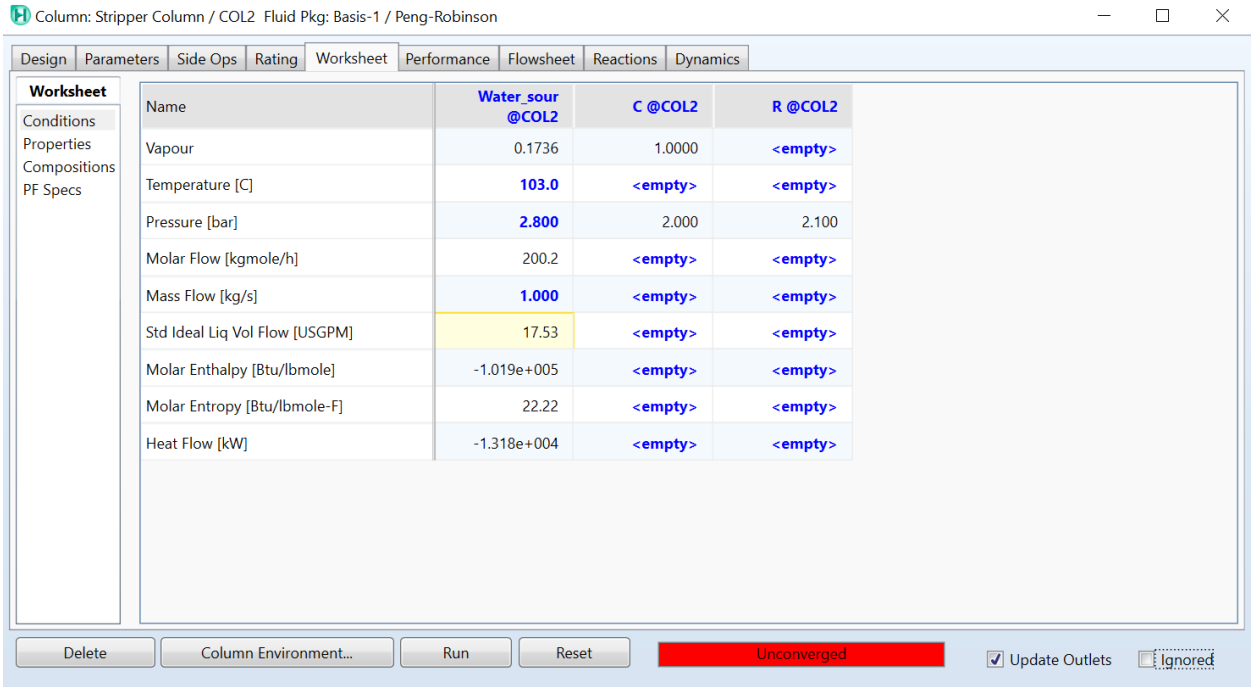

Figure 31. Entering the different conditions 2

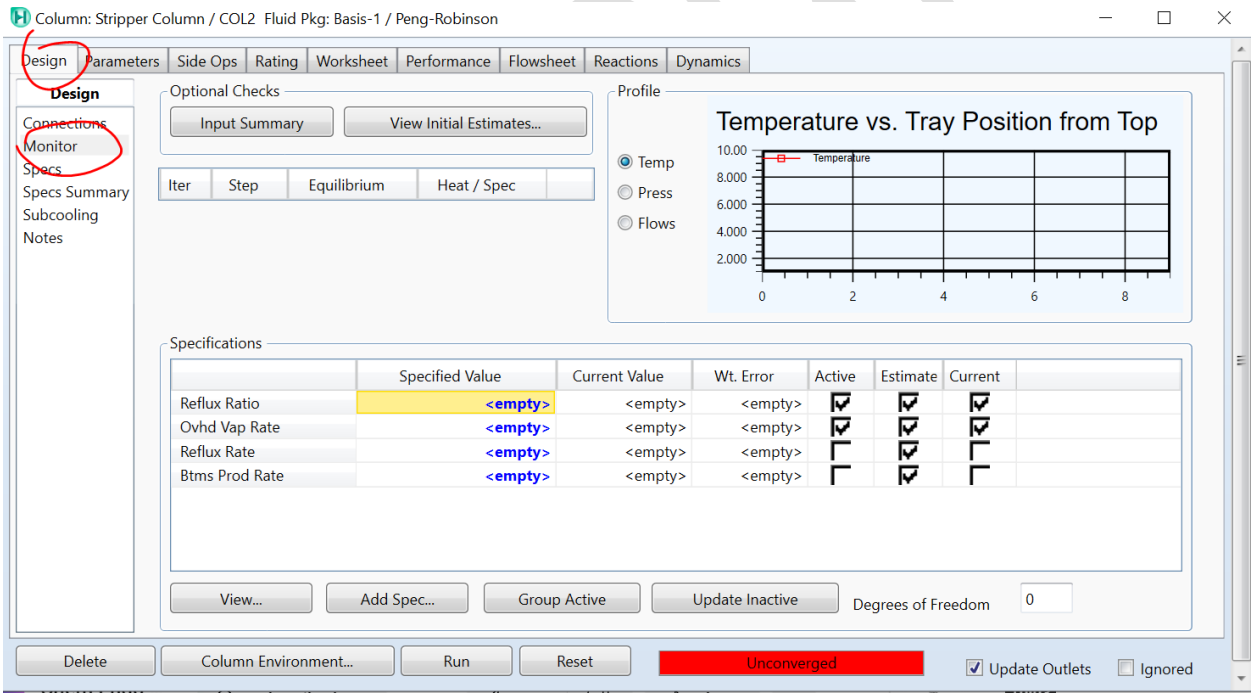

Figure 32. Configuration of the rest parameters

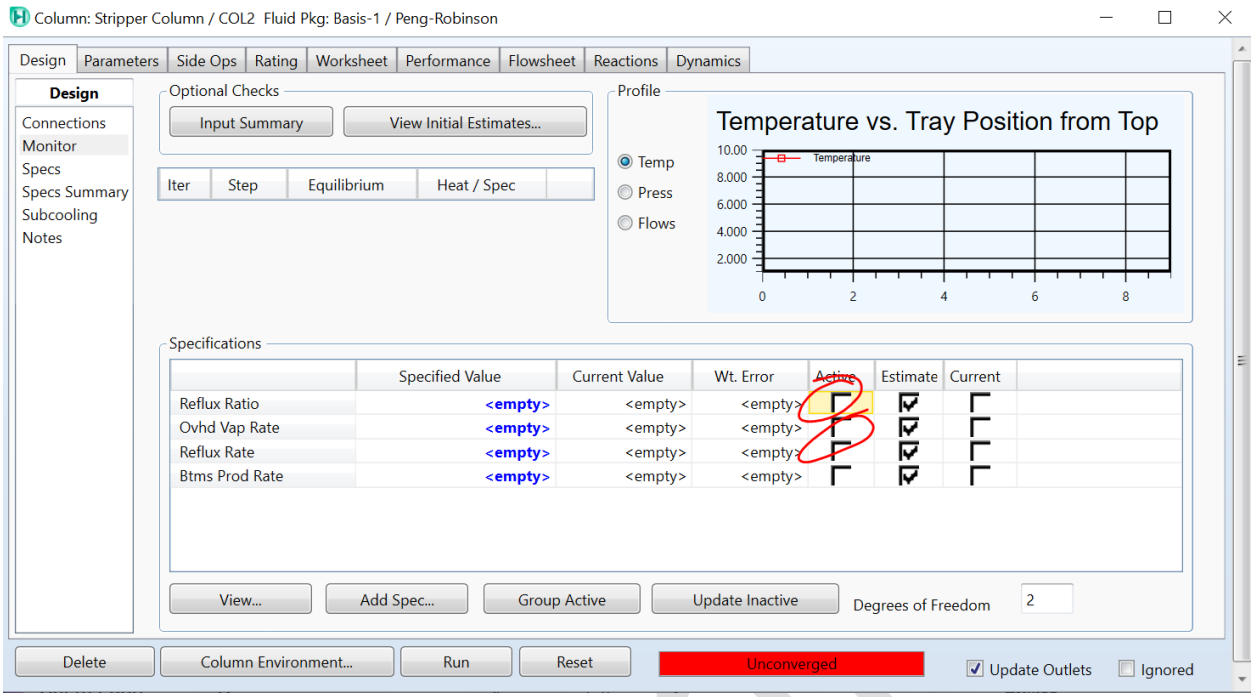

Figure 33. Configuration of the rest parameters

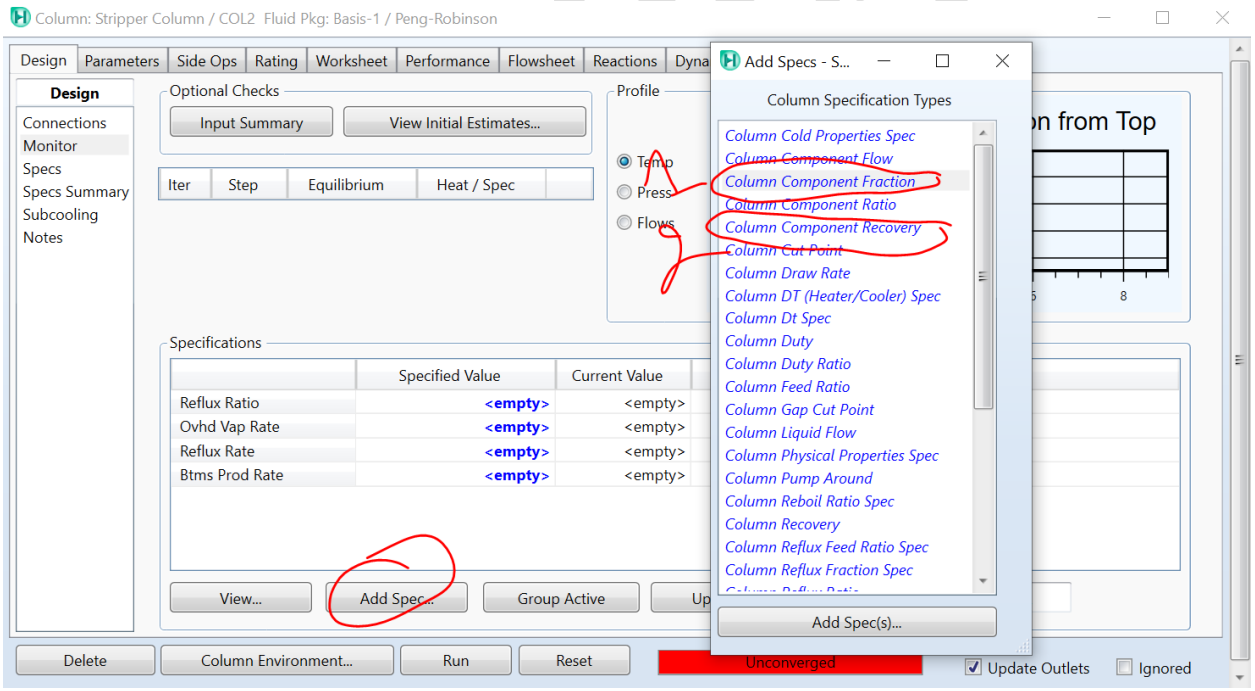

