Chapter II: Simulation of reactions and chemical reactors/bioreactors

II-1- Introduction

In the world of chemistry and biology, understanding and improving different types of reactors is crucial. These reactors can be quite diverse, and they include single conversion reactions (conversion reactor), multiple conversion reactions (conversion reactor), balanced reactions (equilibrium reactor), perfectly stirred reactors (PSR), plug reactors (PR), and catalytic reactors. Each of these has its unique characteristics and complexities, making it a challenge to optimize their performance.

Aspen HYSYS, a powerful simulation tool, is a valuable resource for tackling these challenges. It helps scientists and engineers predict what will happen in these reactors, understand the reactions, and make these systems work better.

This Chapter will explain why Aspen HYSYS is vital for simulating these diverse types of reactors. We'll explore how this software can help us understand and improve these different reactor systems, from making sure single reactions go well to handling more complex reactions and even bioreactors used in pharmaceuticals and other fields. Aspen HYSYS provides the tools and knowledge to make these reactors perform better.

By the end of this chapter, you will have the knowledge and skills to simulate various types of reactors using Aspen HYSYS. This understanding will enable you to model different reactors effectively, making informed decisions, saving time and resources, and ensuring that your work is safer and more efficient. Aspen HYSYS, as a versatile tool, equips you with the capability to employ computer simulations for optimizing the performance of different reactor types, ultimately contributing to a cleaner and more sustainable future across diverse industries.

II-2- Why Simulation of different reactors

The simulation of different reactors using Aspen HYSYS allows engineers and scientists to model and understand a wide range of reactor types and processes.

Aspen HYSYS is a powerful tool that enables the simulation of diverse reactors, including single conversion reactions, multiple conversion reactions, balanced reactions, perfectly stirred reactors (PSR), plug reactors (PR), and catalytic reactors.

Through Aspen HYSYS, users can explore the behavior of these reactors, predict outcomes, and optimize their performance. This versatility empowers individuals to make informed decisions, save time and resources, and enhance safety and efficiency across various industries. The ability to simulate different reactors makes Aspen HYSYS a valuable asset in research, development, and process optimization, ultimately contributing to a cleaner and more sustainable future.

II-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 types of reactors

II-3-1- Conversion Reactors

Conversion reactors are devices used to change one substance into another through a chemical reaction. They are crucial in various industries, from petrochemicals to pharmaceuticals. Aspen HYSYS is a helpful tool for simulating and optimizing conversion reactors. It allows engineers and scientists to understand and predict how these reactors work, making it easier to design efficient processes. Aspen HYSYS aids in improving conversion reactor performance, ensuring that chemical transformations are carried out effectively and yielding desired products. This makes it an invaluable resource for industries that rely on conversion reactors to produce the substances they need.

In order to simulate the conversion reactors, 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.

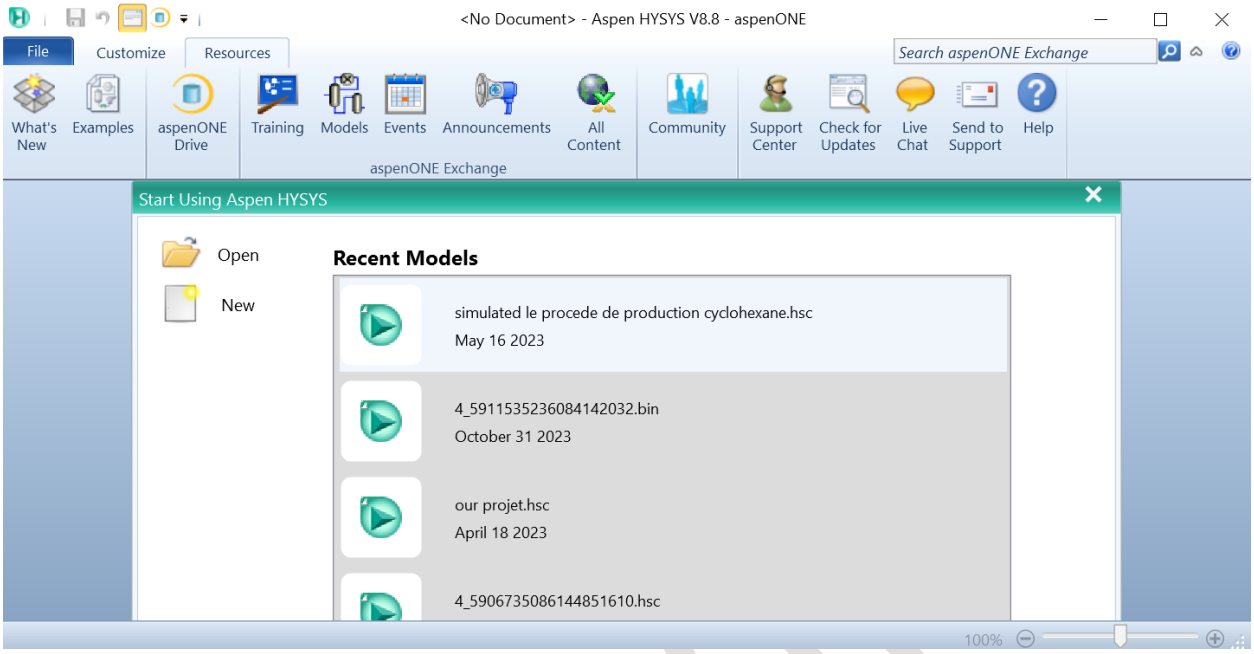

Figure 1. Launch Aspen HYSYS

- **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.

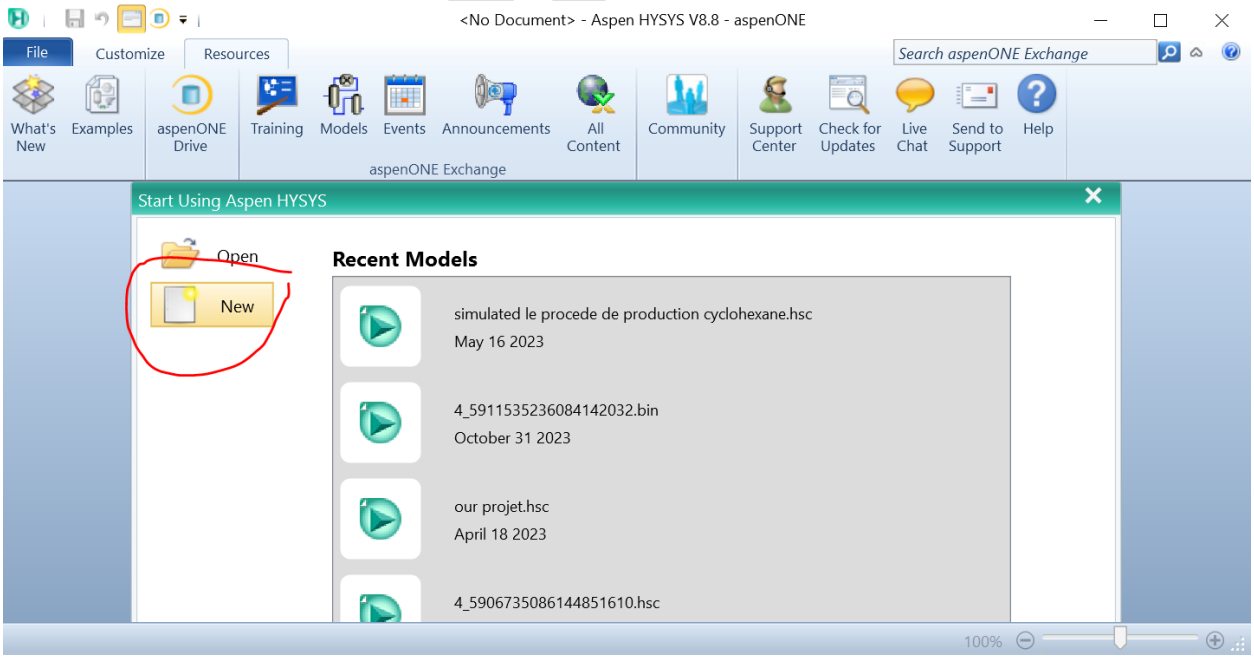

Figure 2. Open a new case

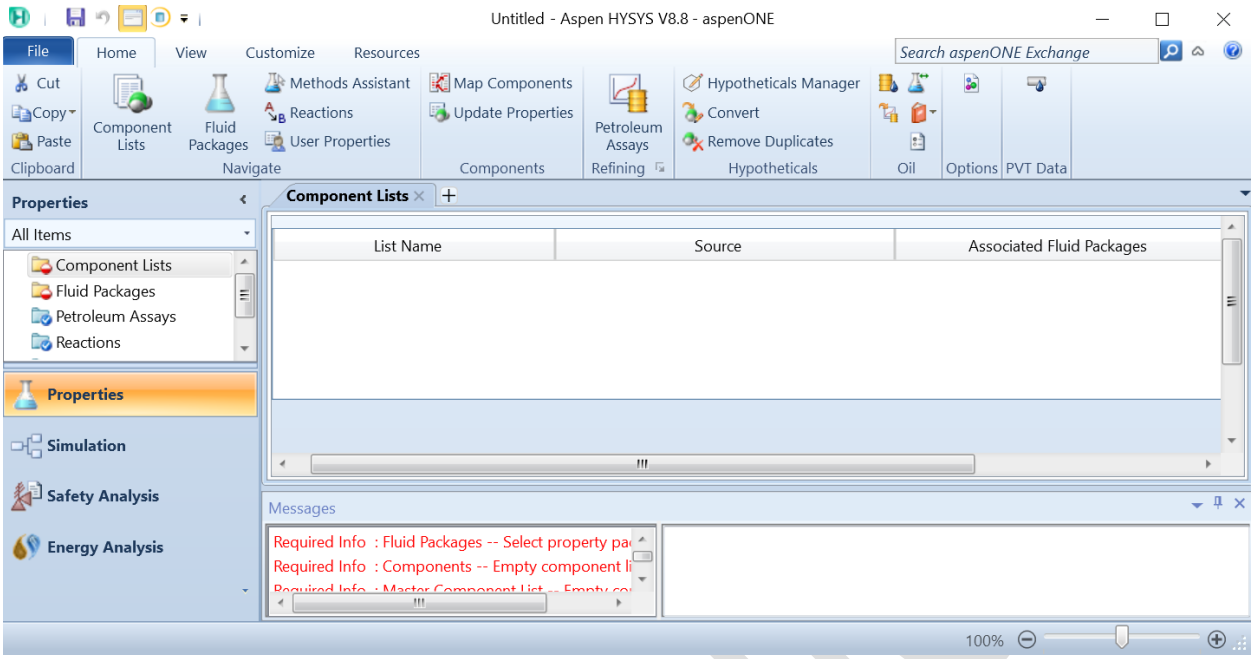

Figure 3. Appeared window after opening a new case or project

- **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.

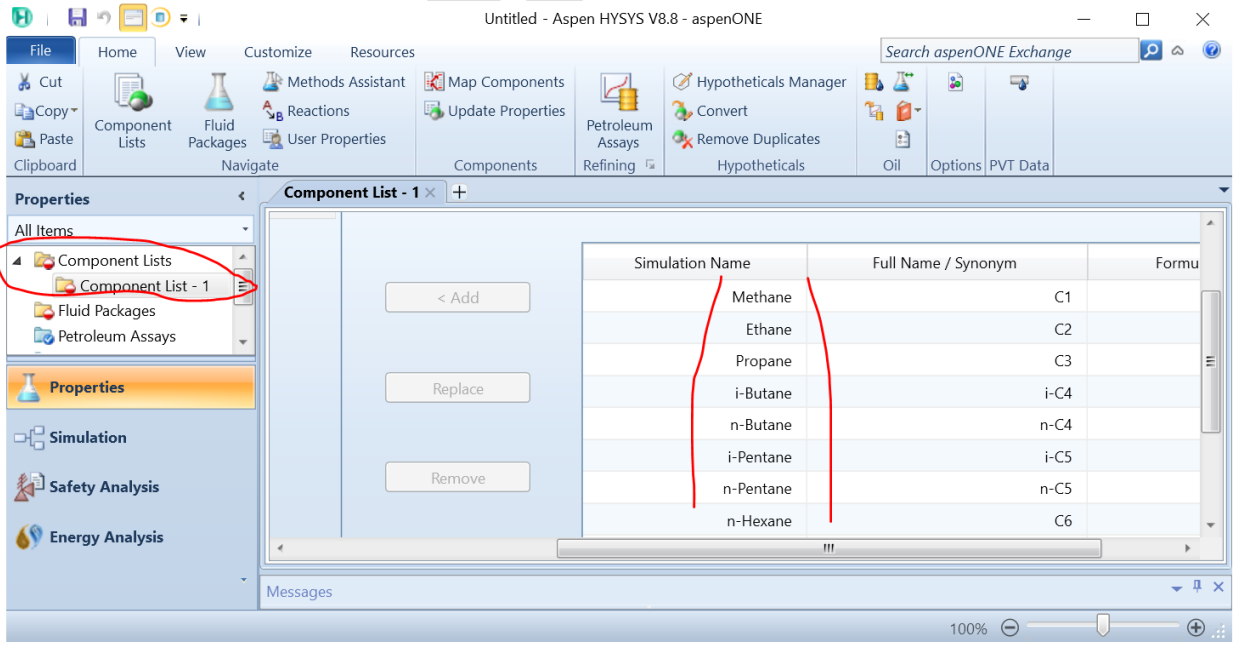

Figure 4. Adding the component list

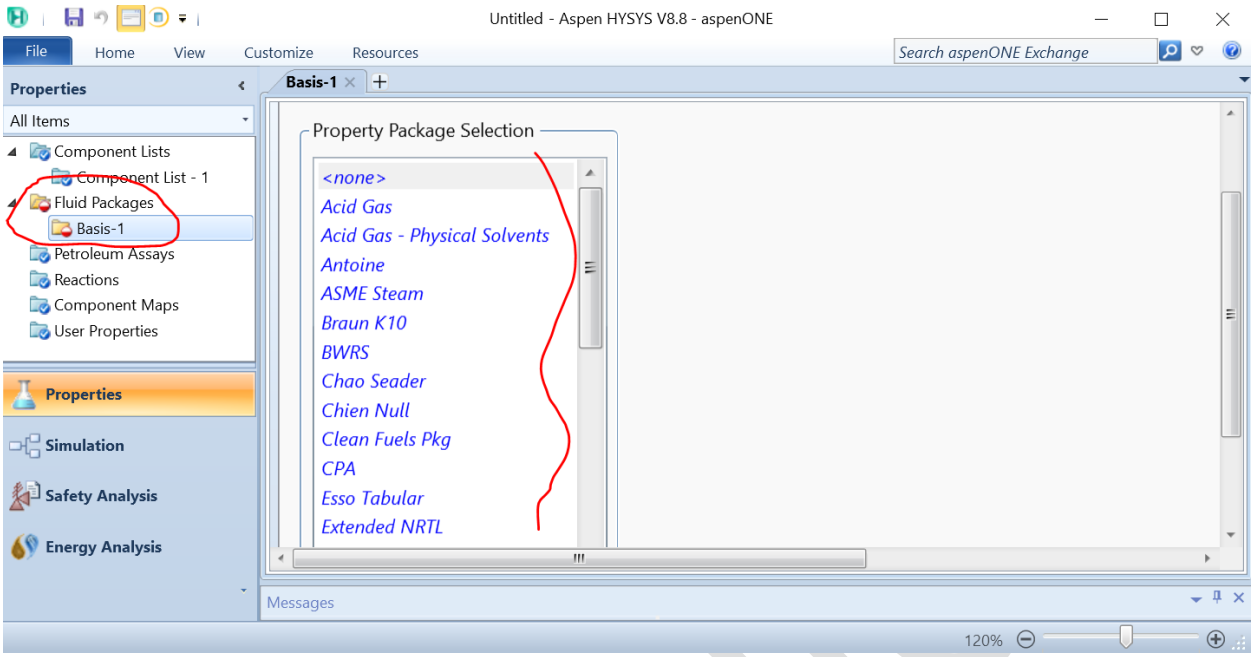

Figure 5. Choose the fluid package

- **Define Reactions:** Specify the chemical reactions that will take place in the reactor. You can input reactants, products, stoichiometry, and kinetics. If you're unsure about the reaction parameters, you may need to consult chemical engineering references or conduct laboratory experiments to gather the necessary data.