Figure 34. Adding of the mentioned new parameters in the example

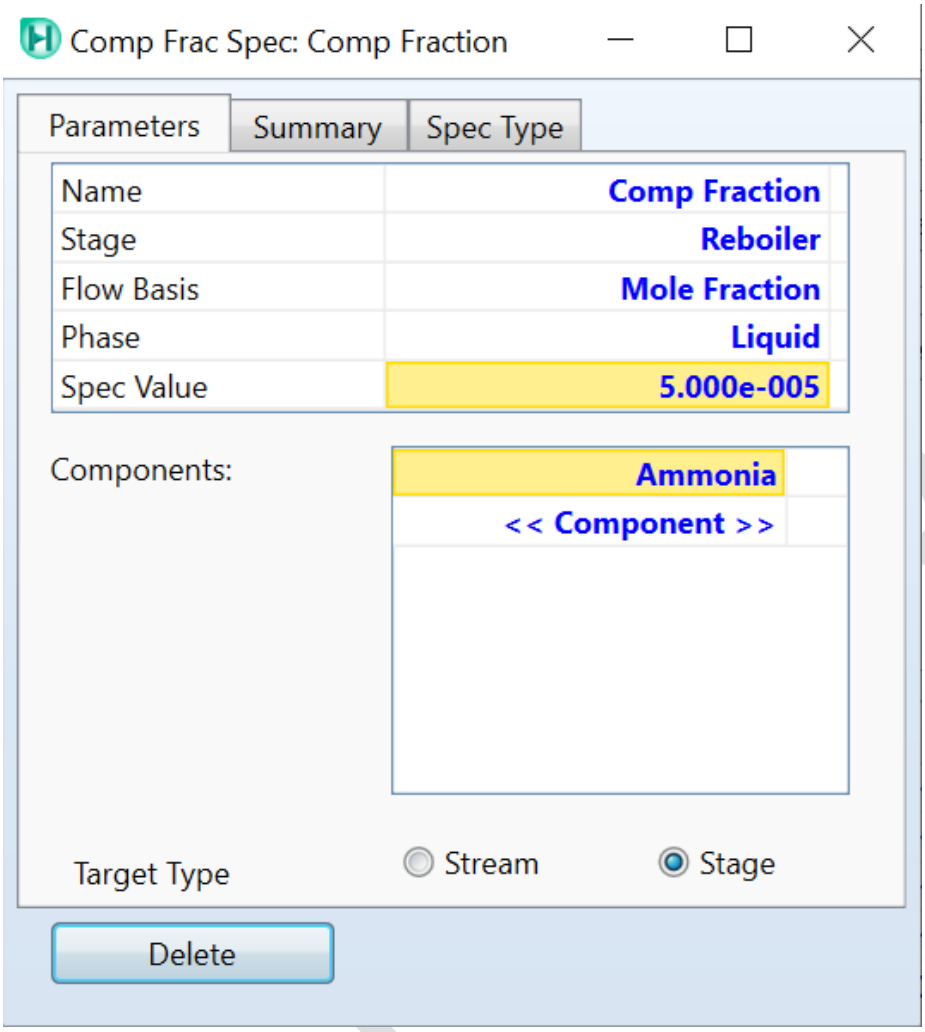

Figure 35. Entering the value required of the Ammonia in the water as a specification

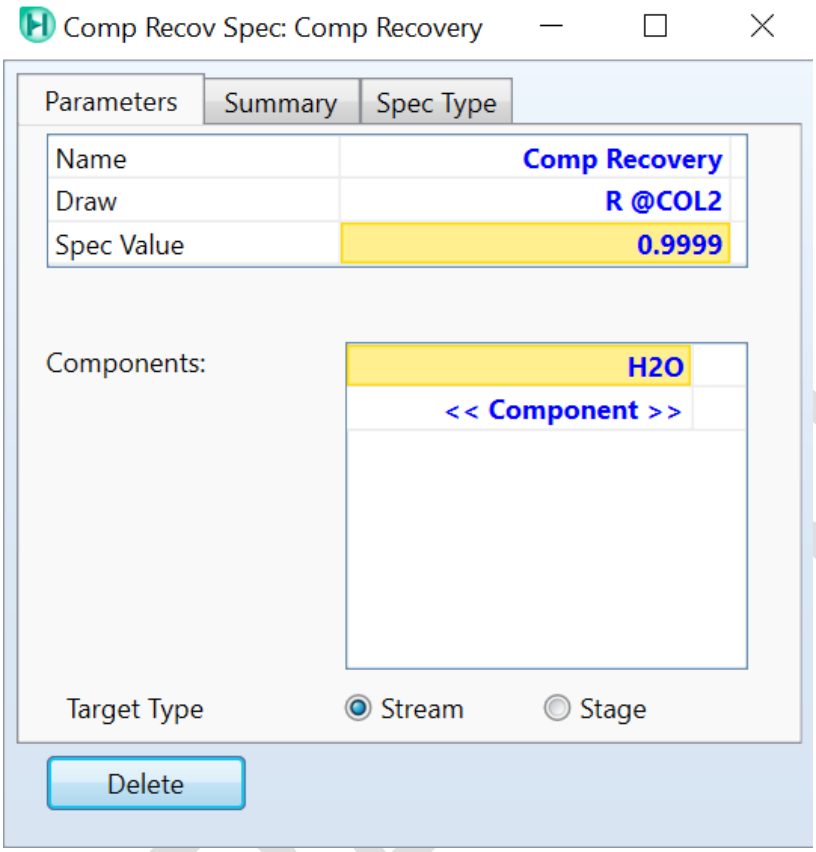

Figure 36. Entering the value required of the water recovery in the water as a specification

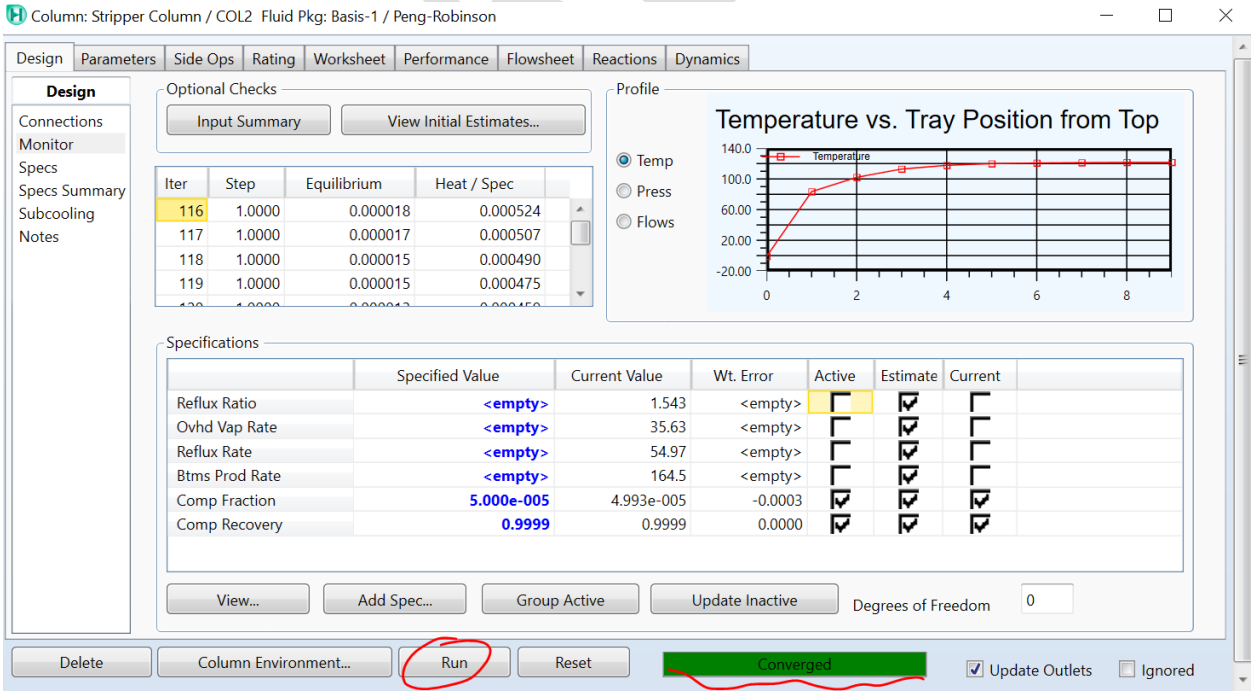

Figure 37. Run the simulation

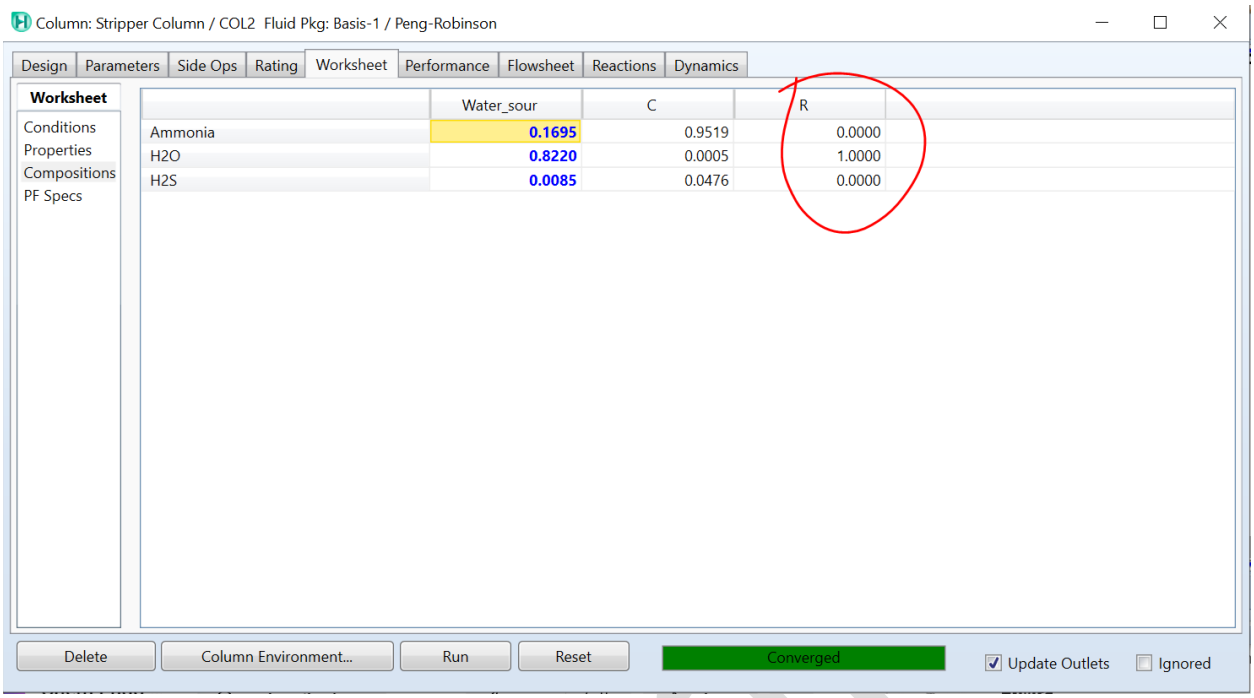

Figure 38. The obtained results 1

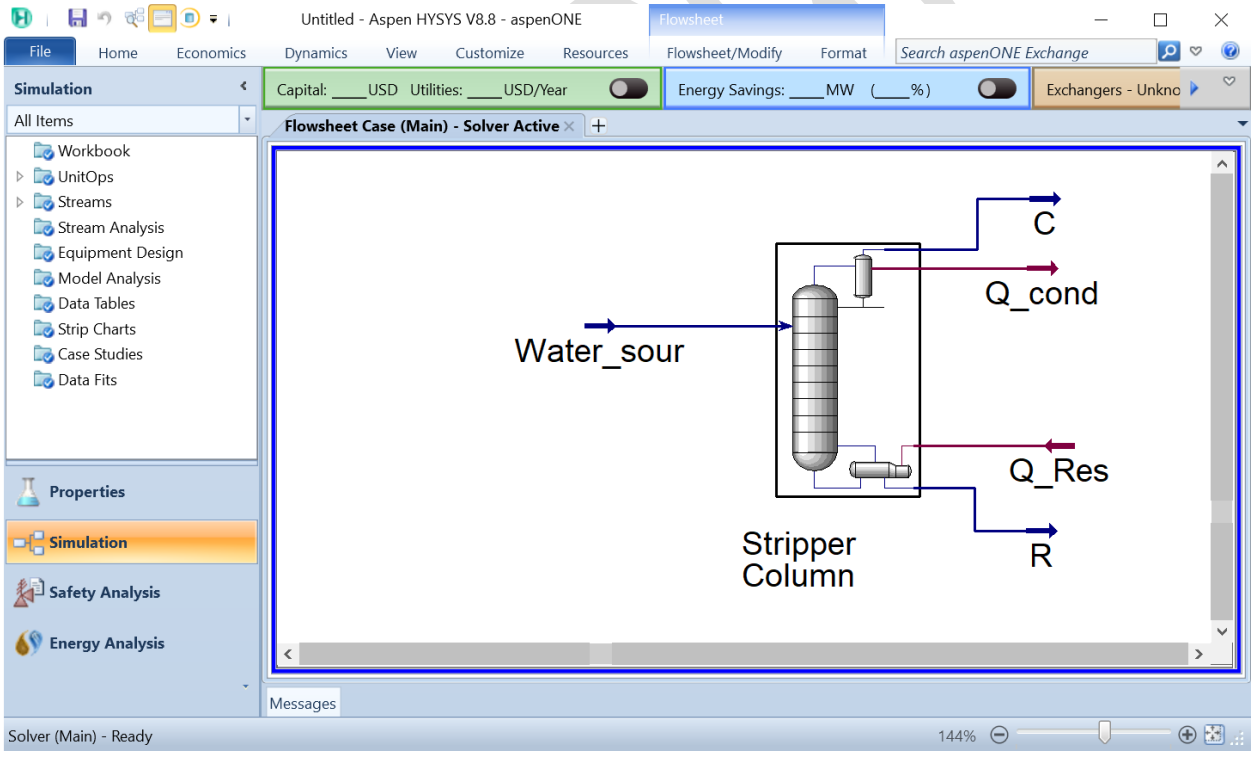

Figure 39. The obtained results 2

These steps provide a general guideline for simulating the stripper column in Aspen HYSYS. However, the specific details and nuances can vary depending on

the type and the complexity of the process involved. It's essential to consult Aspen HYSYS documentation and resources for more in-depth guidance on using the software effectively.

III-3-2- Liquid/Liquid Extraction

In order to perform this simulation, an example has been taken into consideration, and then numerous steps will be followed in order to resolve it.

❖ **Example 1:** Simulate the separation of an equimolar Acetone/Water mixture using 3-Methylhexane as the solvent in an Aspen HYSYS liquid-liquid extraction column.
Parameters:

- Feed: Equimolar Acetone/Water mixture at 25°C, 50 kgmole/h, and 1.2 bar.