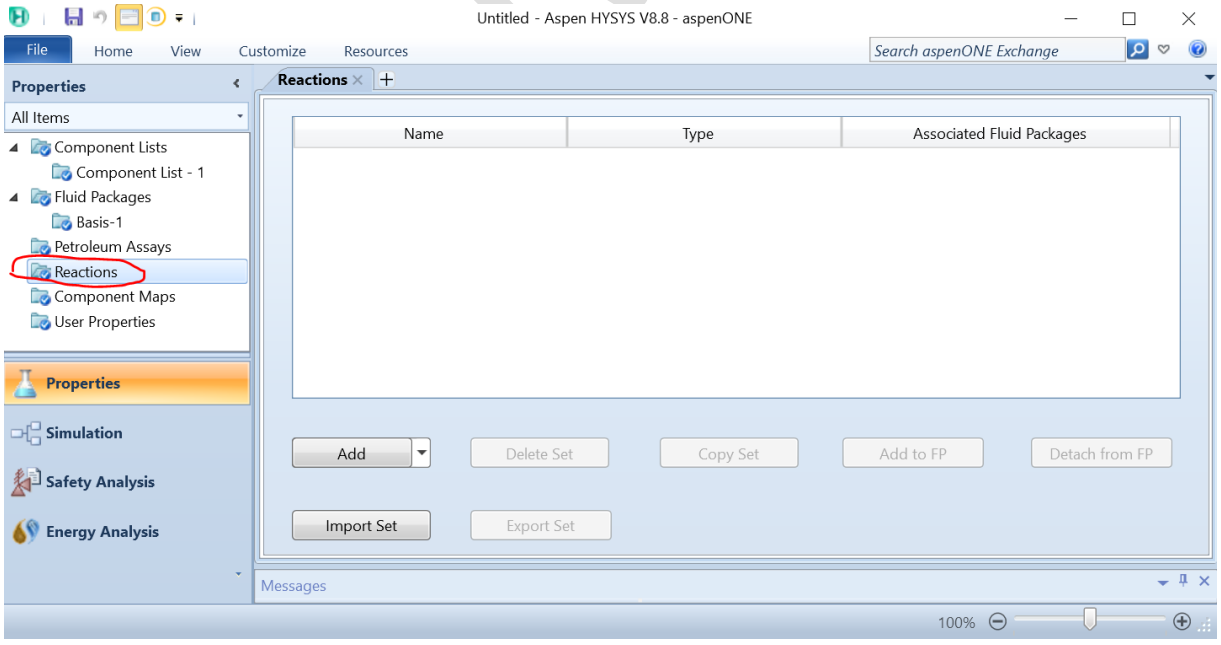

Figure 6. Setting up the reactions

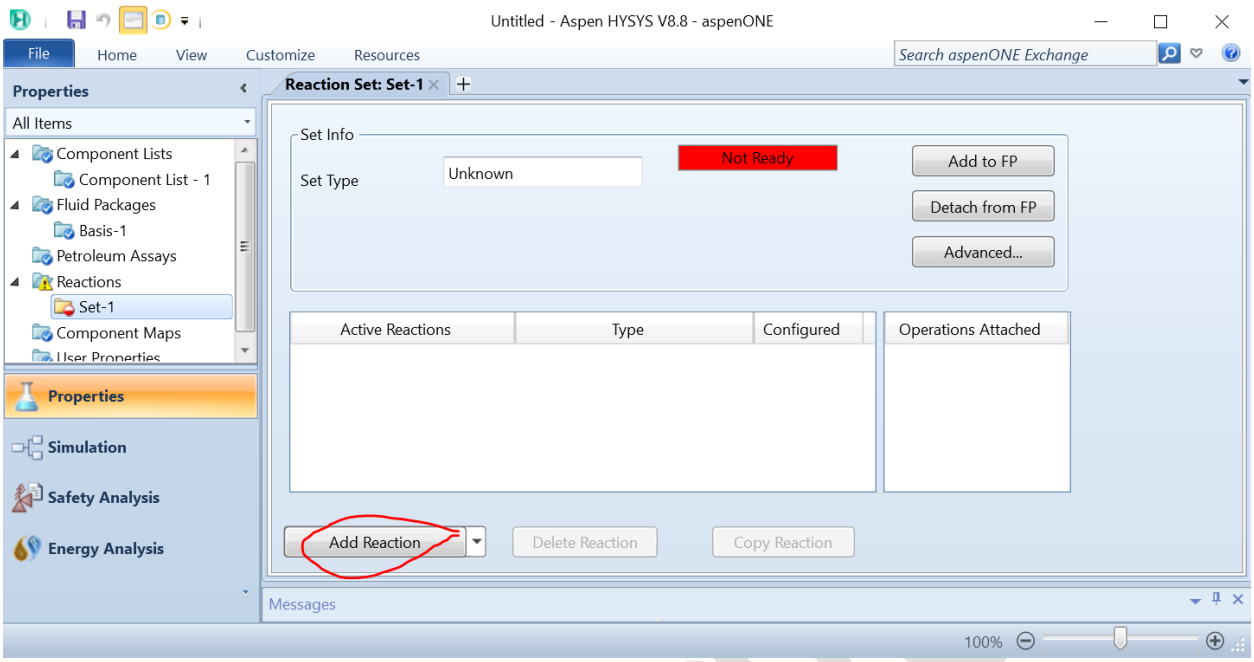

Figure 7. Add reactions

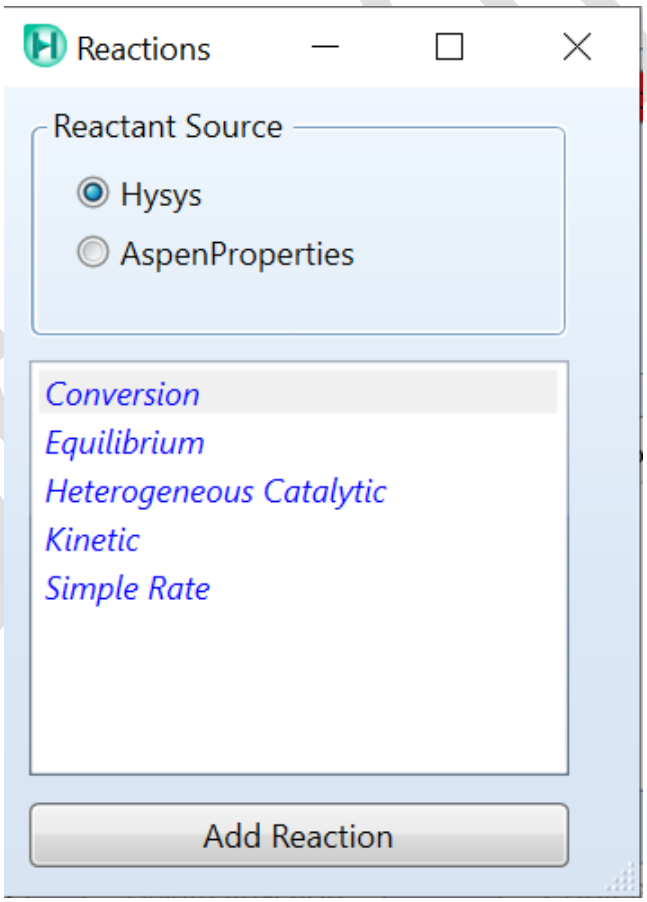

Figure 8. Choose the reaction type

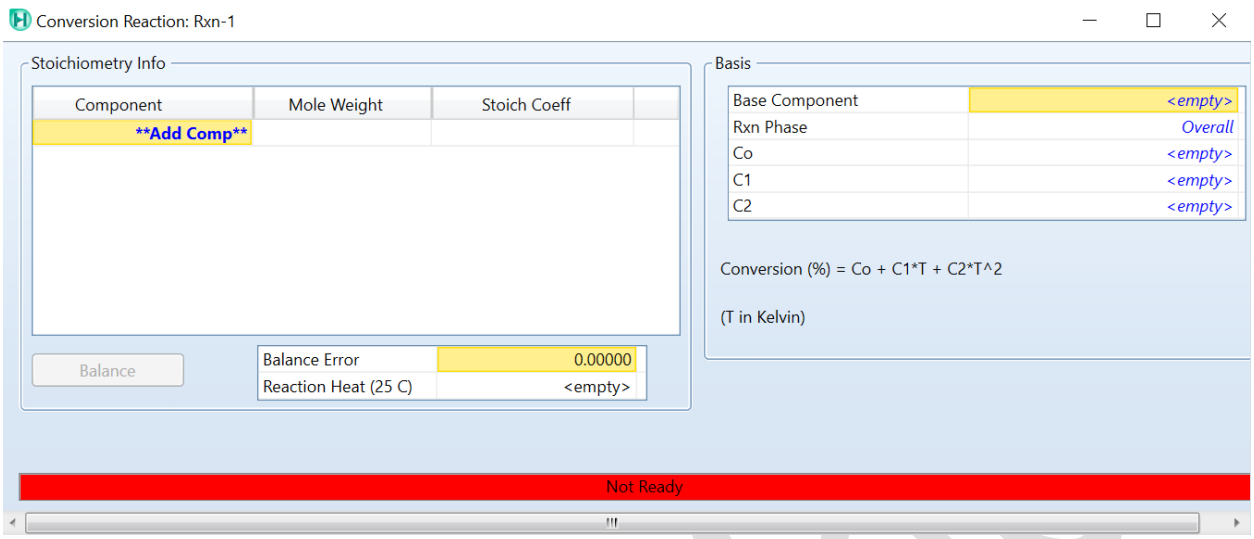

Figure 9. Insert the different parameters of the reaction

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

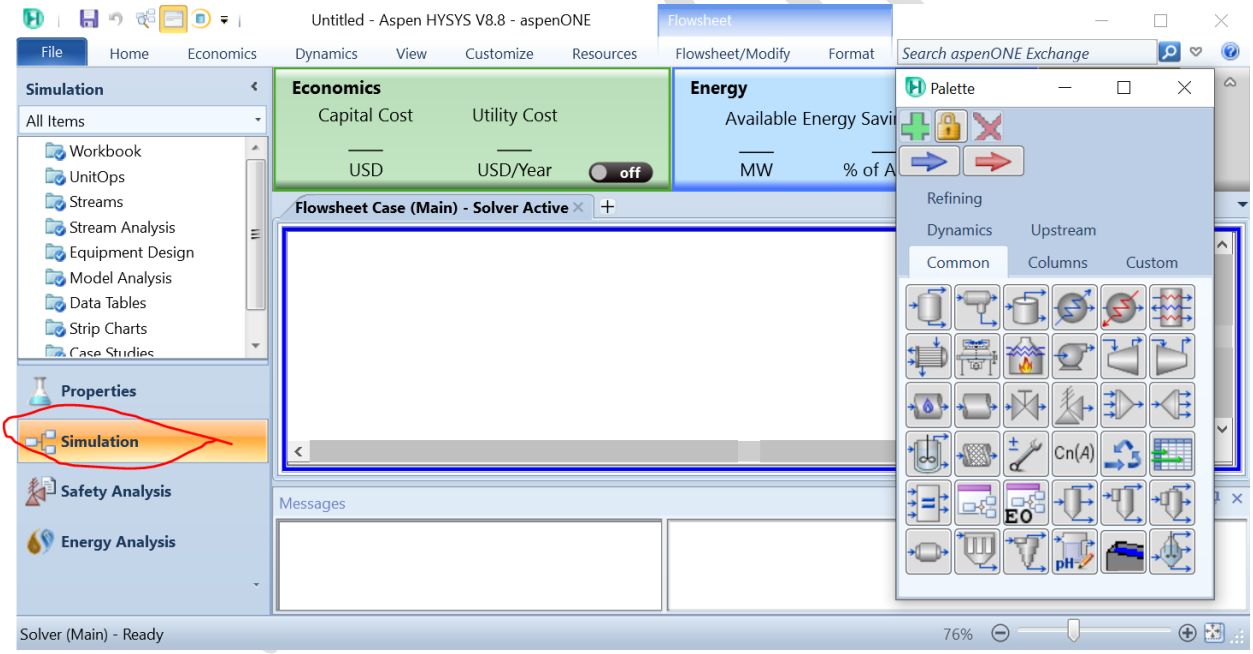

Figure 10. clicking on Simulation Icon

- **Add Reactor:** from the Palette, add a reactor by selecting the reactor type you want to simulate, in our case conversion reactor.