- Solvent: 3-Methylhexane at 25°C, 200 kgmole/h, and 3 bar.
- Column: 10 stages, top stage pressure: 104 kPa, bottom stage pressure: 200 kPa.

In order to solve this example, and simulate this process, it is necessary to follow up the previous mentioned steps, starting by selecting the component list, then the fluid package going then to the simulation environment and select the extraction column from the palette.

However, the other steps in setting the different parameters of the extractor are similar to the steps employed to set up the different parameters of the stripper and also the absorber, in which the number of stages should be assumed, also the top and bottom pressures, the different conditions of the solvent and the mixture, the next pictures depicted the necessary steps in order to perform this process and also the obtained results at the end of the simulation.

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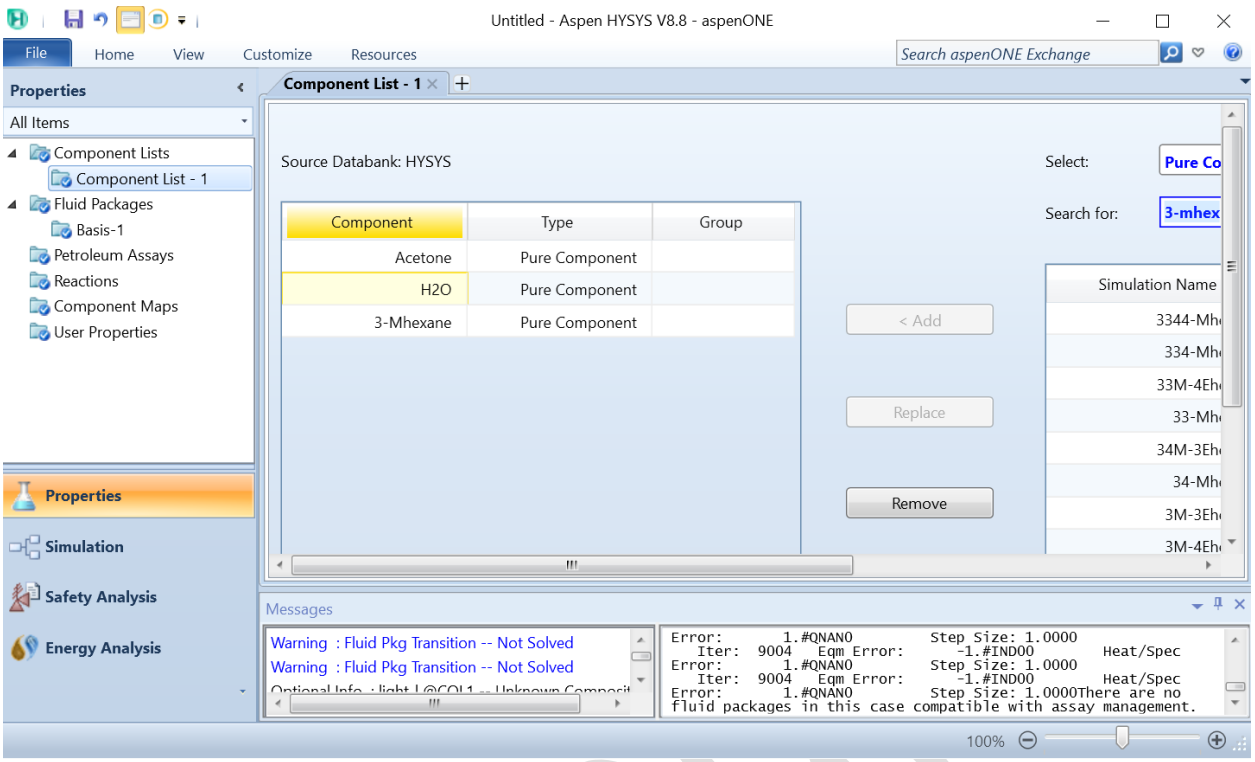