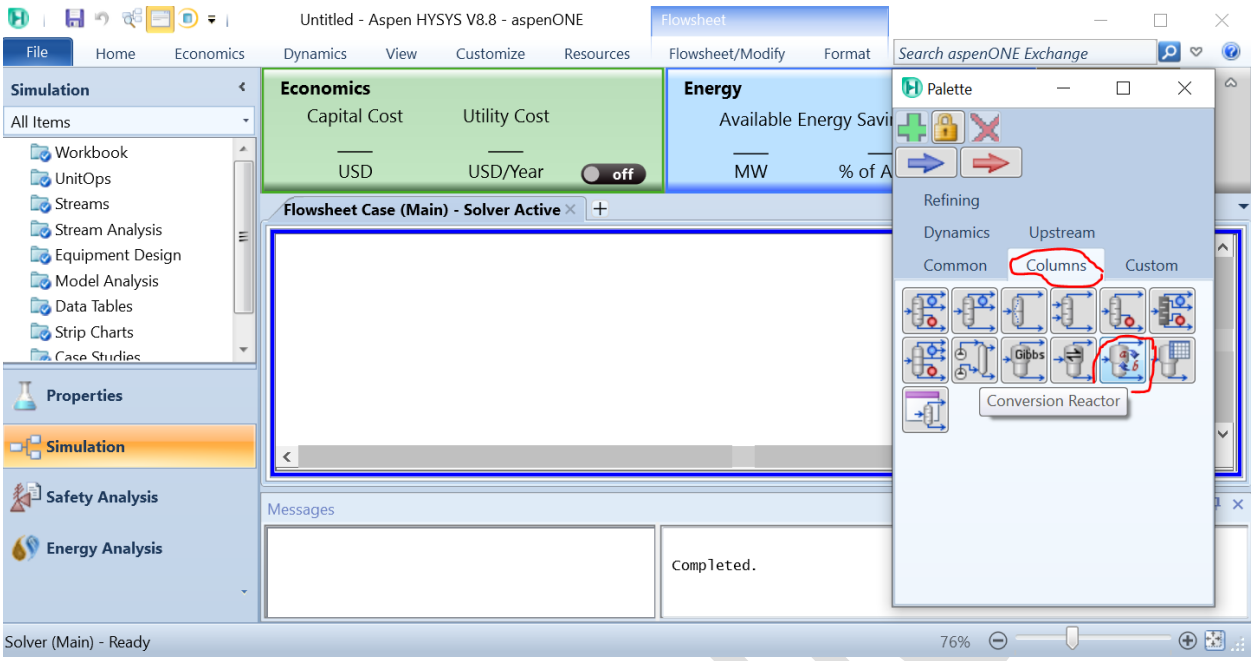

Figure 11. Conversion reaction from the palette

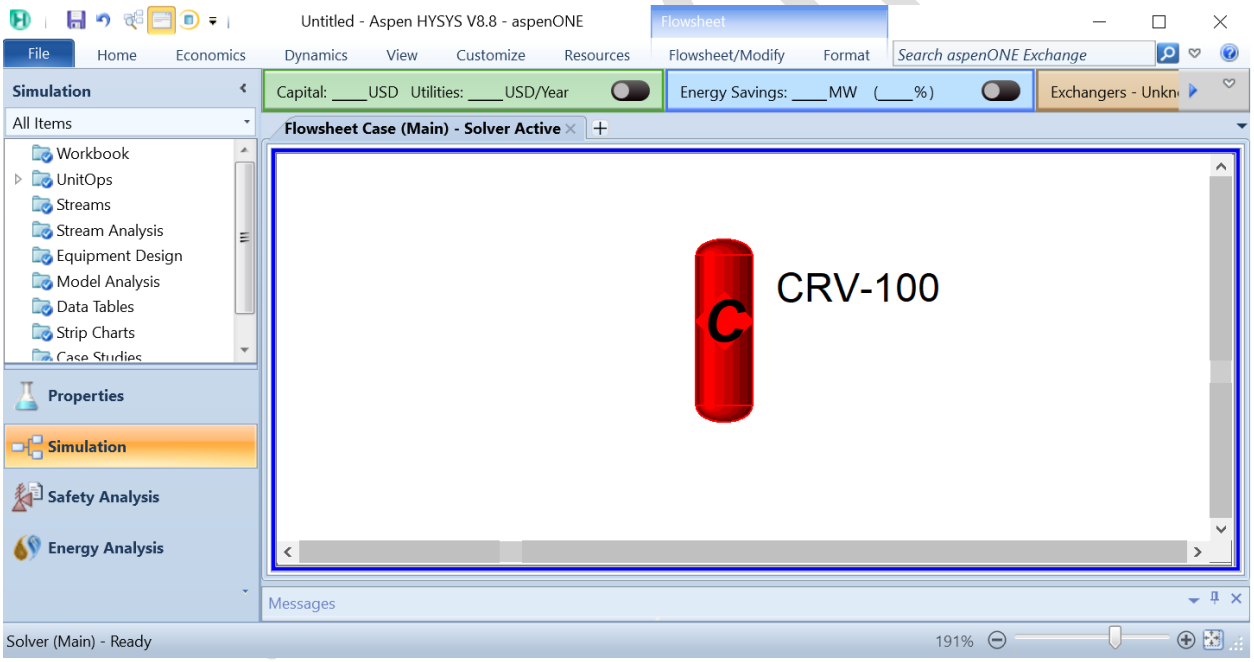

Figure 12. Add the reactor to the PFD

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

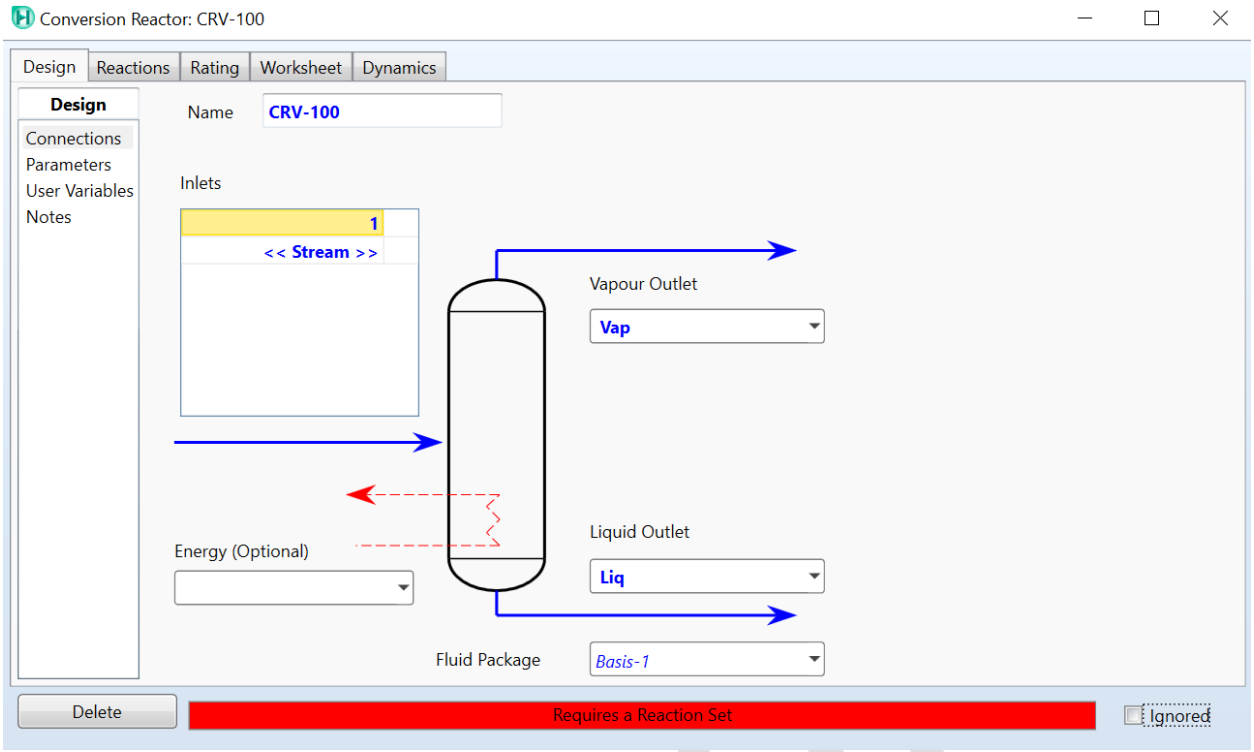

Figure 13. Setting the streams in the reactor

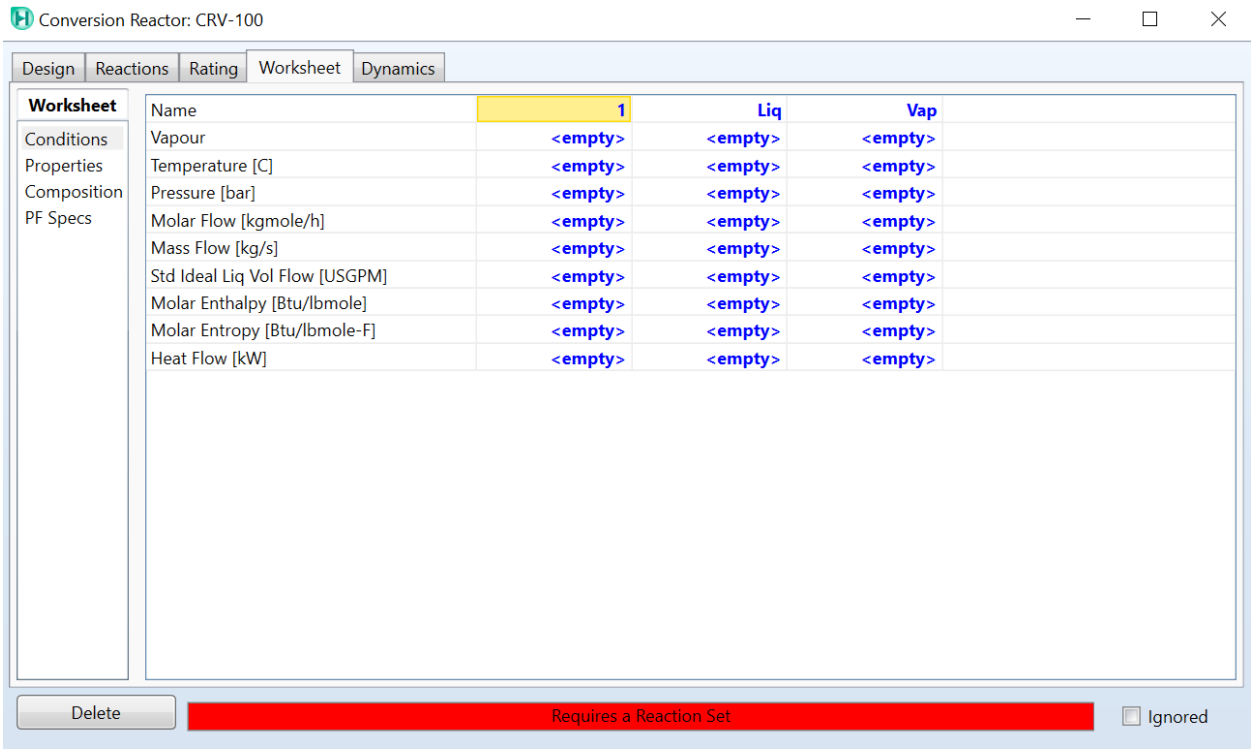

Figure 14. Insert the different parameters of the fluxes

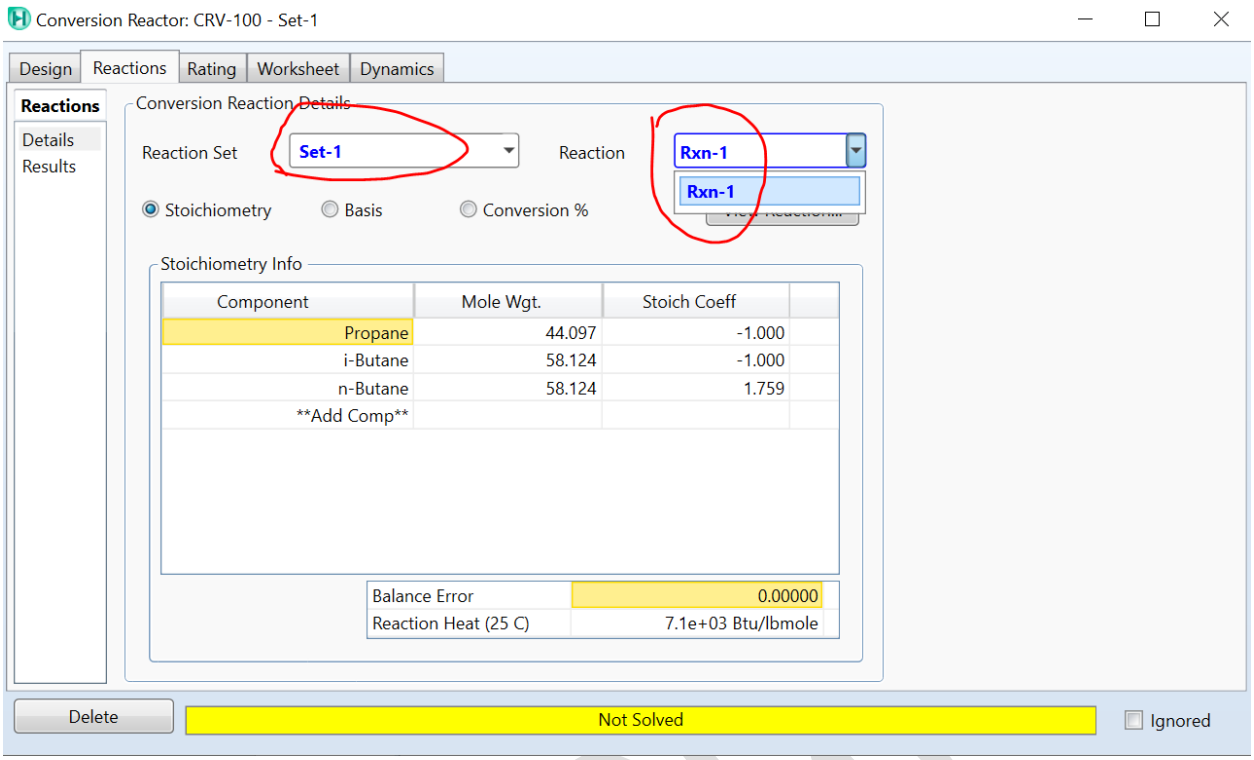

Figure 15. Adding reaction set

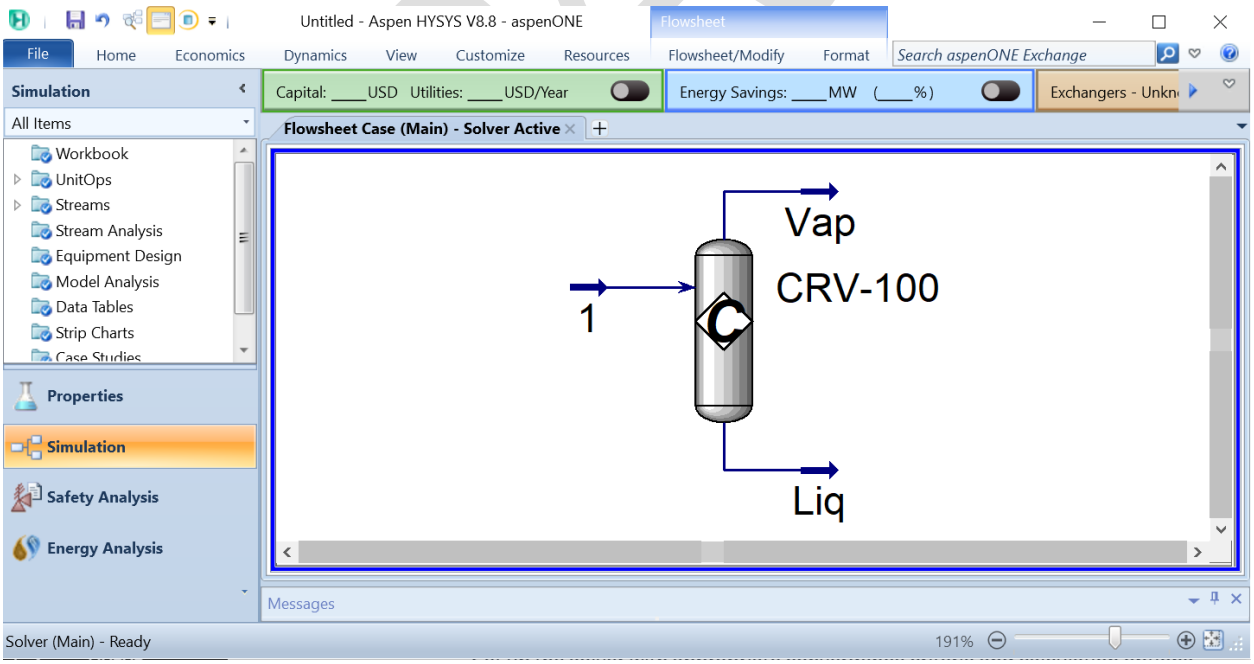

Figure 16. Getting the results

These steps provide a general guideline for simulating conversion reactors in Aspen HYSYS. However, the specific details and nuances can vary depending on the type of reactor and the complexity of the chemical reactions involved. It's

essential to consult Aspen HYSYS documentation and resources for more in-depth guidance on using the software effectively.

However, more details will be discussed and be practiced in the PW sessions, in which numerous examples of this type of reactors will be studied.

II-3-2- Equilibrium Reactors

Equilibrium reactors are a specific type of chemical reactor that operate under conditions where the reactants and products are in a state of chemical equilibrium. In chemical equilibrium, the forward and reverse reactions occur at the same rate, and there is no net change in the concentrations of the reactants and products over time. This type of reactor is commonly used in processes where it's necessary to maintain a particular chemical composition.

In order to simulate the equilibrium reactors, 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.

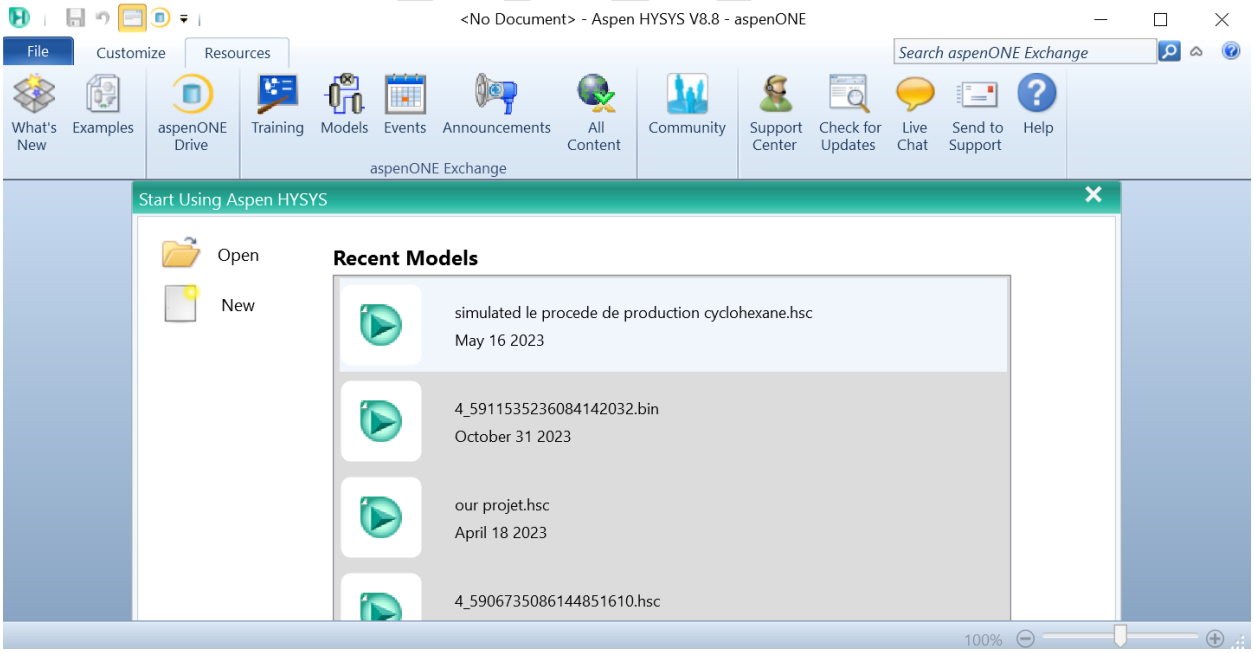

Figure 17. Launch Aspen HYSYS

- **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.

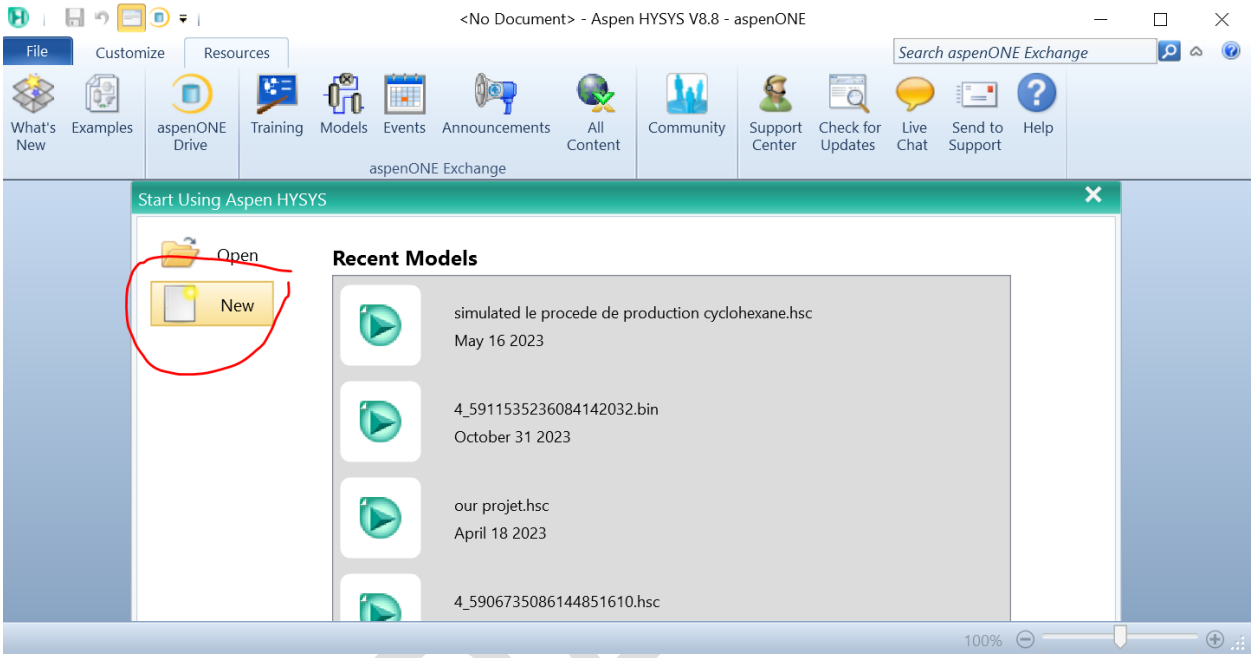

Figure 18. Open a new case

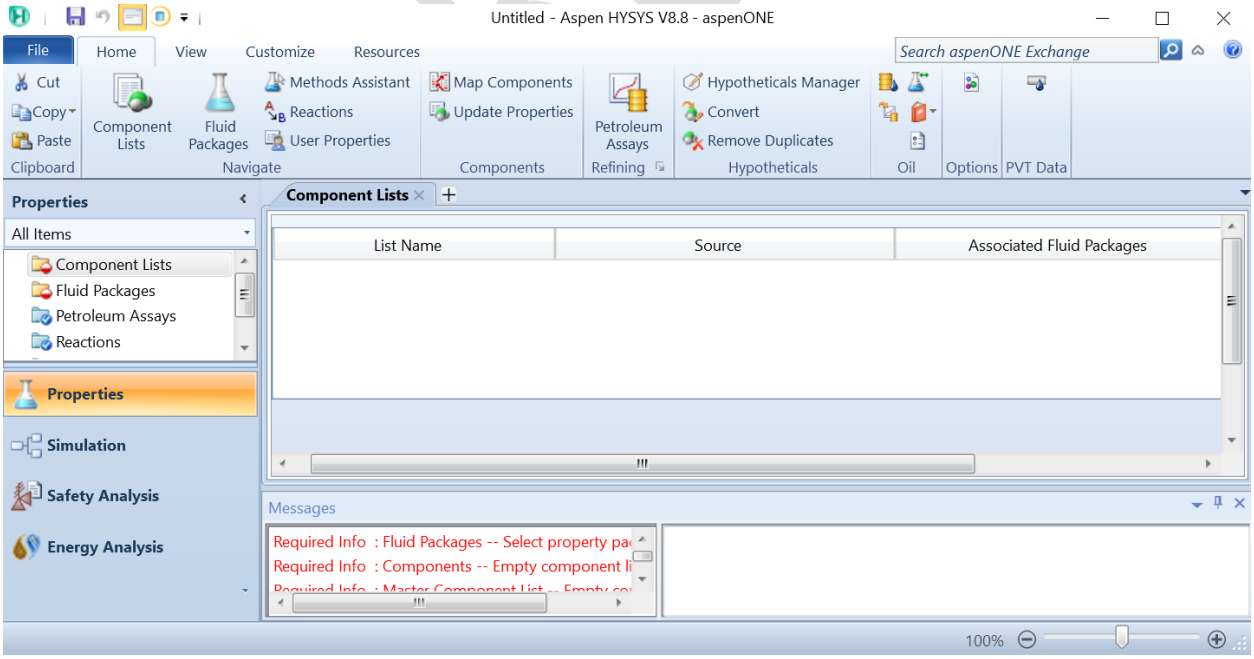

Figure 19. Appeared window after opening a new case or project

- **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.

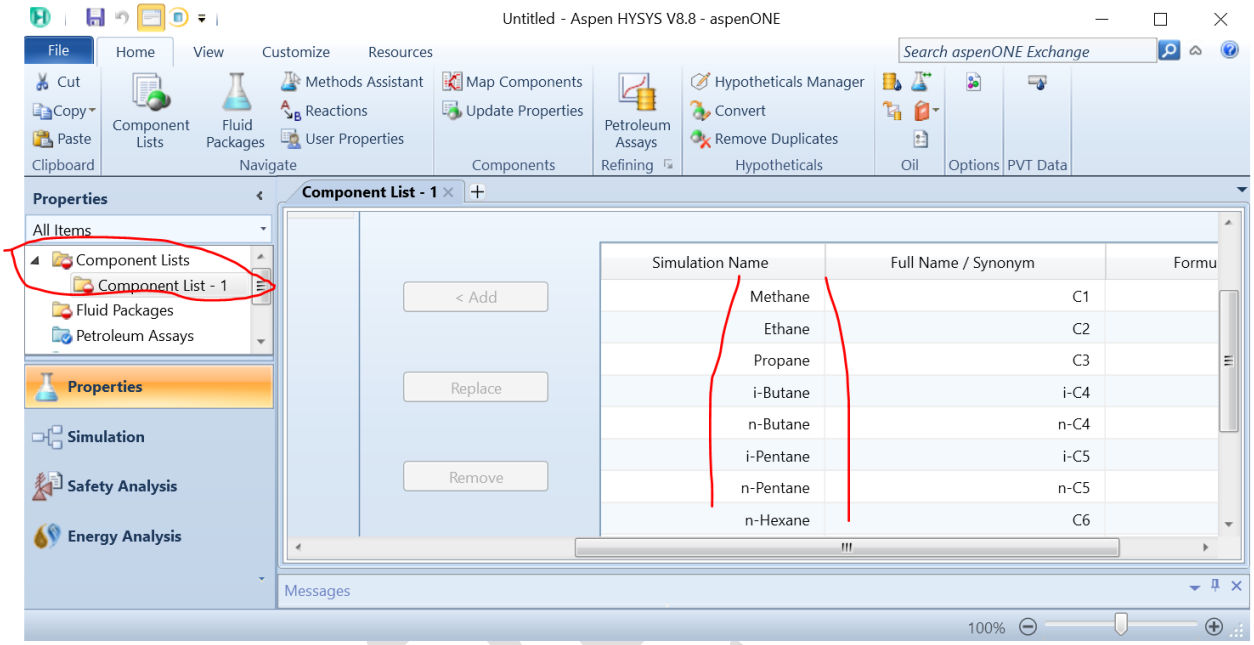

Figure 20. Adding the component list

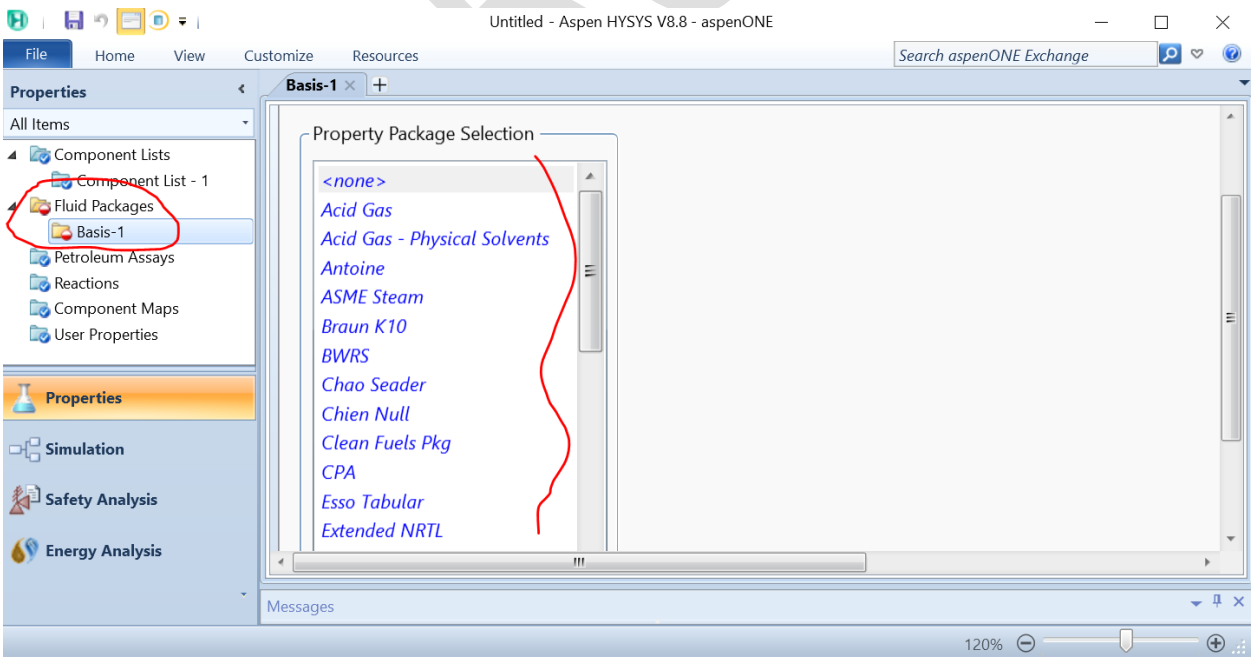

Figure 21. Choose the fluid package

- **Define Reactions:** Specify the chemical reactions that will take place in the reactor. You can input reactants, products, stoichiometry, and kinetics. If you're unsure about the reaction parameters, you may need to consult chemical engineering references or conduct laboratory experiments to gather the necessary data.