Figure 40. Setting component list

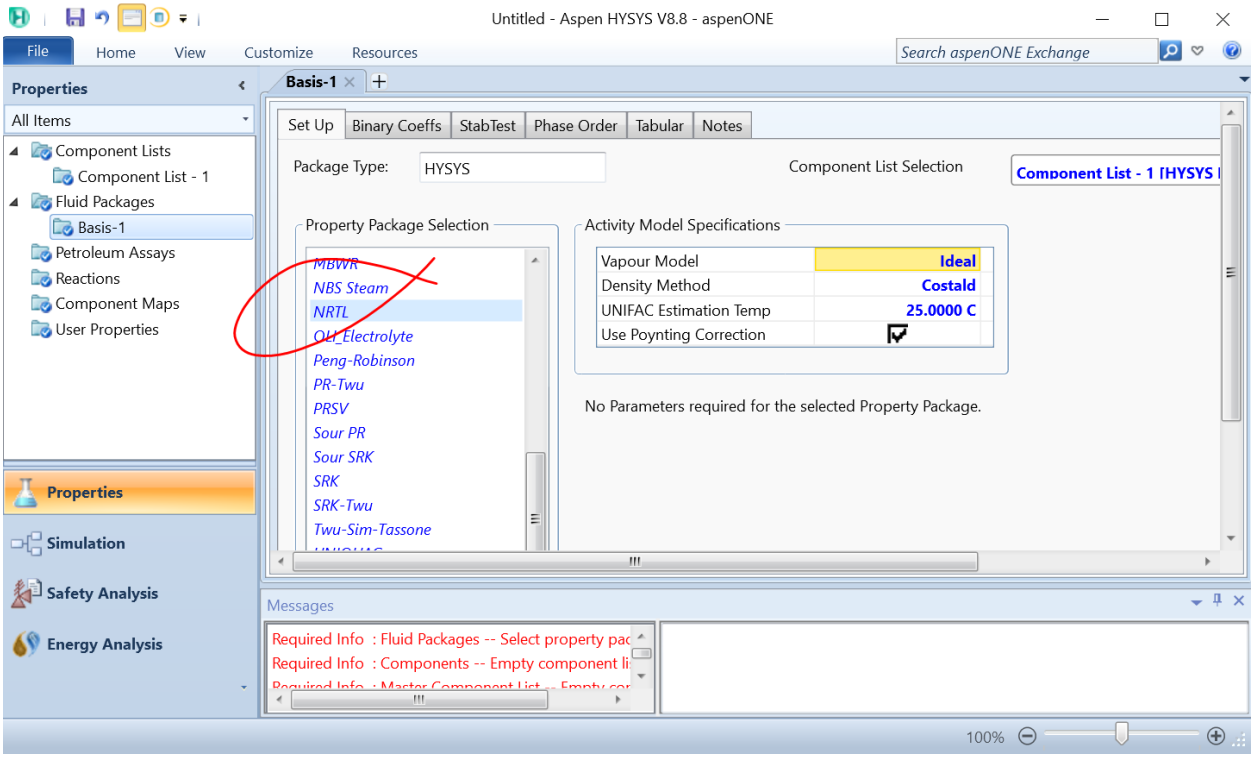

Figure 39. Setting fluid package

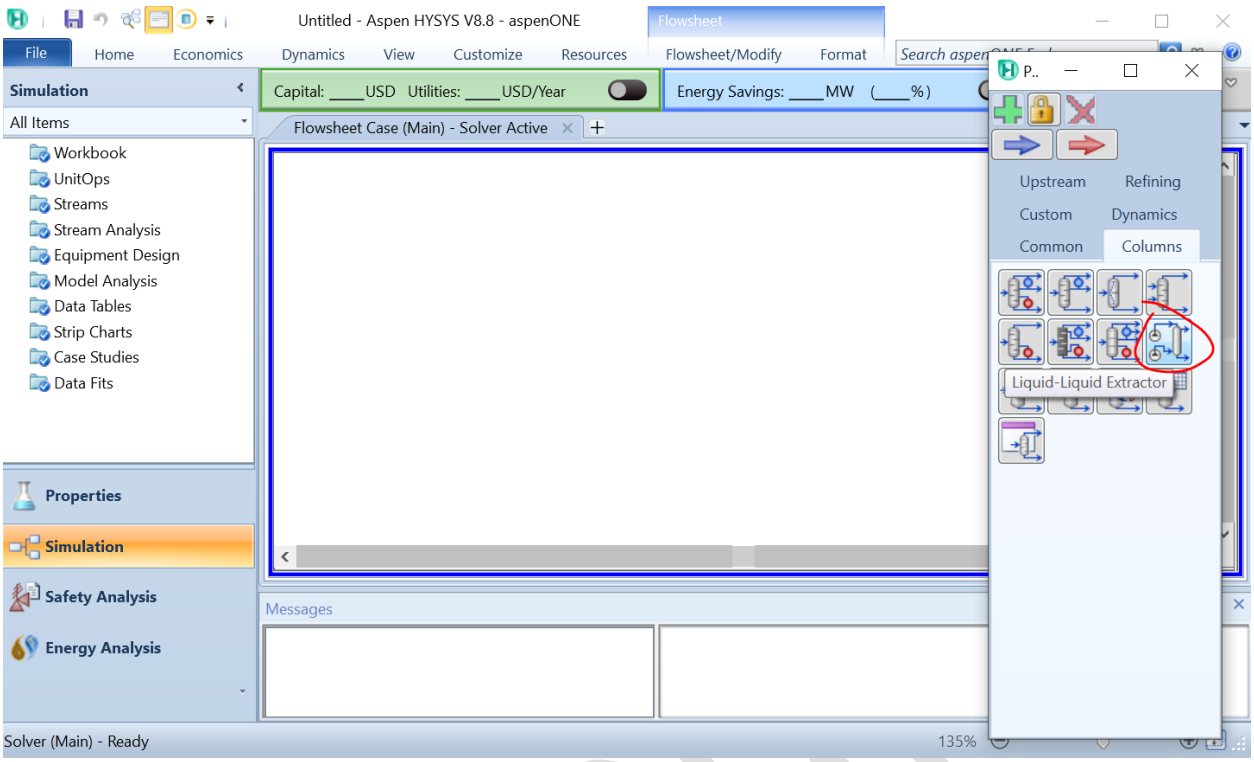

Figure 41. Selection of extraction column from the palette

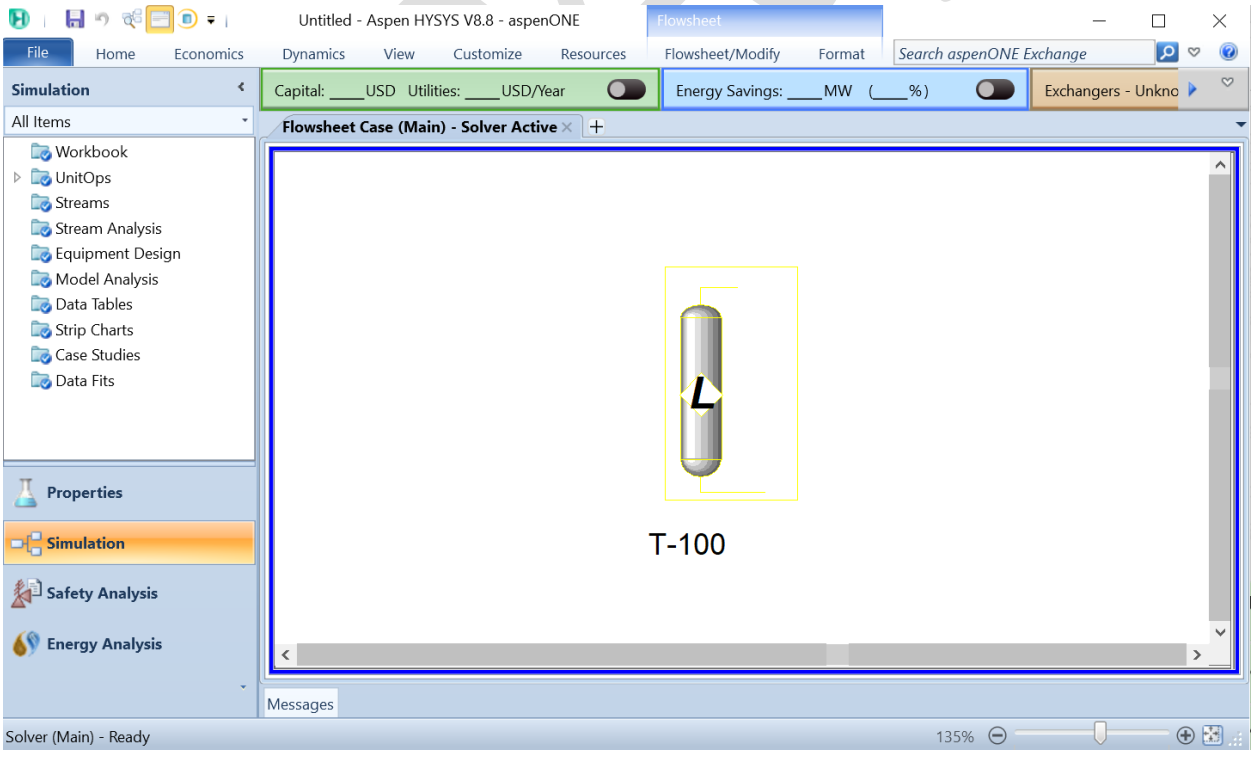

Figure 42. Putting it into the PFD

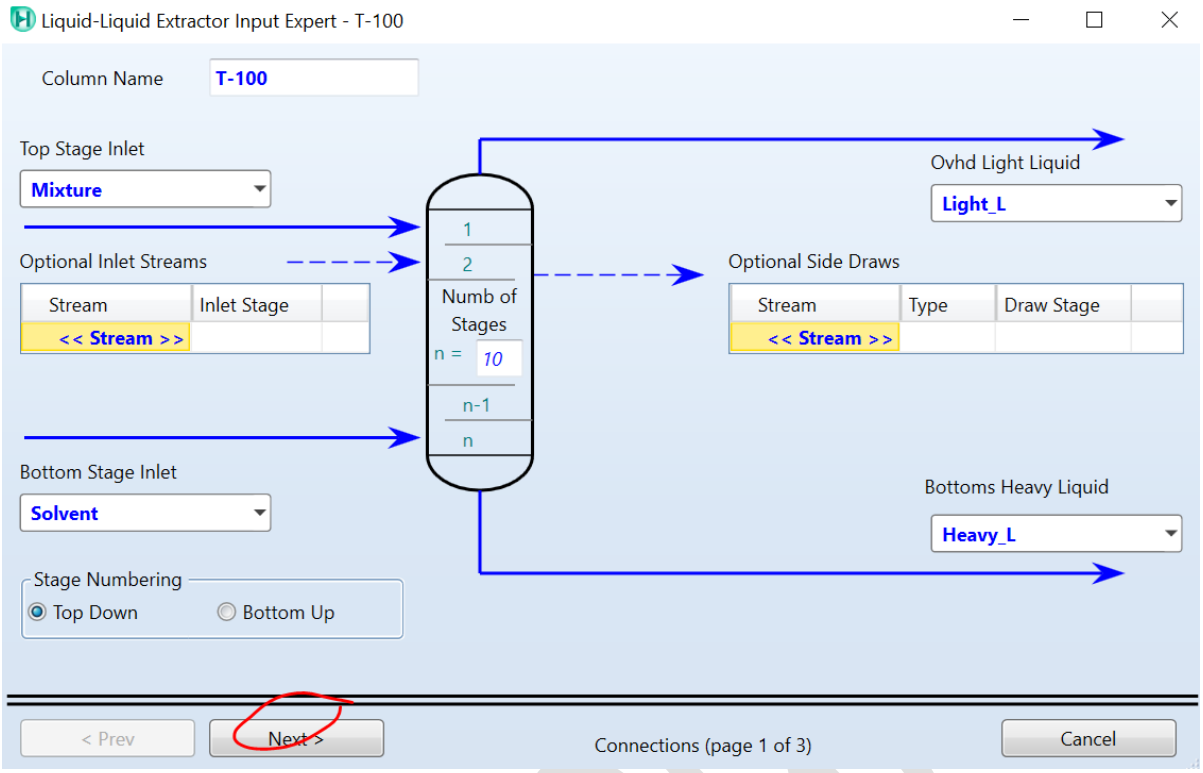

Figure 43. Setting the parameters of the extractor 1

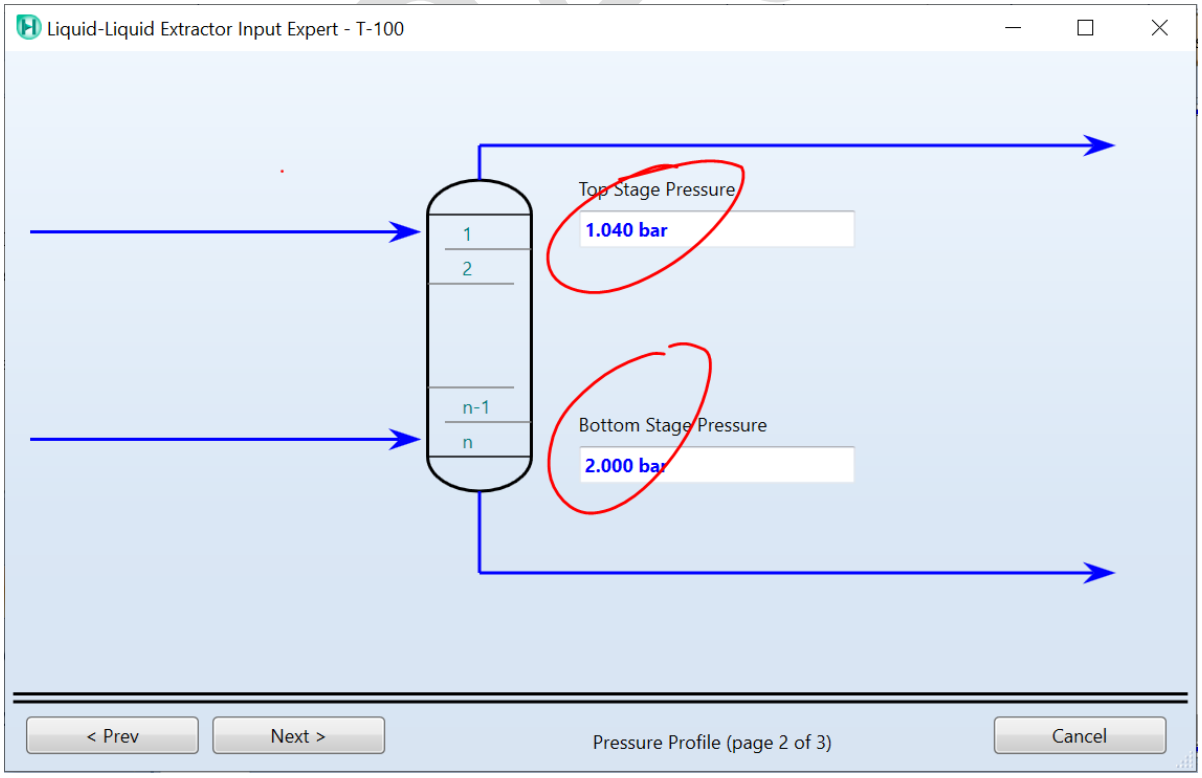

Figure 44. Setting the parameters of the extractor 2

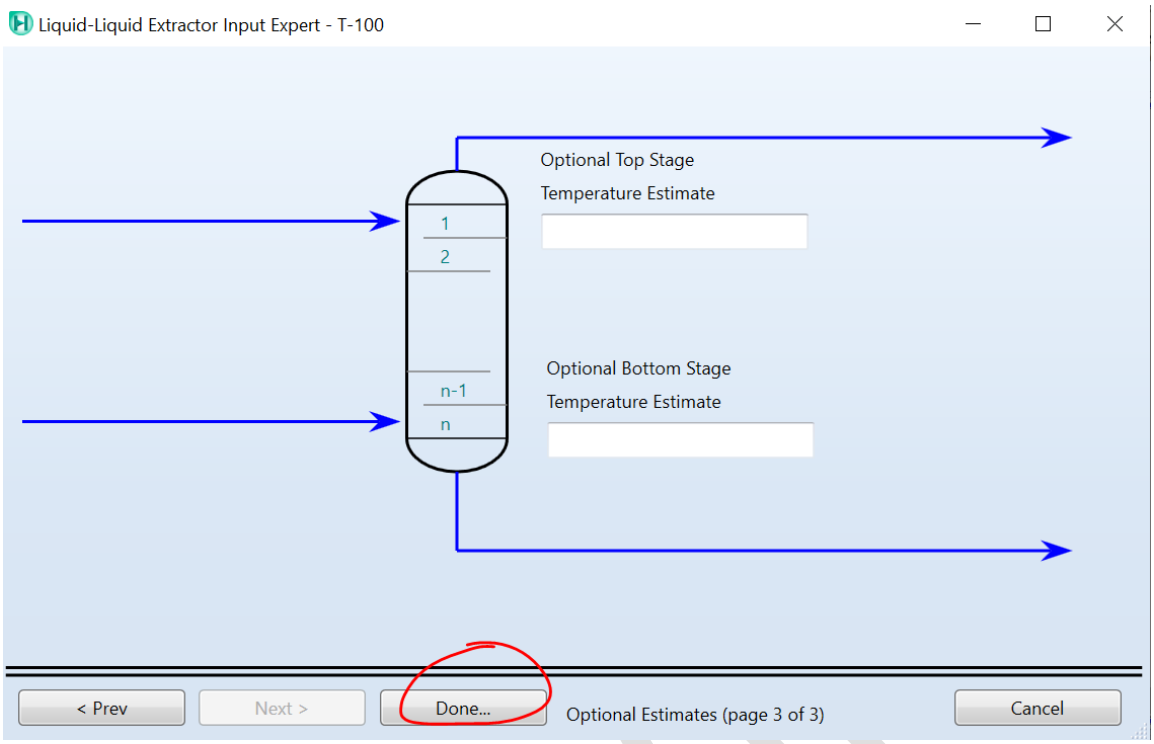