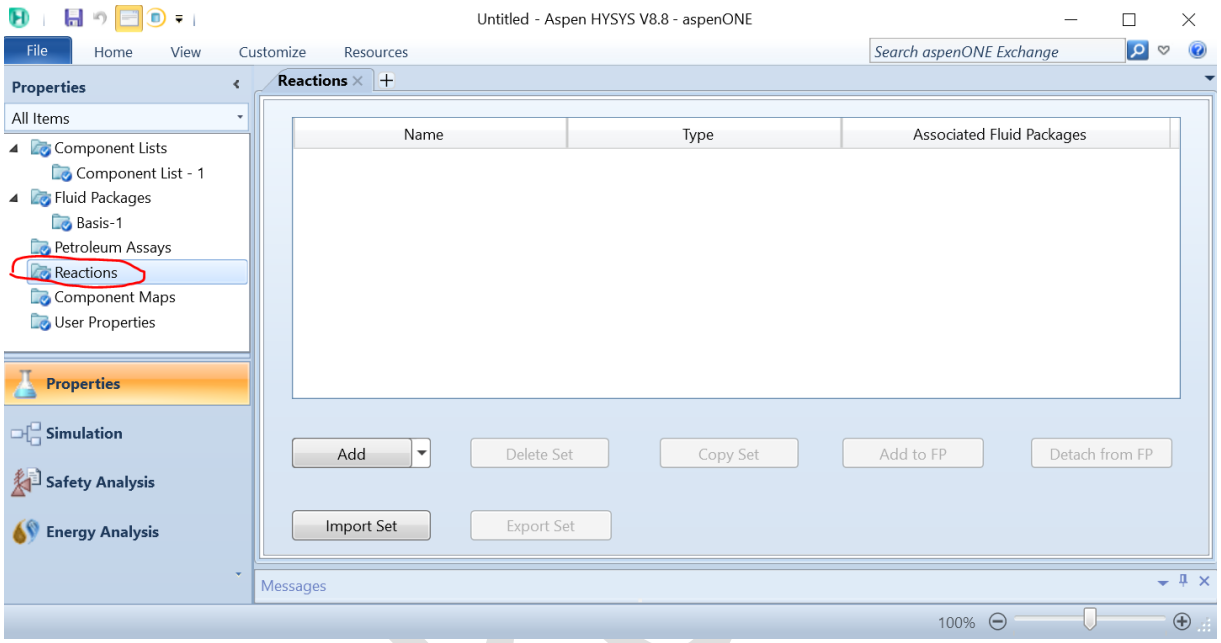

Figure 22. Setting up the reactions

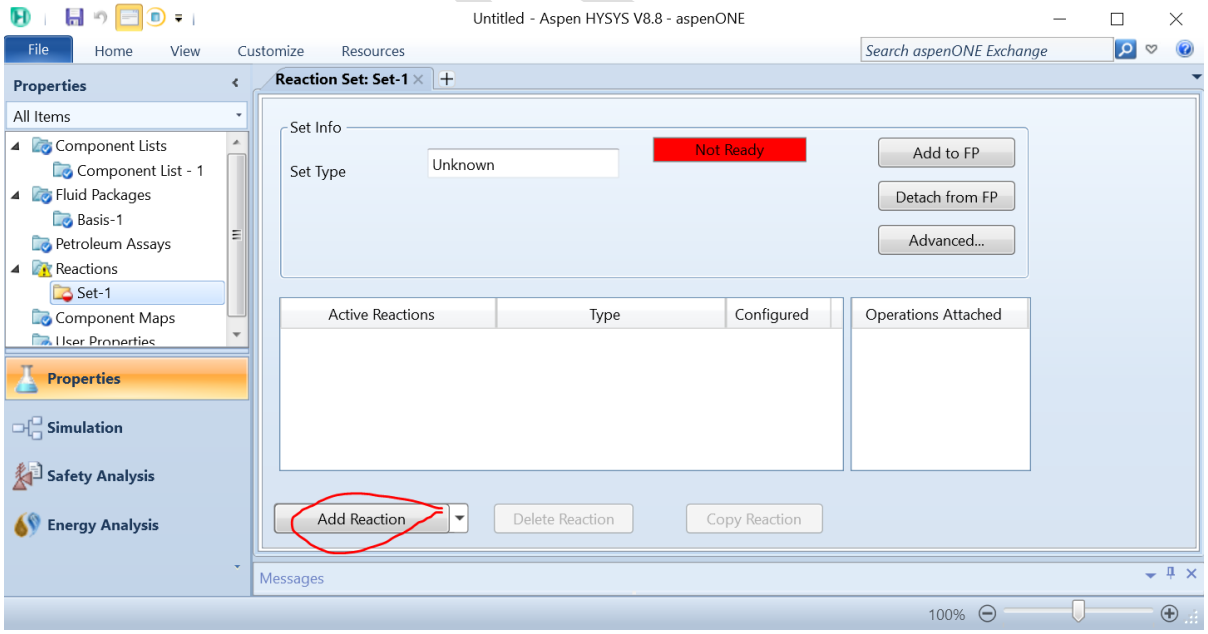

Figure 23. Add reactions

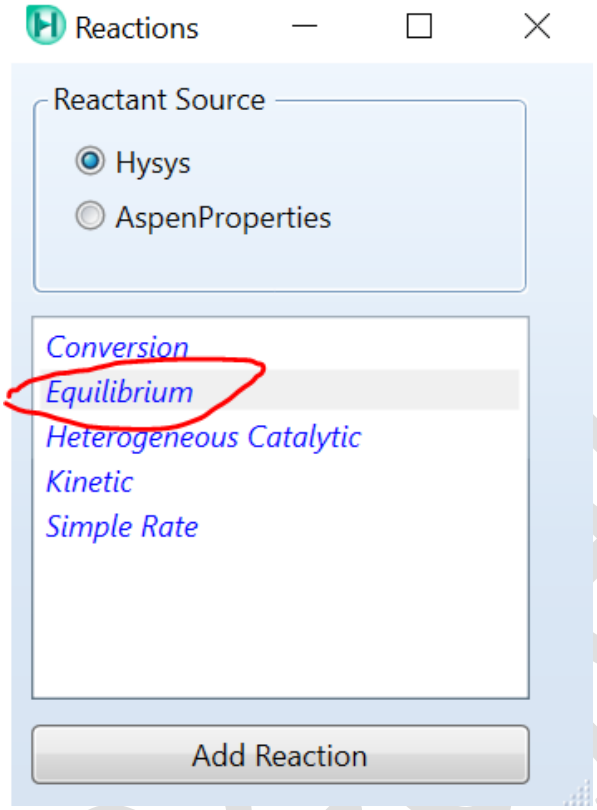

Figure 24. Choose the reaction type

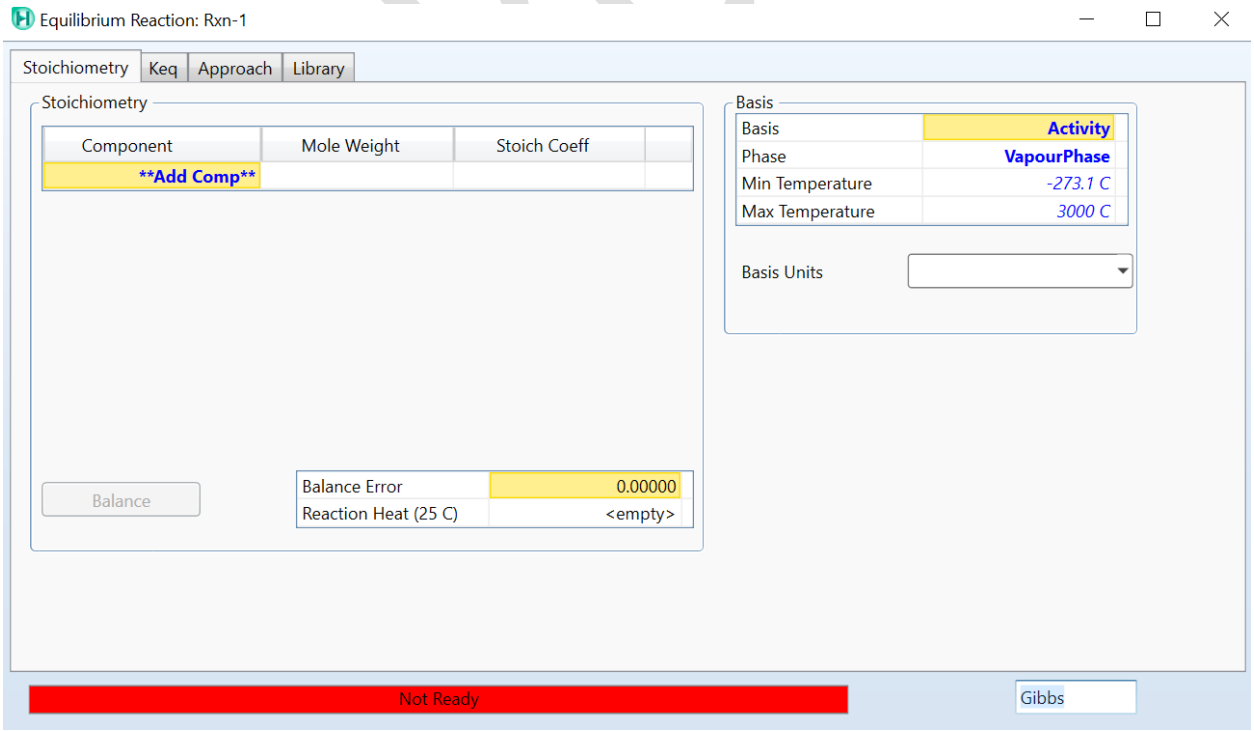

Figure 25. Insert the different parameters of the reaction

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

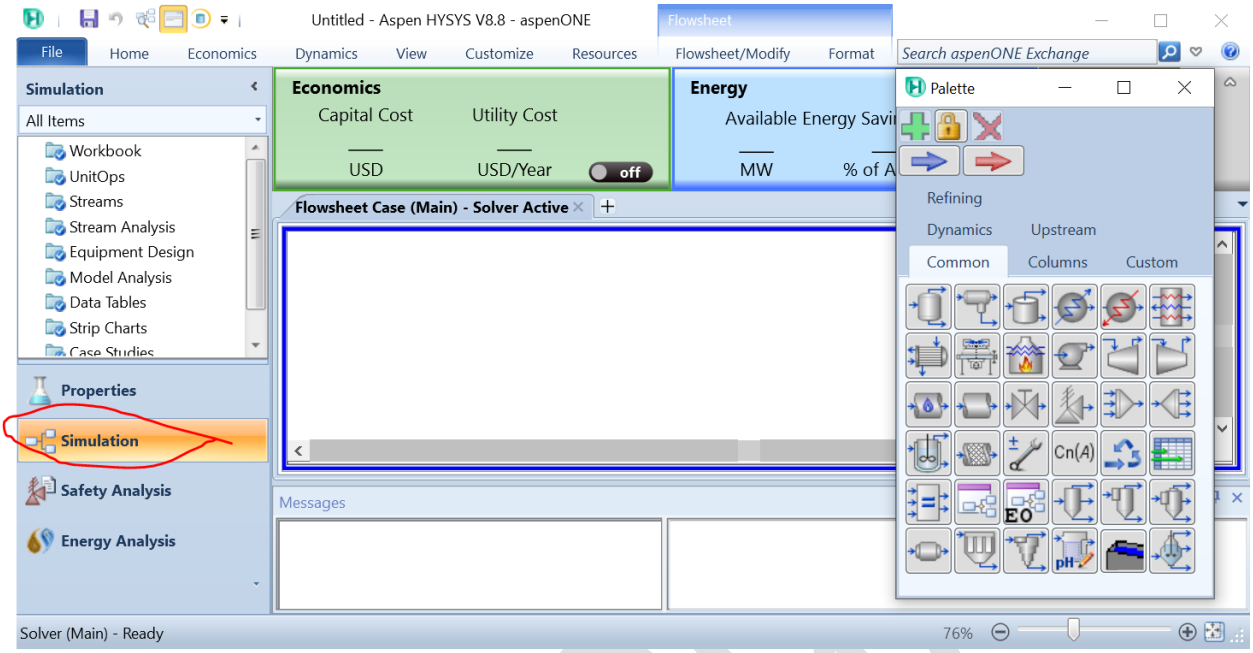

Figure 26. clicking on Simulation Icon

- **Add Reactor:** from the Palette, add a reactor by selecting the reactor type you want to simulate, in our case equilibrium reactor.