Figure 45. Setting the parameters of the extractor 3

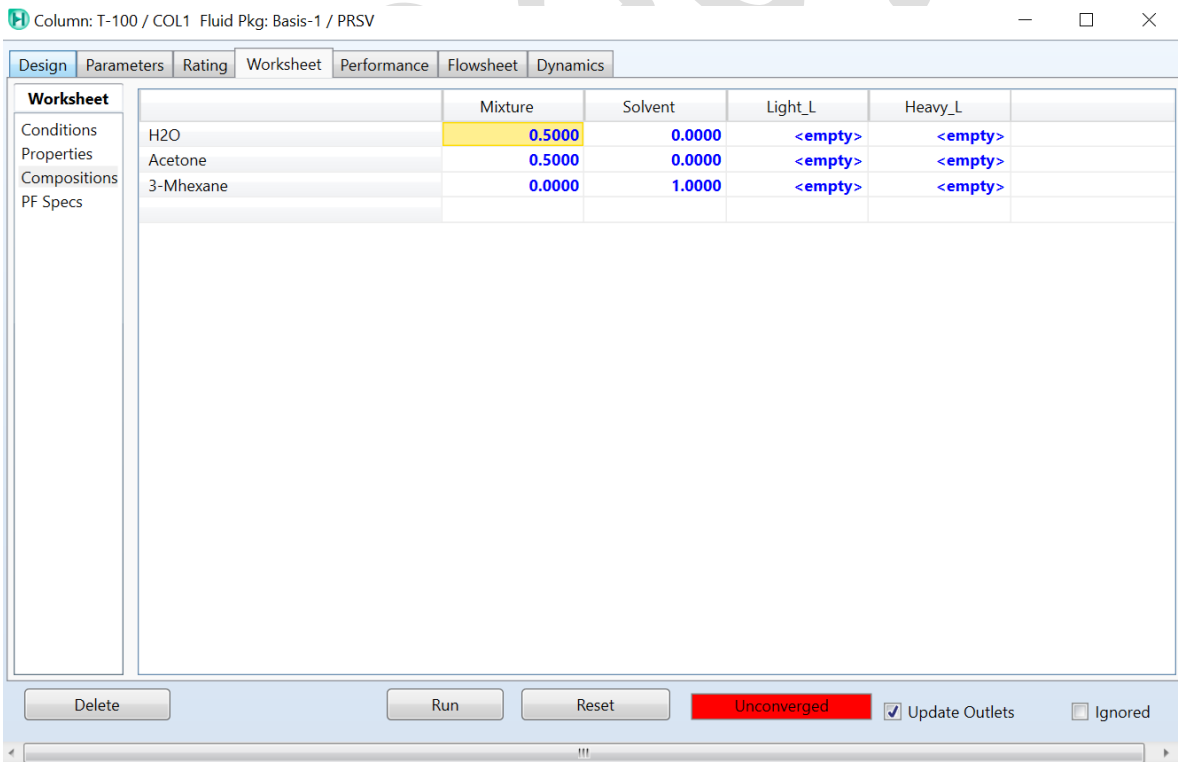

Figure 46. Setting the compositions

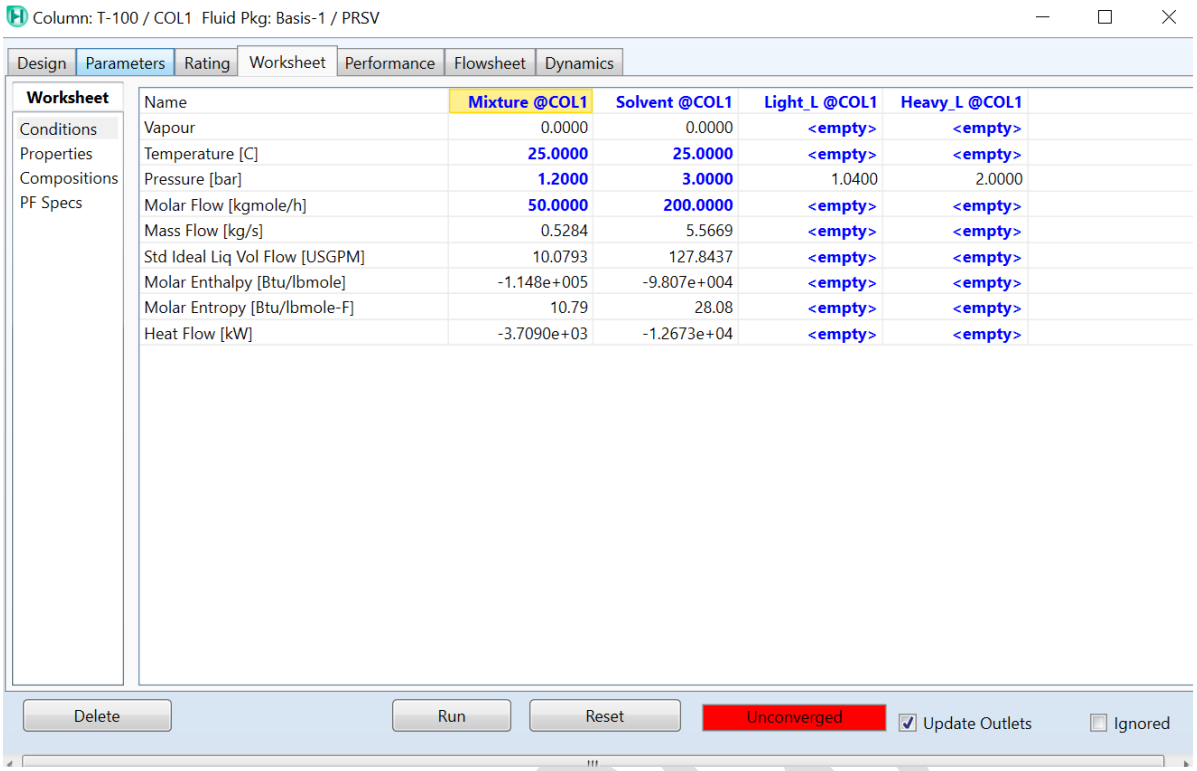

Figure 47. Setting the different parameters and conditions

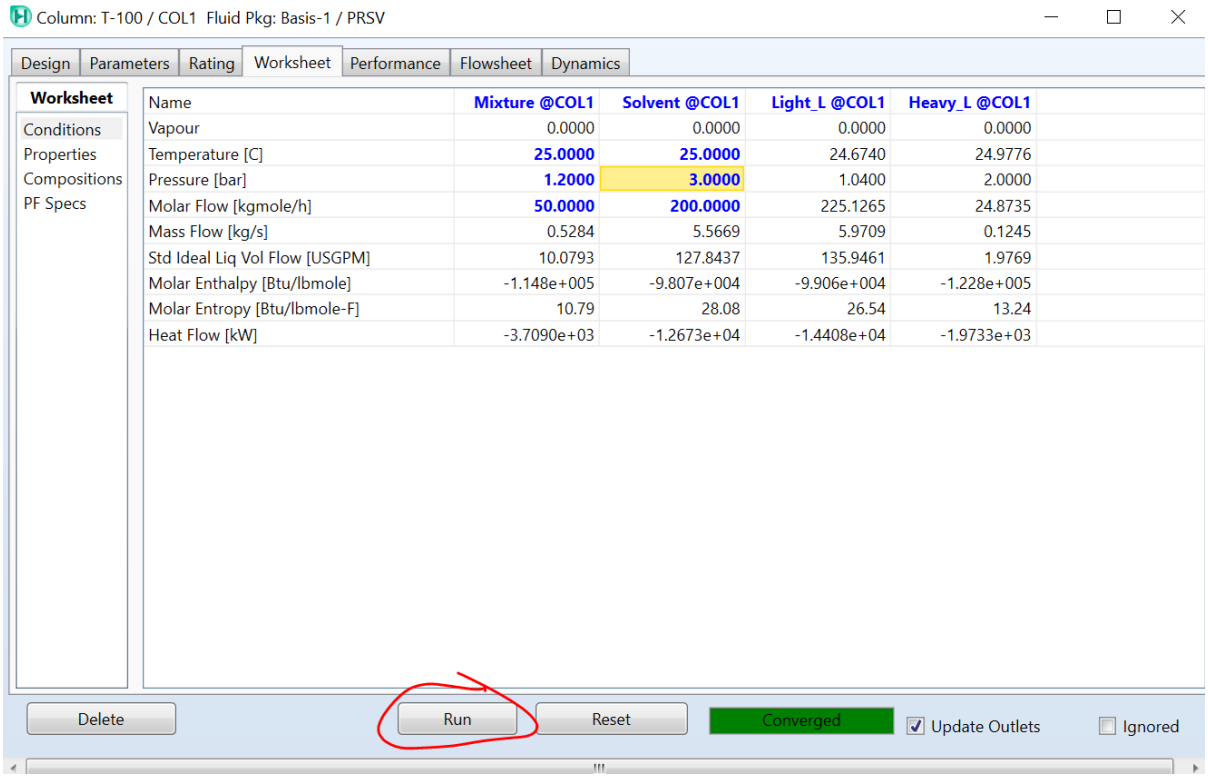

Figure 48. Run the simulation and get the results

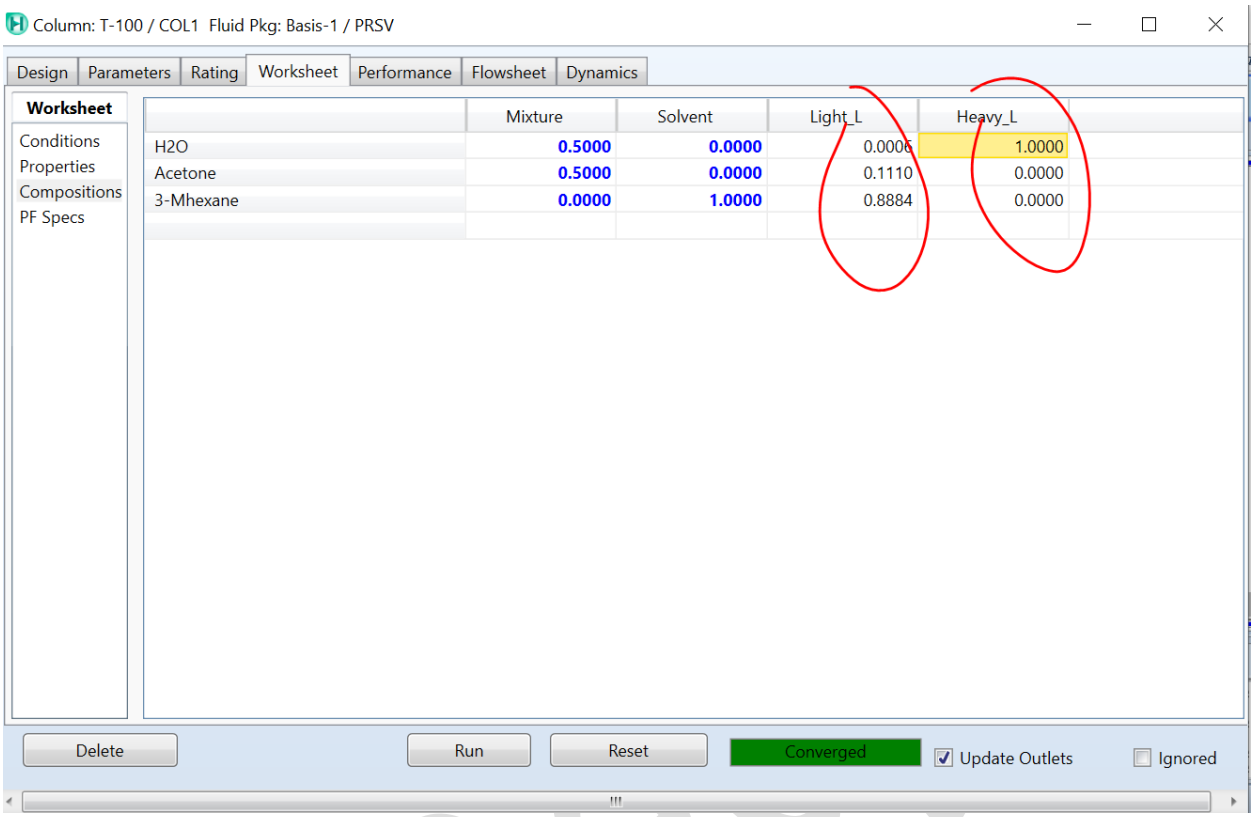

Figure 49. Check of the composition

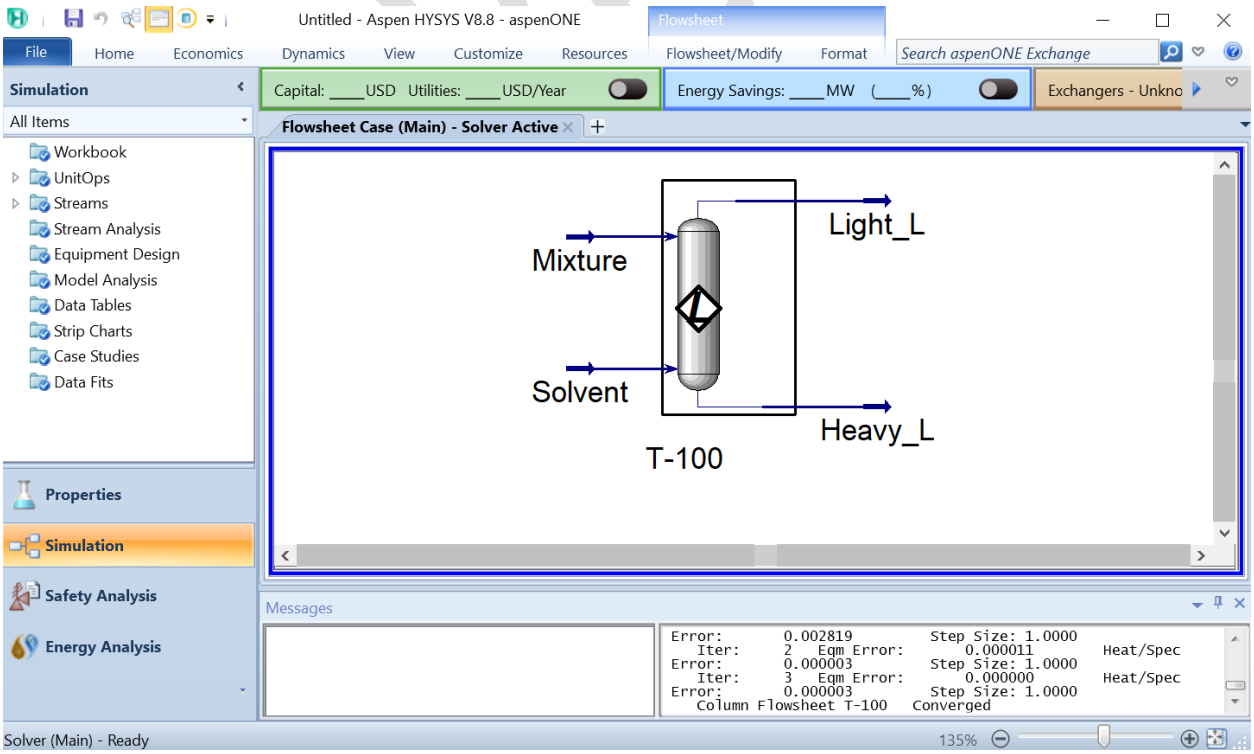

Figure 50. The obtained results

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