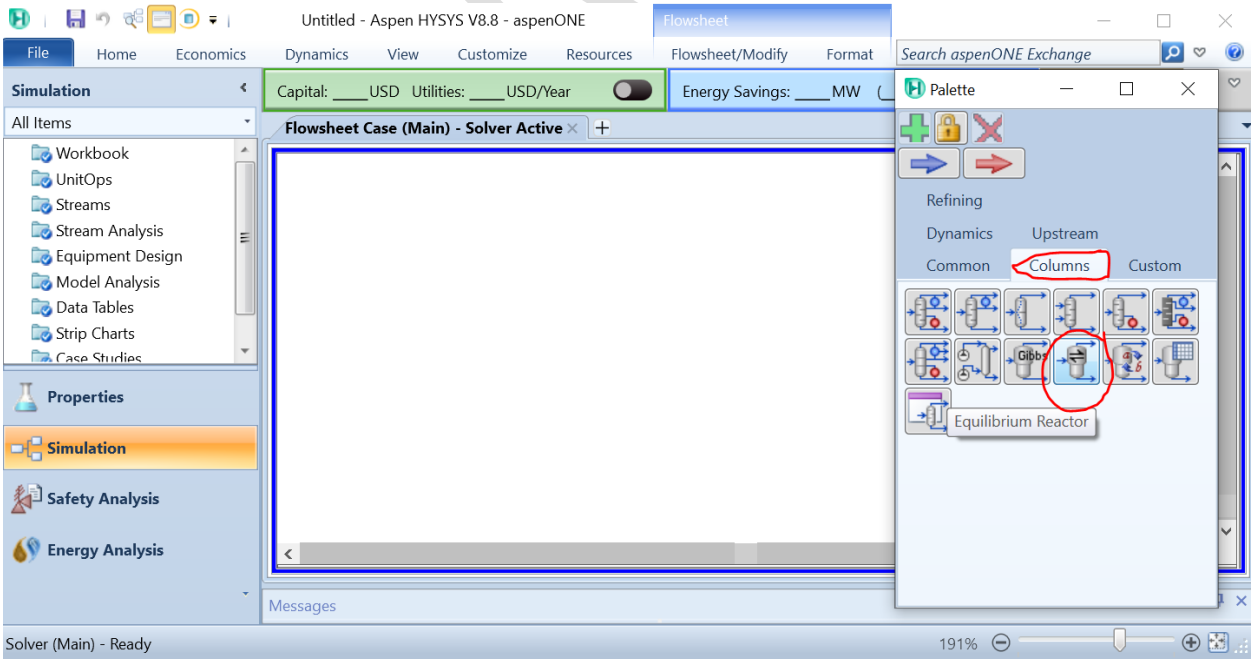

Figure 27. Equilibrium reactor from the palette

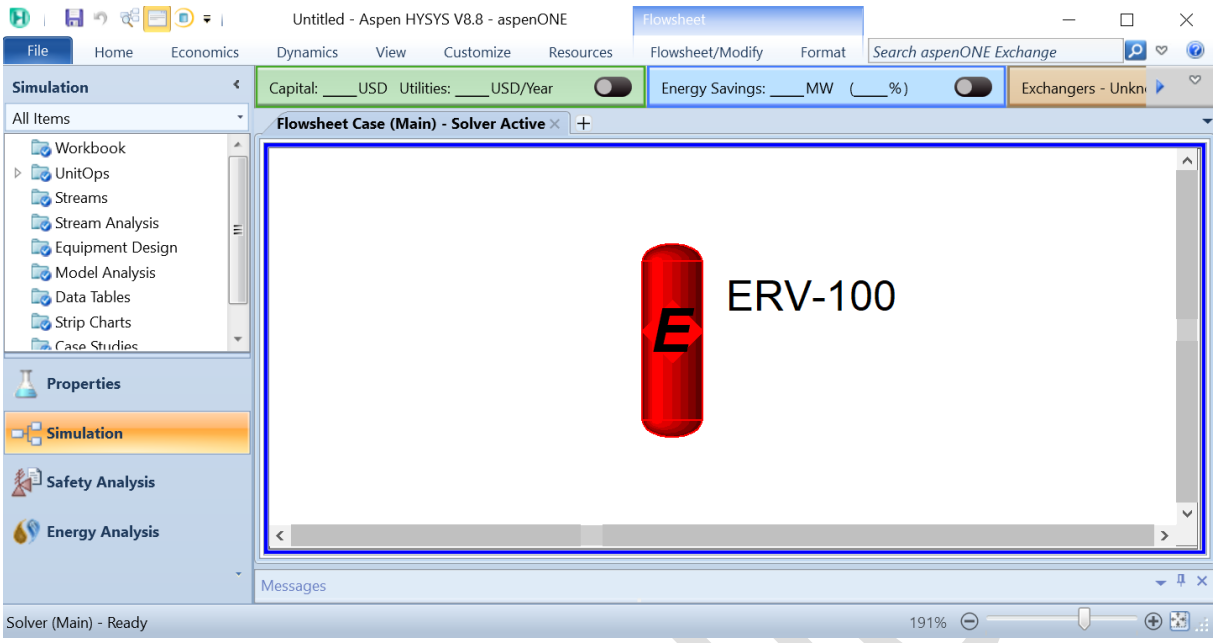

Figure 28. Add the reactor to the PFD

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

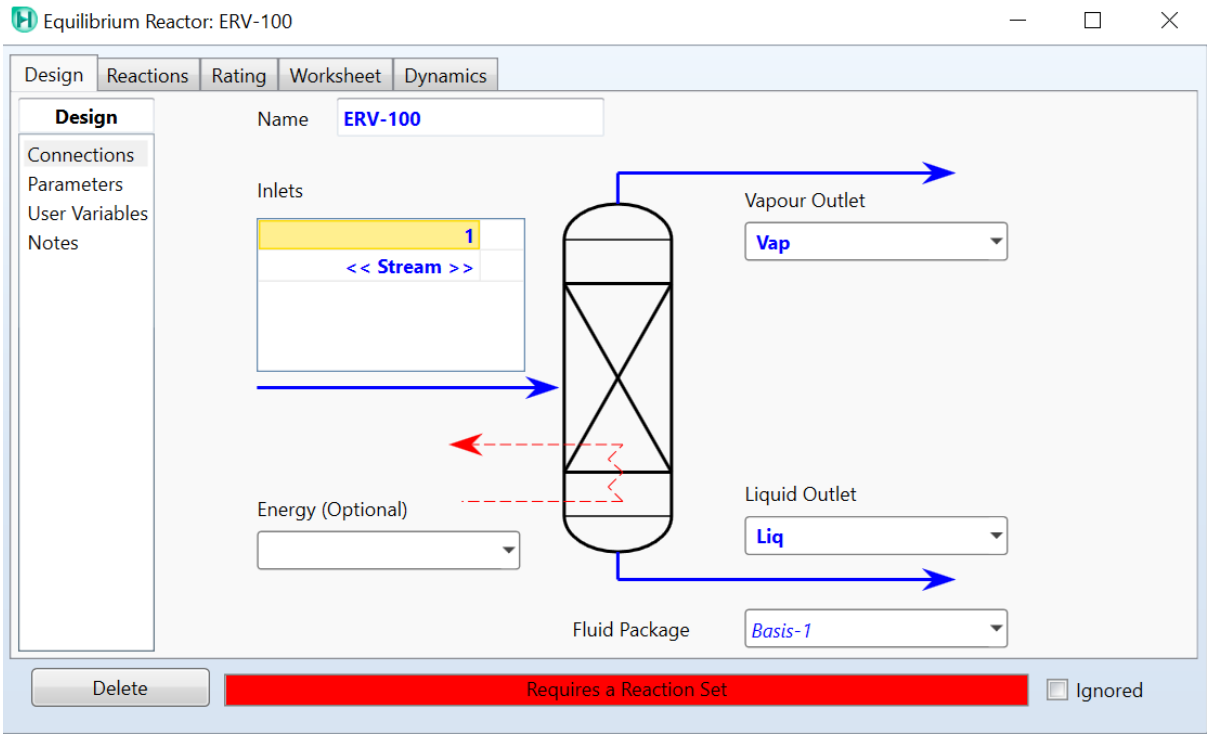

Figure 29. Setting the streams in the reactor

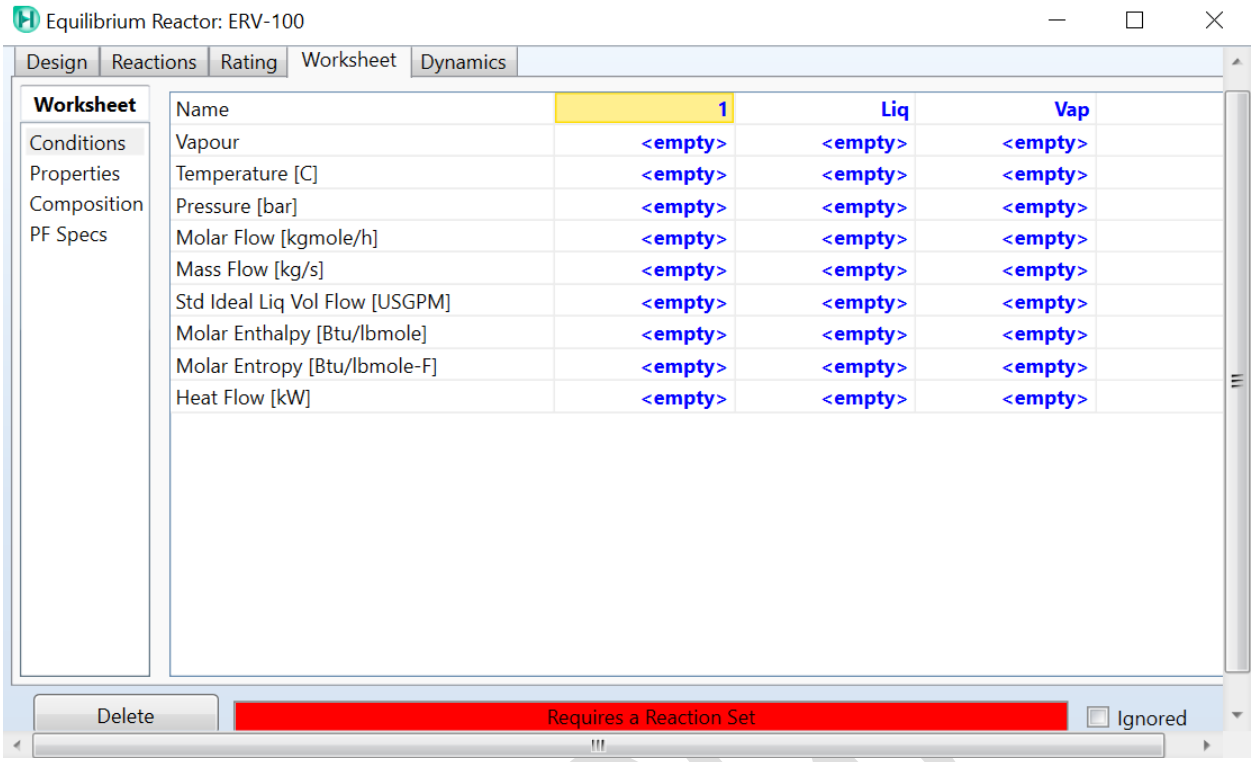

Figure 30. Insert the different parameters of the fluxes

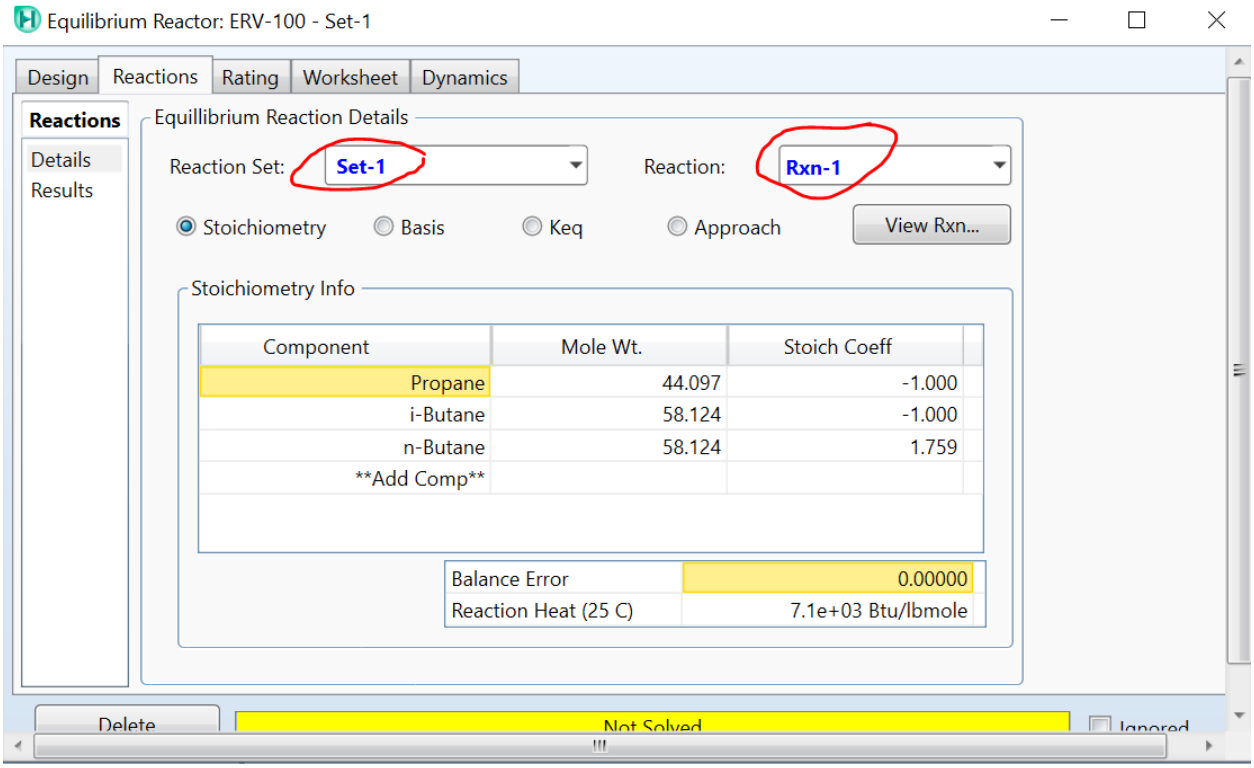

Figure 31. Adding reaction set

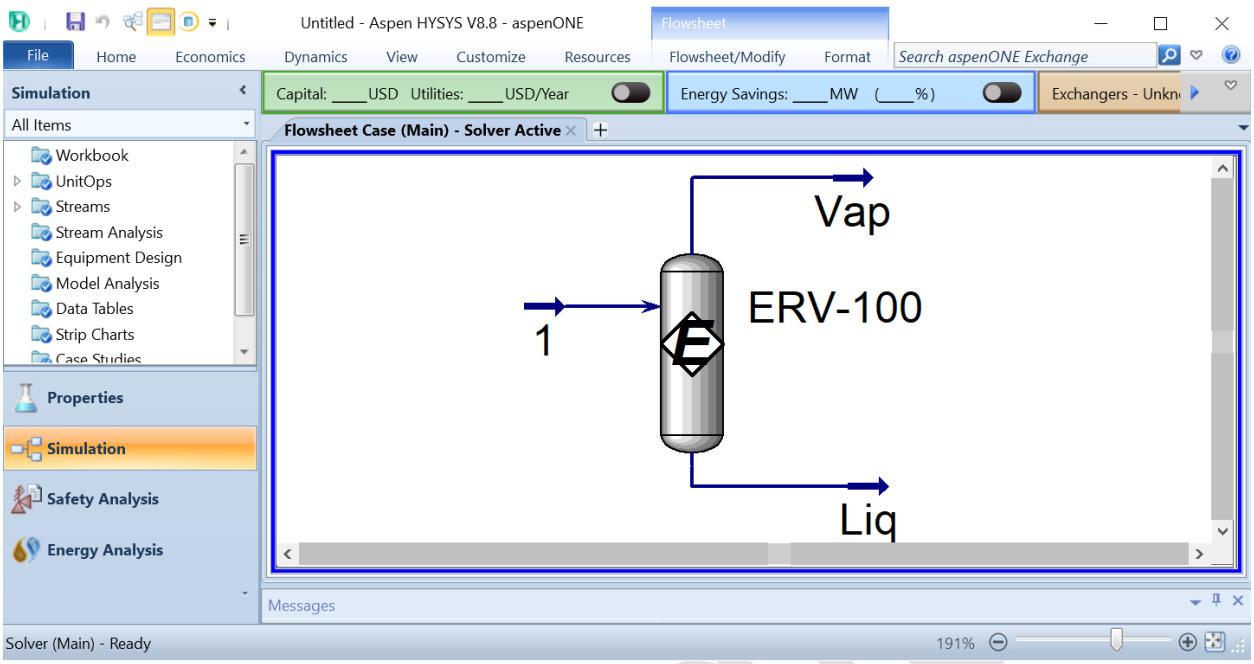

Figure 32. Getting the results

Please note that equilibrium reactors are typically used for reactions where the composition of reactants and products needs to be precisely controlled. Aspen HYSYS provides a platform for modeling and understanding these reactors, ensuring that chemical processes are maintained at equilibrium, as required for various industrial applications.

However, more details will be discussed and be practiced in the PW sessions, in which numerous examples of this type of reactor will be studied.

II-3-3- Perfectly Stirred Reactors (RPR)

Stirred reactors, often referred to as Continuous Stirred-Tank Reactors (CSTR), are a type of chemical reactor used in various industries to mix and react substances continuously. These reactors maintain a well-mixed environment where reactants are continuously fed, and products are continuously withdrawn. Aspen HYSYS can be employed to simulate stirred reactors, helping engineers and scientists understand and optimize their performance.

In order to simulate the equilibrium reactors, there are numerous steps that should be followed using Aspen Hysys, they can be presented as points as follows:

For the first steps, starting by lunching Aspen Hysys, Selecting the component list,

and the fluid package, the same previous steps should be followed, as illustrated in Figures 1 to 7, then, for the type of reaction, it should be chosen according to your target and objective, for example it could be a kinetic type

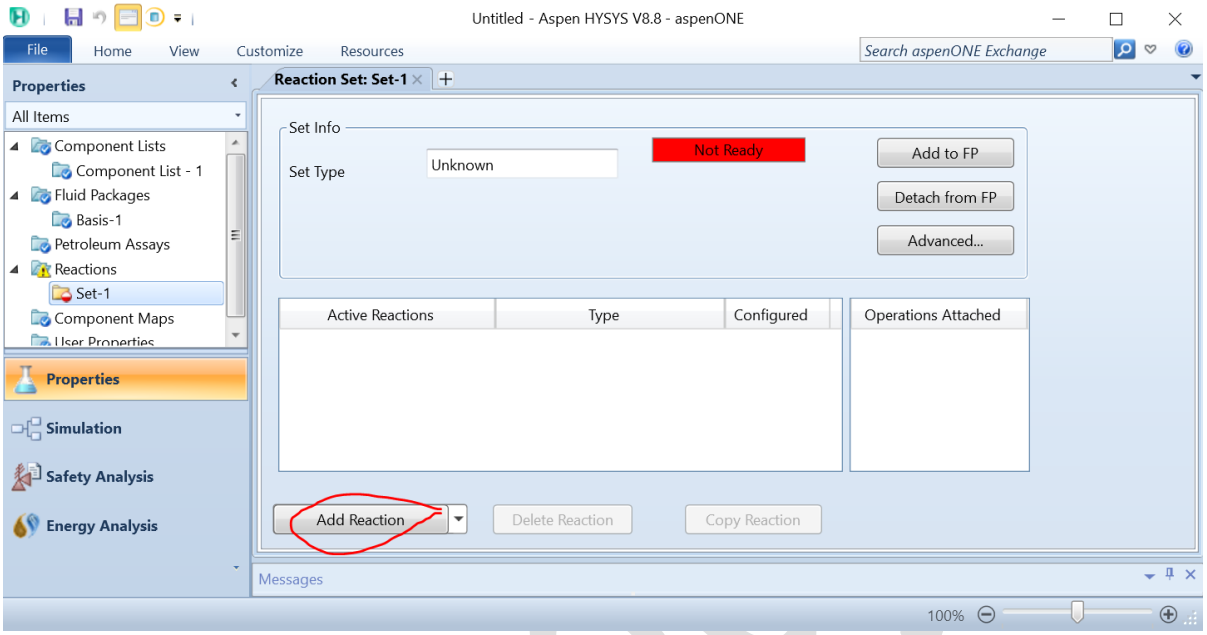

Figure 33. Add reactions

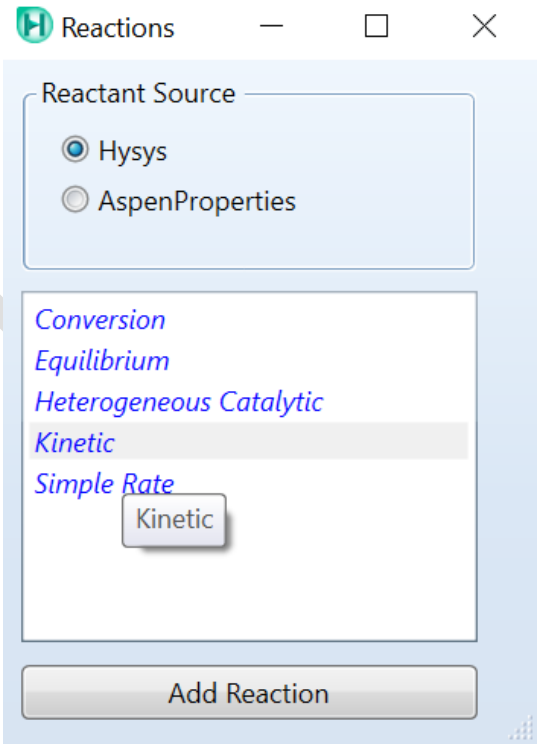

Figure 34. Choose the reaction type

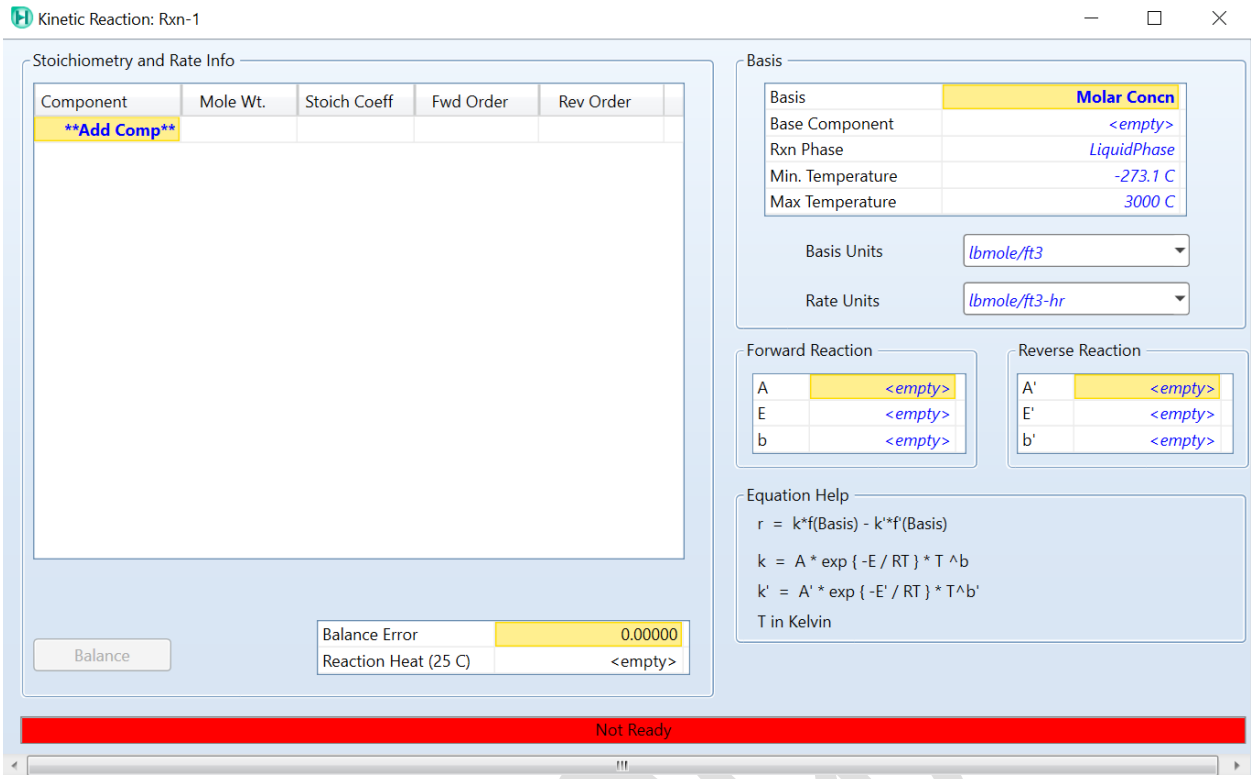

Figure 35. Insert the different parameters of the reaction

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

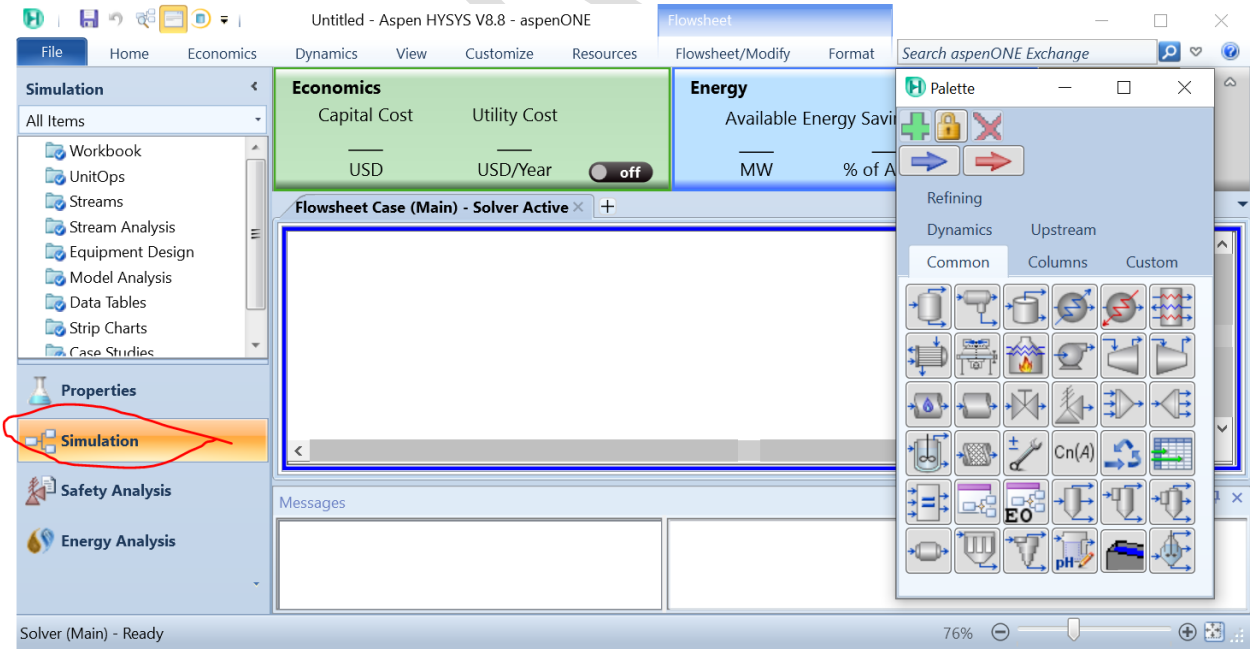

Figure 36. clicking on Simulation Icon

- **Add Reactor:** from the Palette, add a reactor by selecting the reactor type you want to simulate, in our case equilibrium reactor.

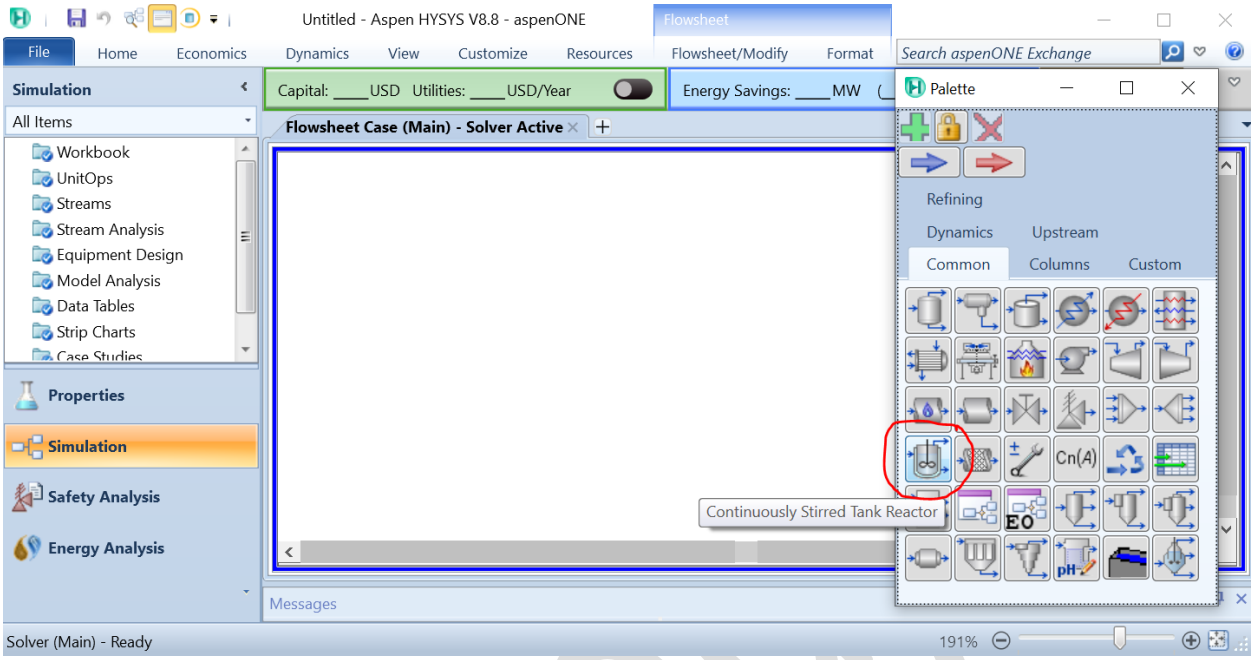

Figure 37. Stirred reactor from the palette

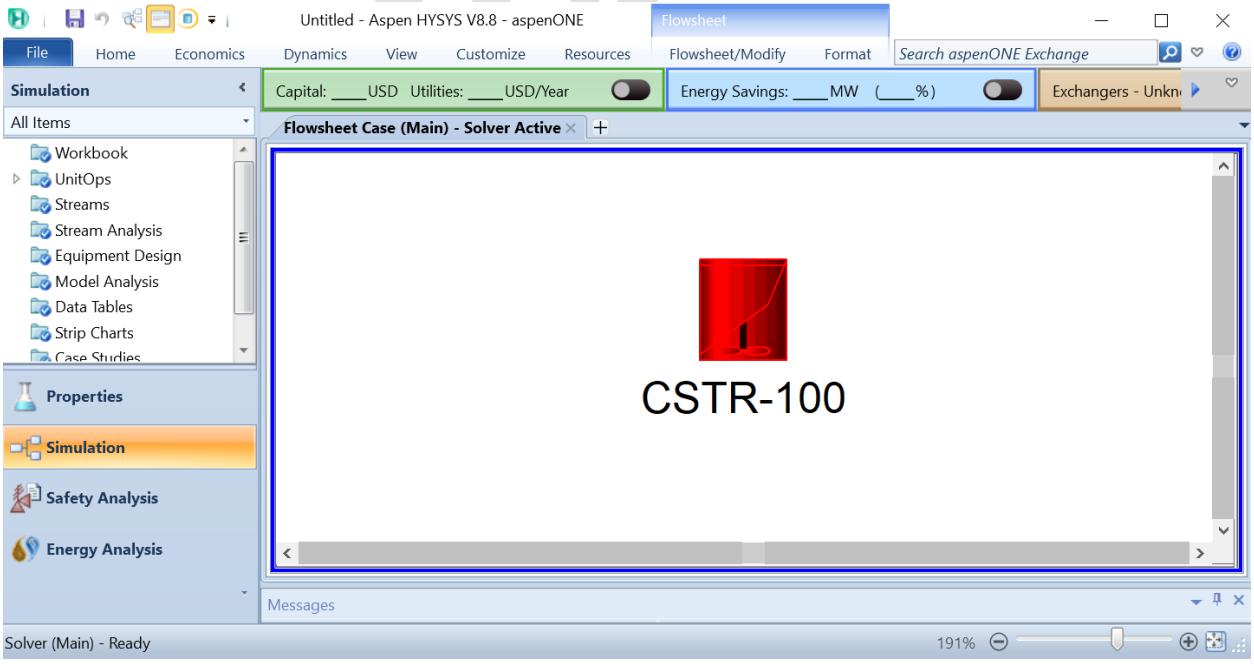

Figure 38. Add the reactor to the PFD

- **Set Operating Conditions:** Define the operating conditions of the reactor, such as temperature, pressure, and flow rates. These conditions significantly

impact the reaction rate and product formation.

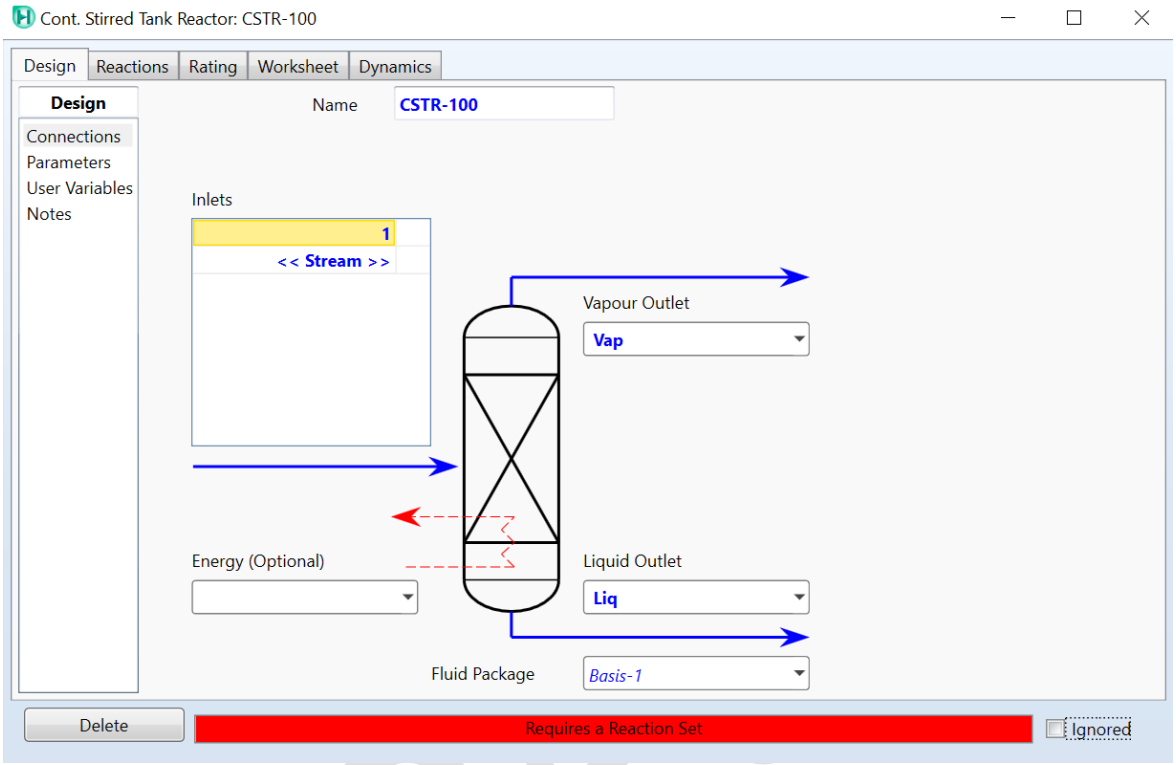

Figure 39. Setting the streams in the reactor

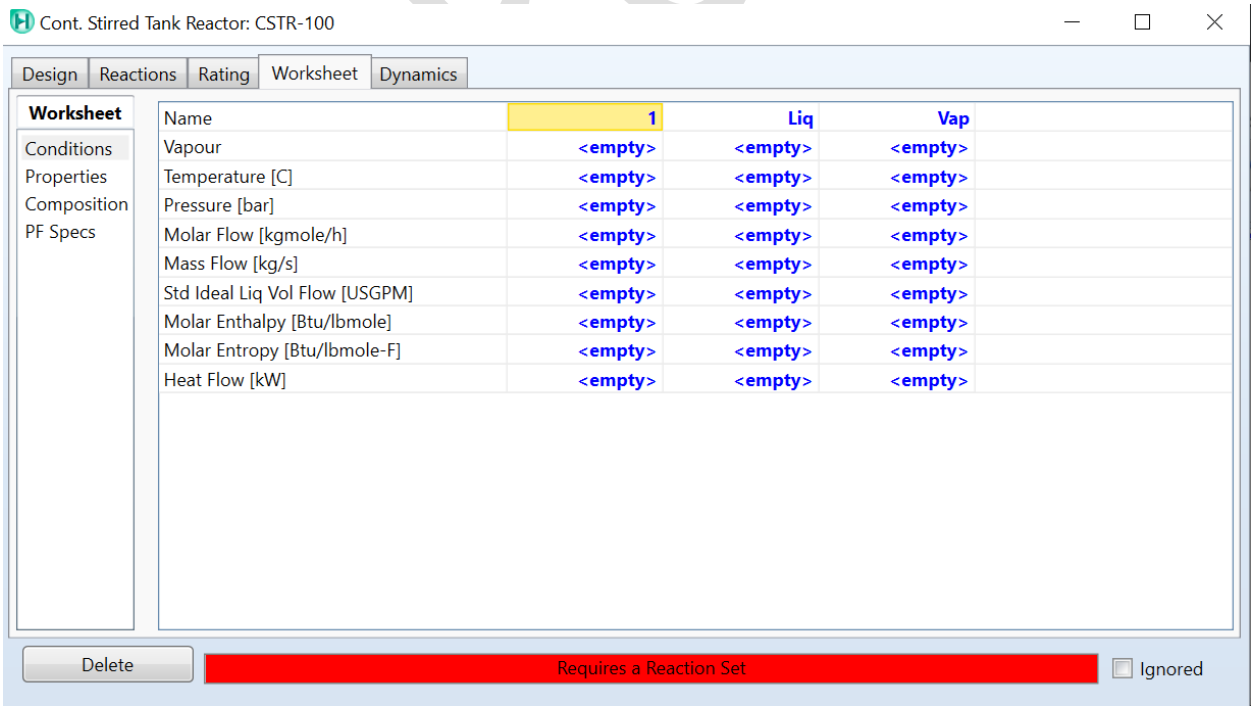

Figure 40. Insert the different parameters of the fluxes

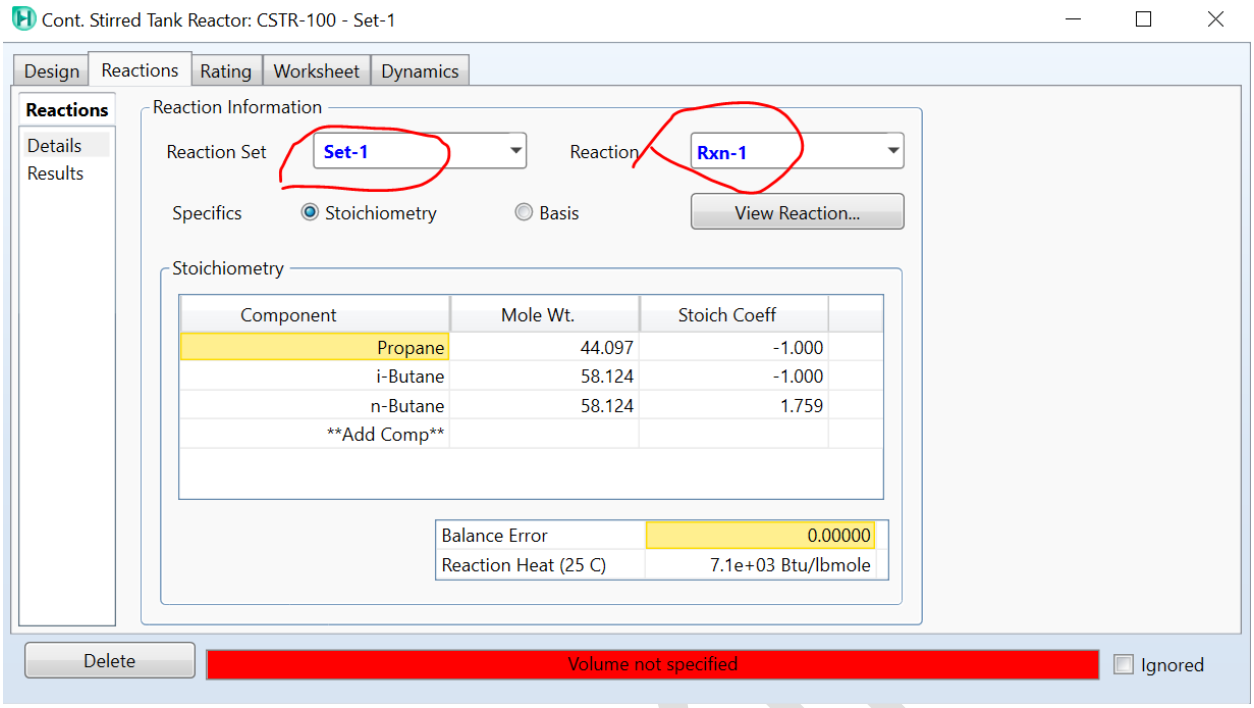

Figure 41. Adding reaction set

After adding the reaction set and the different conditions, it is necessary to add some associated parameters such as volume of the reactor, as a means to calculate the different related parameters, this will be discussed in the PW sessions.

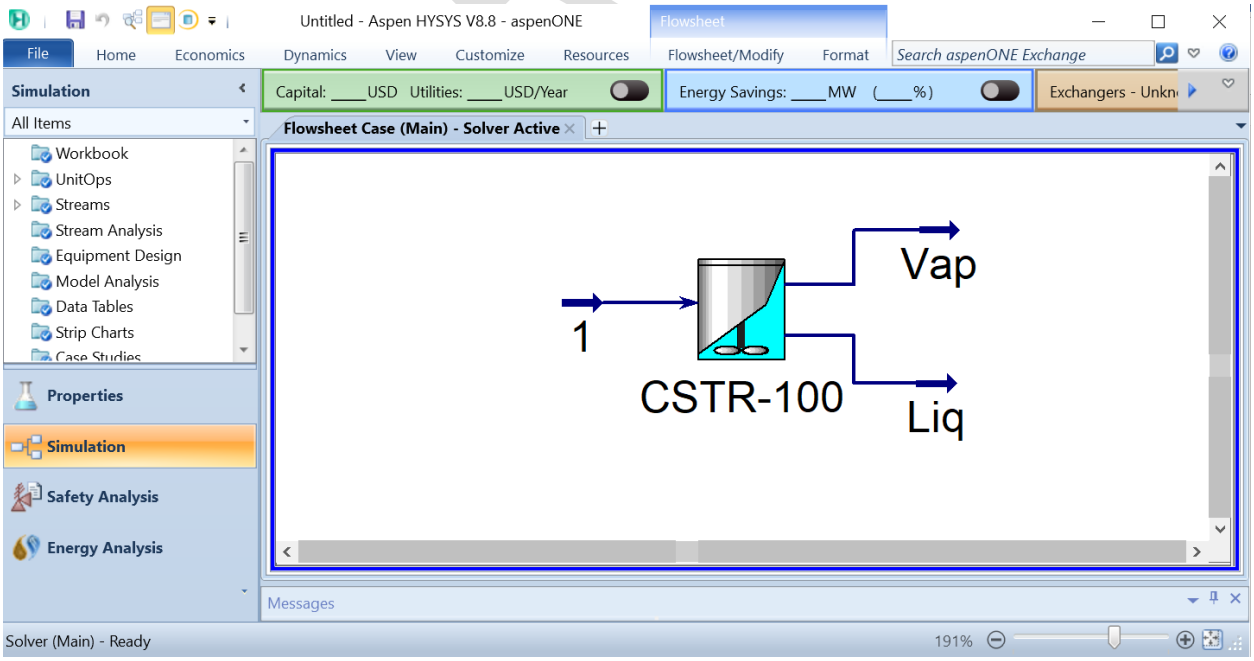

Figure 42. Getting the results

These steps offer a simplified guide to simulating stirred reactors using Aspen HYSYS. Keep in mind that the specifics can vary based on your specific reactor and reaction requirements. Aspen HYSYS serves as a valuable tool for understanding and optimizing the performance of stirred reactors, making it an essential resource in various industries where these reactors are used for chemical processing and production.

However, more details will be discussed and be practiced in the PW sessions, in which numerous examples of this type of reactor will be studied.

II-3-4- Plug Reactors (RP)

Plug reactors, also known as Plug Flow Reactors (PFR), are a type of chemical reactor used in various industrial processes to facilitate continuous and controlled chemical reactions. Unlike stirred reactors, where the contents are thoroughly mixed, plug reactors allow reactants to flow through the reactor without significant mixing, creating a "plug" of reactants that move through the reactor in a straight, continuous path. Aspen HYSYS can be employed to simulate plug reactors, aiding engineers and scientists in understanding and optimizing their behavior.

In order to simulate the Plug reactors, there are numerous steps that should be followed using Aspen Hysys, they can be presented as points as follows:

To initiate the process, begin by launching Aspen Hysys and selecting the component list and fluid package, following the same sequence as depicted in Figures 1 to 7. Subsequently, when determining the type of reaction, it should align with your specific goals and objectives; for instance, you may opt for a kinetic reaction type.

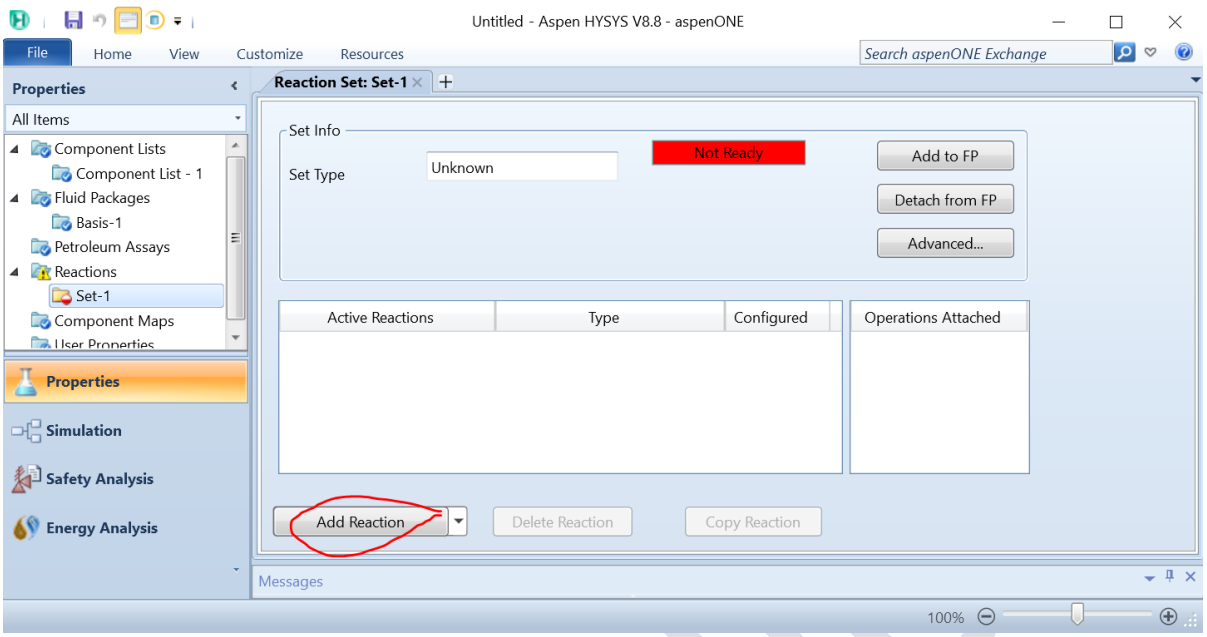

Figure 43. Add reactions

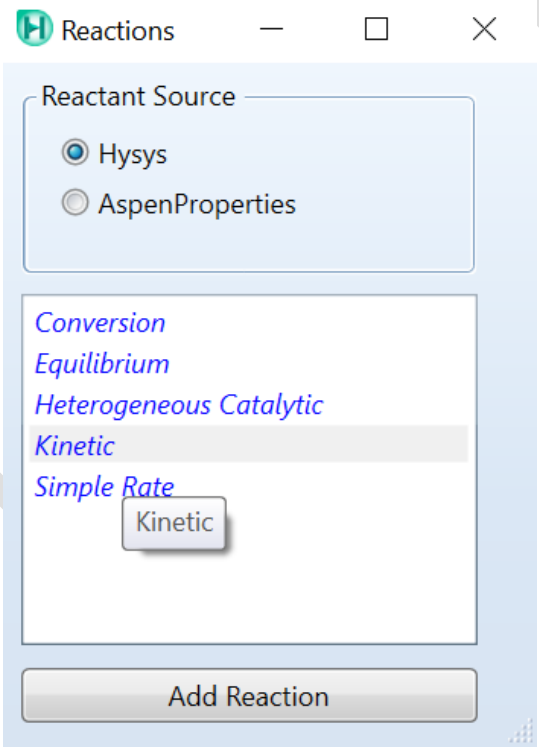

Figure 44. Choose the reaction type

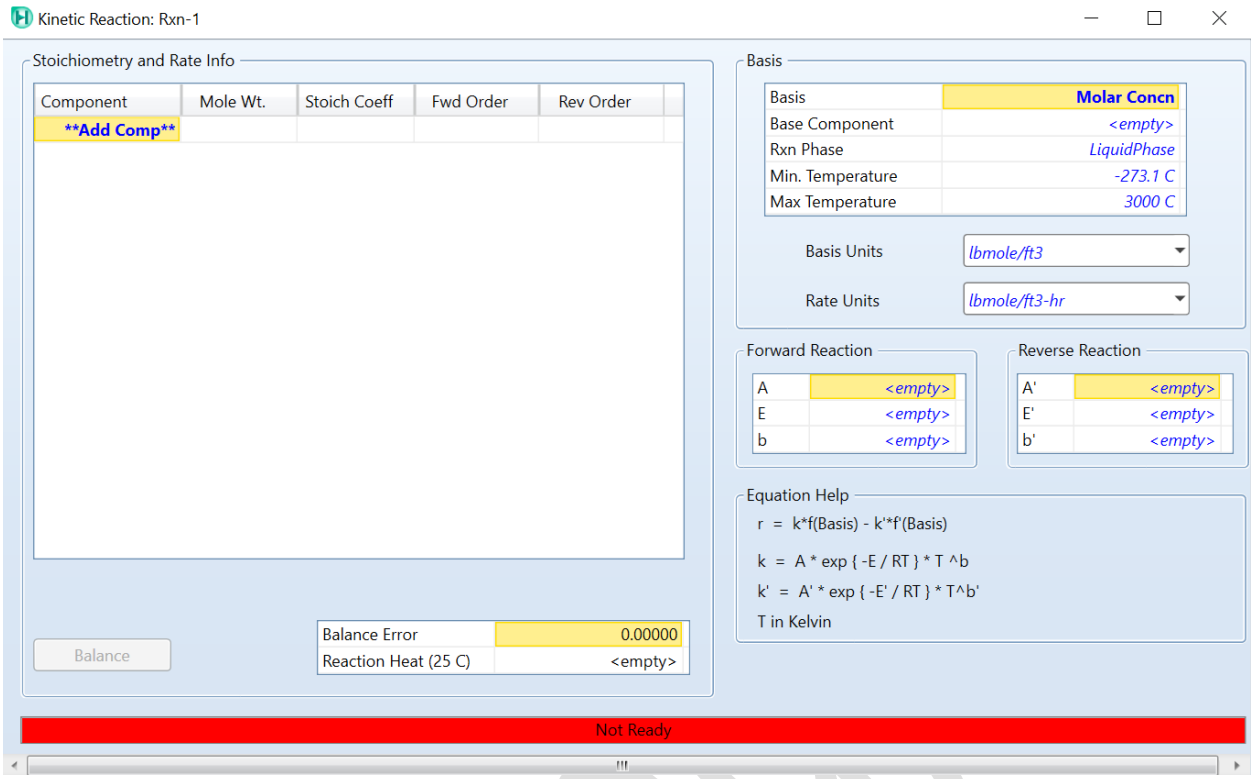

Figure 45. Insert the different parameters of the reaction

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

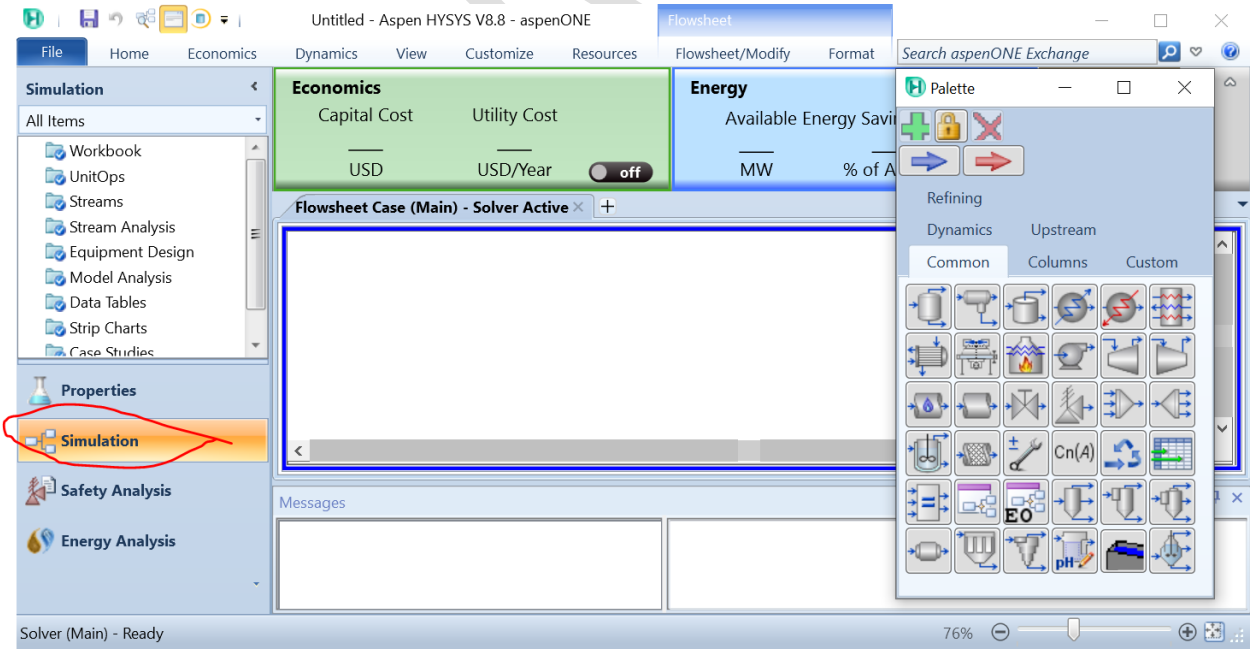

Figure 46. clicking on Simulation Icon

- **Add Reactor:** from the Palette, add a reactor by selecting the reactor type you want to simulate, in our case equilibrium reactor.

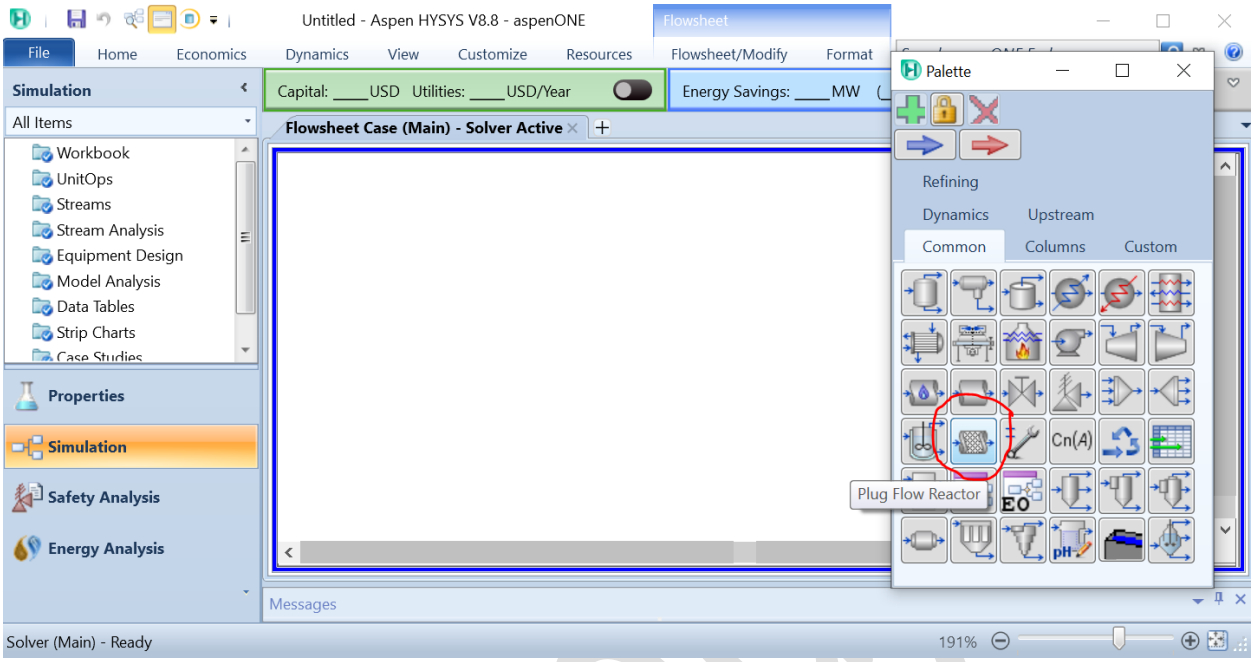

Figure 47. Plug flow reactor from the palette

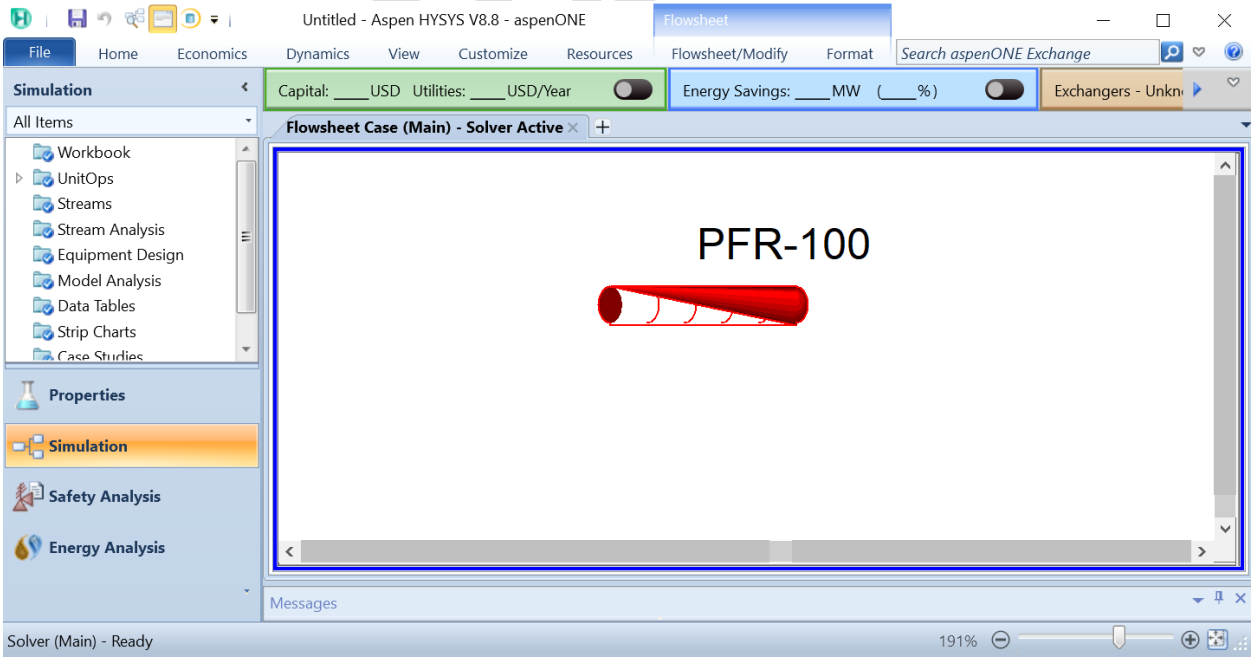

Figure 48. Add the reactor to the PFD

- **Set Operating Conditions:** Define the operating conditions of the reactor, such as temperature, pressure, and flow rates. These conditions significantly

impact the reaction rate and product formation.

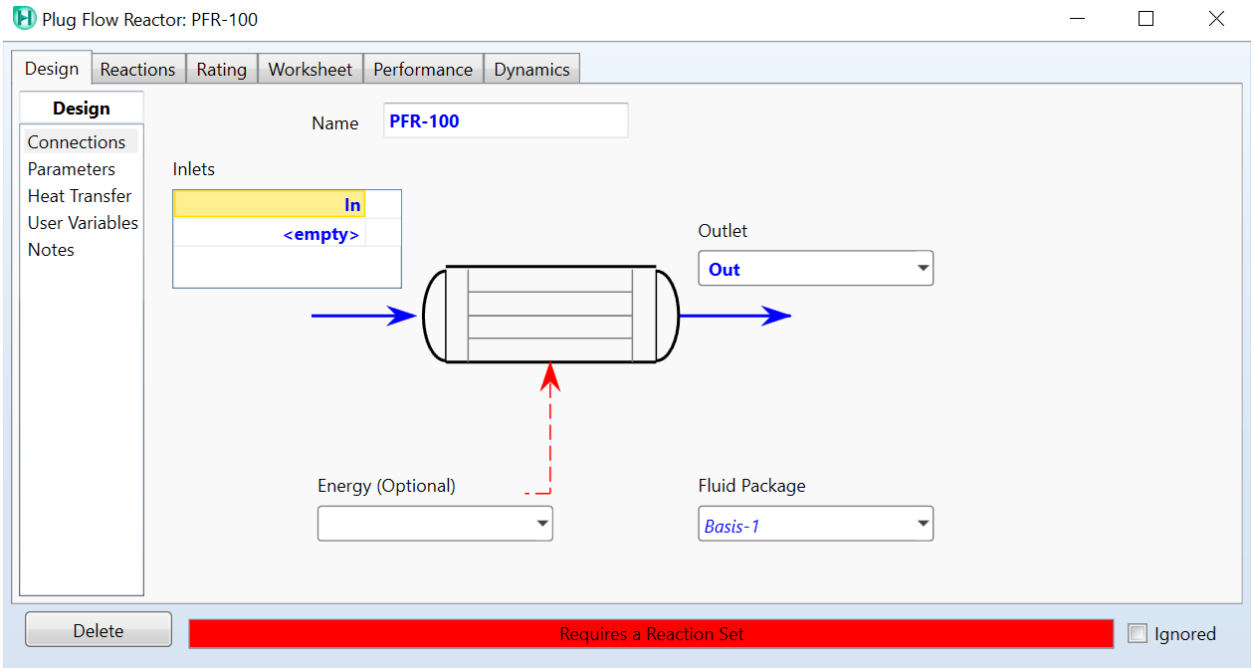

Figure 49. Setting the streams in the reactor

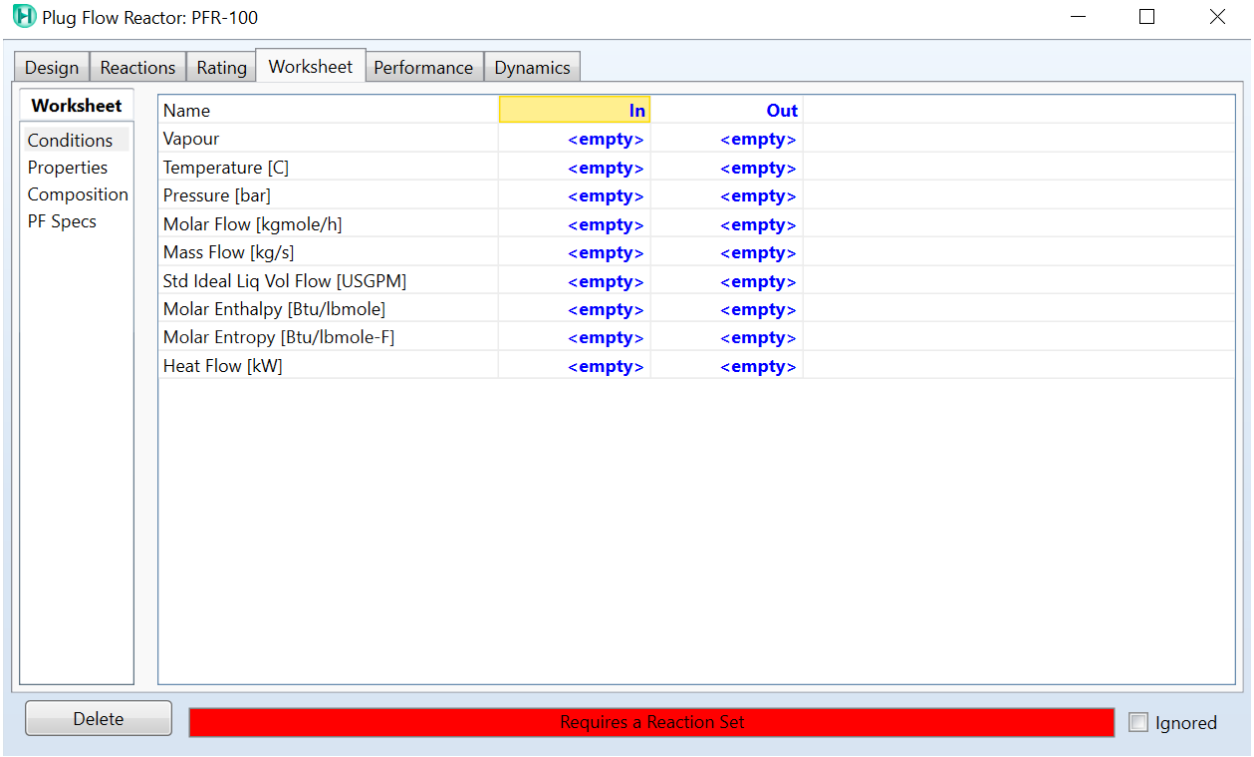

Figure 50. Insert the different parameters of the fluxes

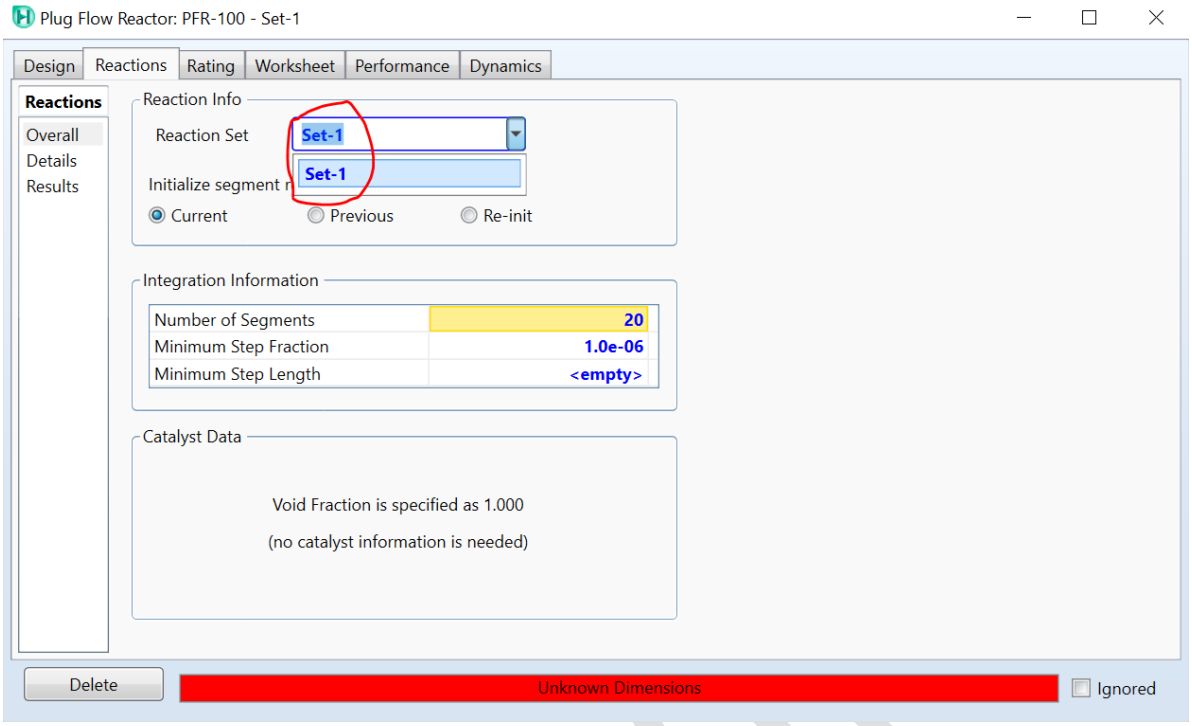

Figure 51. Adding reaction set

After adding the reaction set, it is necessary to add some associated parameters such as the length of the plug flow reactor, its diameter, and the pressure drops, in order to calculate the different related parameters, this could be discussed in details in the PW sessions.

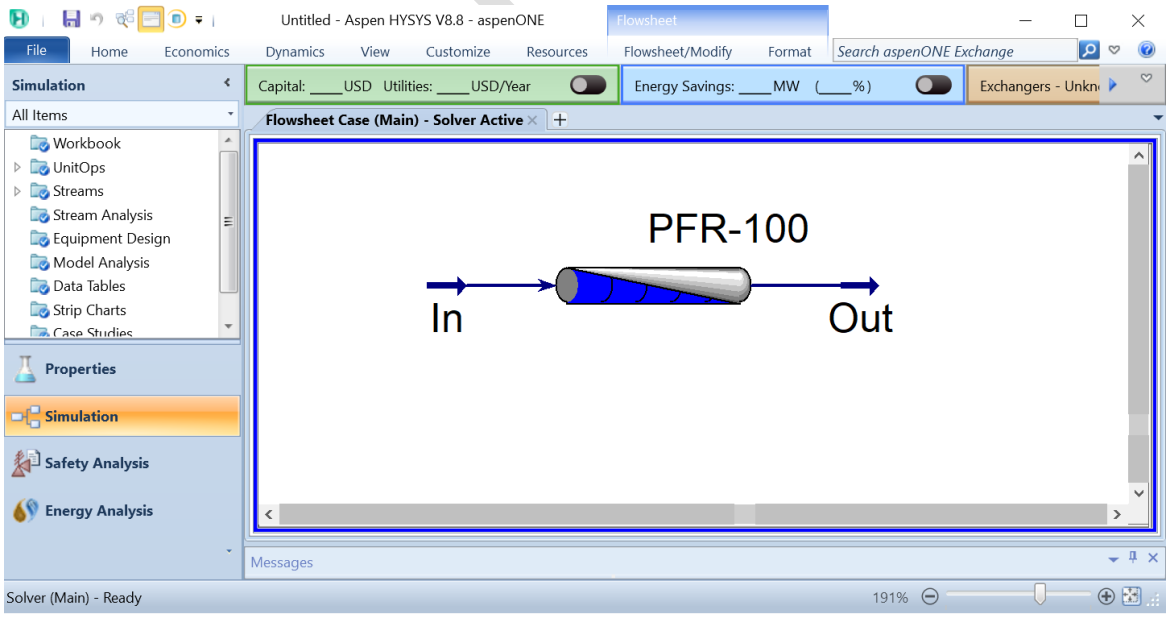

Figure 52. Getting the results

These steps provide a streamlined overview of simulating plug reactors within Aspen HYSYS. The precise procedures can differ depending on the unique characteristics of the reactor and the particular demands of the reaction. Aspen HYSYS proves to be a valuable resource for understanding and enhancing the efficiency of plug reactors, especially in scenarios where precise control and limited mixing are crucial for specific chemical reactions.

However, more details will be discussed and be practiced in the PW sessions, in which numerous examples of this type of reactor will be studied.

II-3-5- Catalytic reactors

Catalytic reactors are essential in many chemical processes where catalysts are used to facilitate chemical reactions, making them happen more efficiently and at lower temperatures. These reactors play a crucial role in industries such as petrochemicals, chemicals, and environmental engineering. Simulating catalytic reactors in Aspen HYSYS can help engineers and scientists understand and optimize these complex systems.

To simulate Catalytic reactors using Aspen Hysys, a series of steps must be adhered to, commence by initiating Aspen Hysys and choosing the component list and fluid package, following the prescribed sequence detailed in Figures 1 to 7. Following this, when defining the reaction type, ensure it corresponds to your distinct objectives and goals. For example, you might consider selecting a catalytic reaction type.

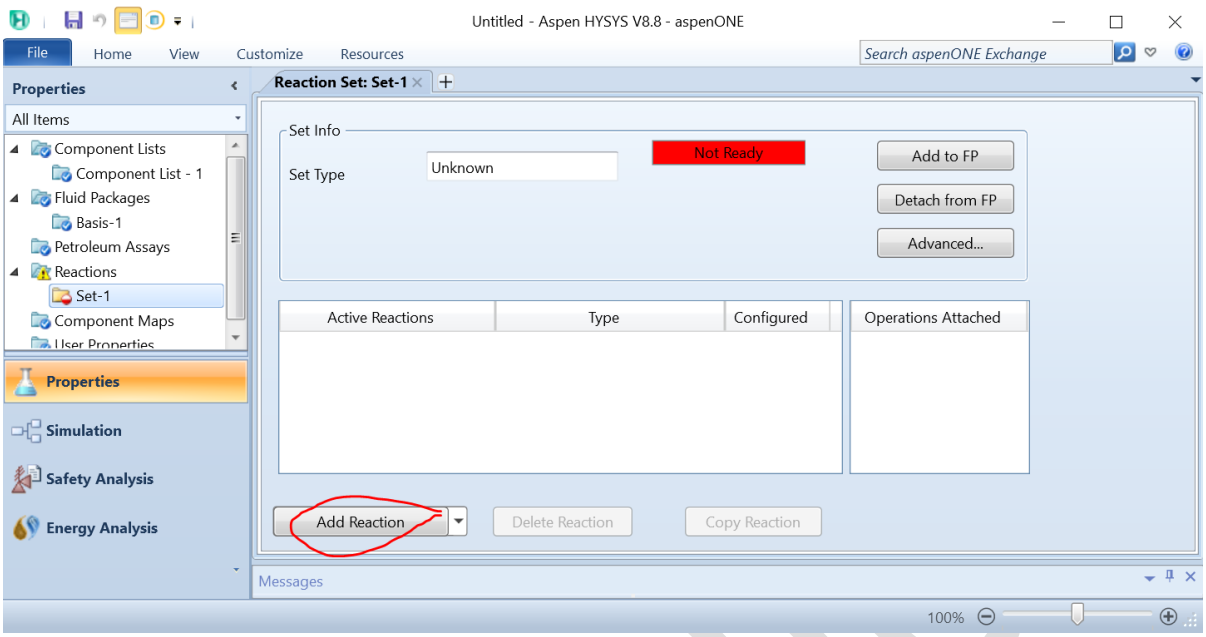

Figure 53. Add reactions

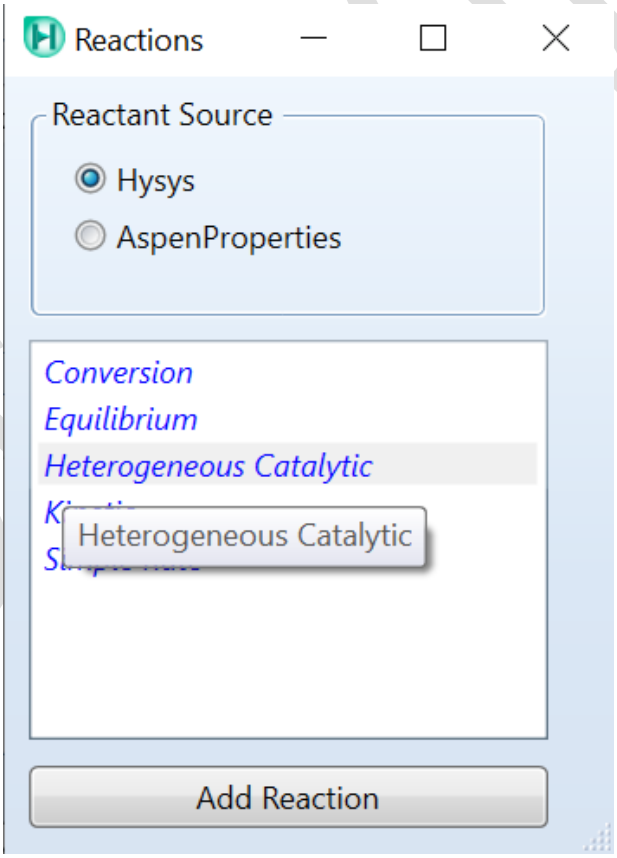

Figure 54. Choose the reaction type

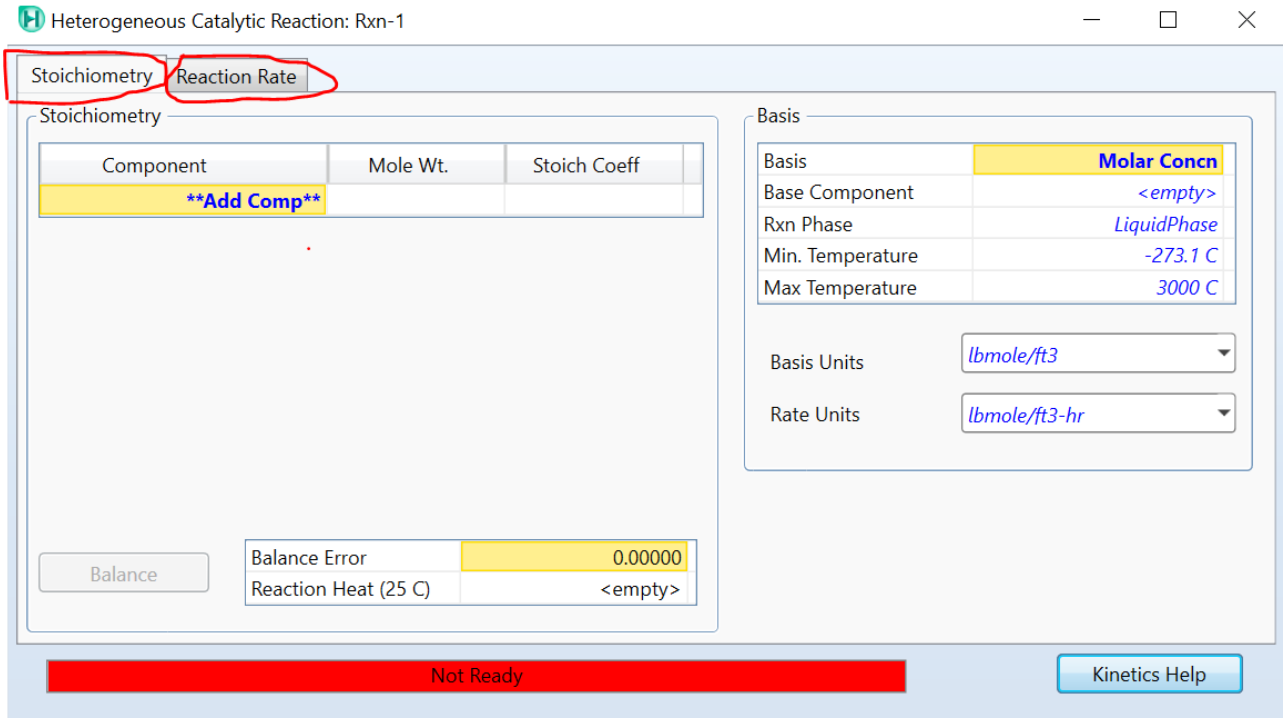

Figure 55. Insert the different parameters of the reaction

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

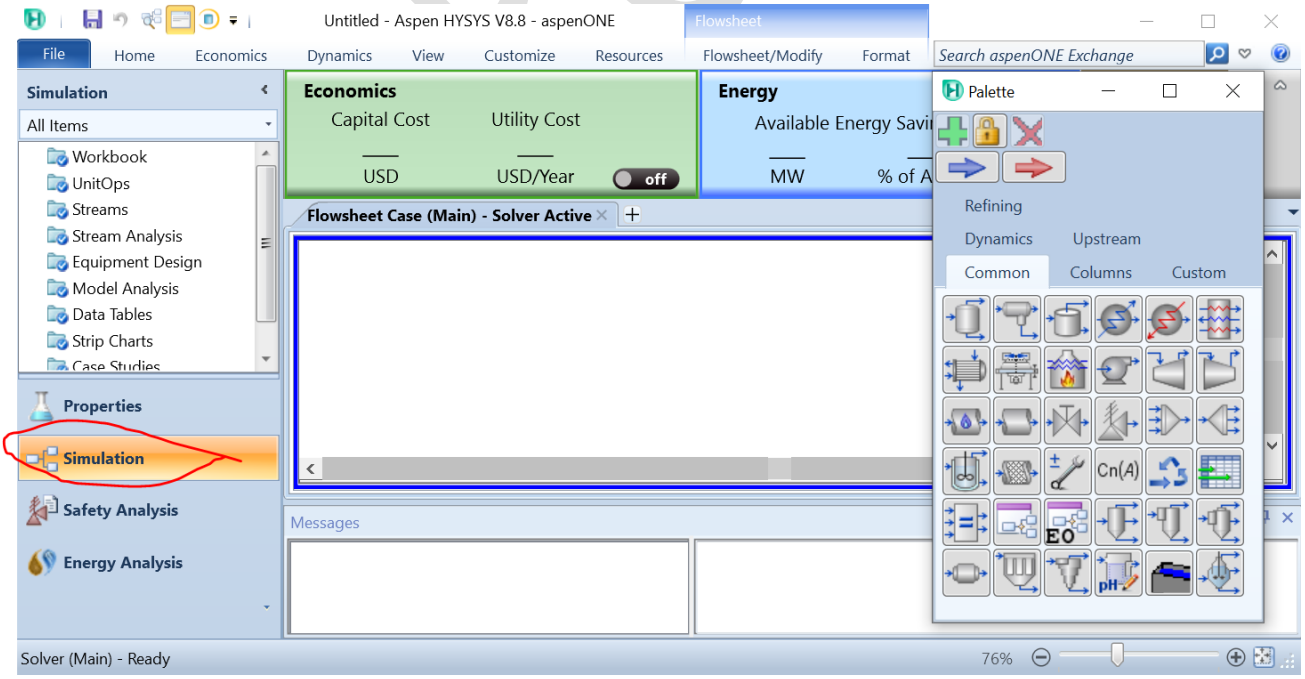

Figure 56. clicking on Simulation Icon

It is necessary to mention that a Plug Flow Reactor (PFR) is often chosen to simulate catalytic reactions in Aspen Hysys and other chemical engineering simulations for several reasons:

- ✓ **Realistic Representation:** PFR models provide a more realistic representation of the actual flow and behavior in a catalytic reactor. In a PFR, reactants flow through the reactor in a continuous, streamlined manner, which is often the case in real-world catalytic reactors.
- ✓ **Suitable for Complex Reactions:** PFRs can handle complex catalytic reactions involving multiple reactants and intermediates, making them versatile for a wide range of industrial applications.
- ✓ **Improved Mass and Heat Transfer:** PFRs promote better mass and heat transfer due to the one-dimensional flow, allowing for more precise modeling of reaction kinetics and heat exchange in catalytic systems.
- ✓ **Enhanced Residence Time Control:** PFRs enable precise control of reactant residence time, which is crucial in catalytic reactions to optimize conversion and selectivity.
- ✓ **Easy Implementation:** Aspen Hysys and similar simulation software typically offer built-in models for PFRs, making it relatively straightforward to set up and analyze catalytic reactions in a PFR configuration.
- ✓ **Effective Parameter Tuning:** PFR models allow for the adjustment of key parameters like reactor length, flow rates, and reaction kinetics to optimize reactor performance and meet specific process goals.

In summary, the choice of a Plug Flow Reactor in Aspen Hysys for simulating catalytic reactions is driven by its ability to provide a realistic representation of catalytic systems, enable complex reaction modeling, offer control over residence time, and facilitate parameter tuning for process optimization.

- ➢ **Add Reactor:** from the Palette, add a reactor by selecting the reactor type you want to simulate, in our case equilibrium reactor.

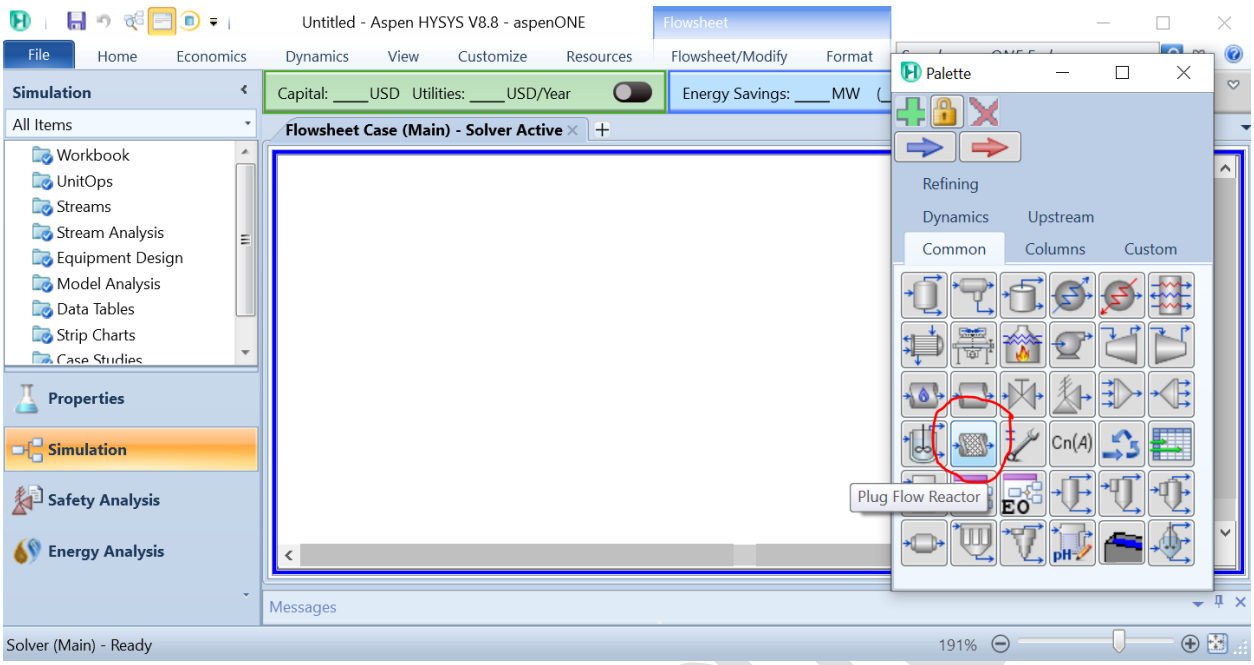

Figure 57. Plug flow reactor from the palette

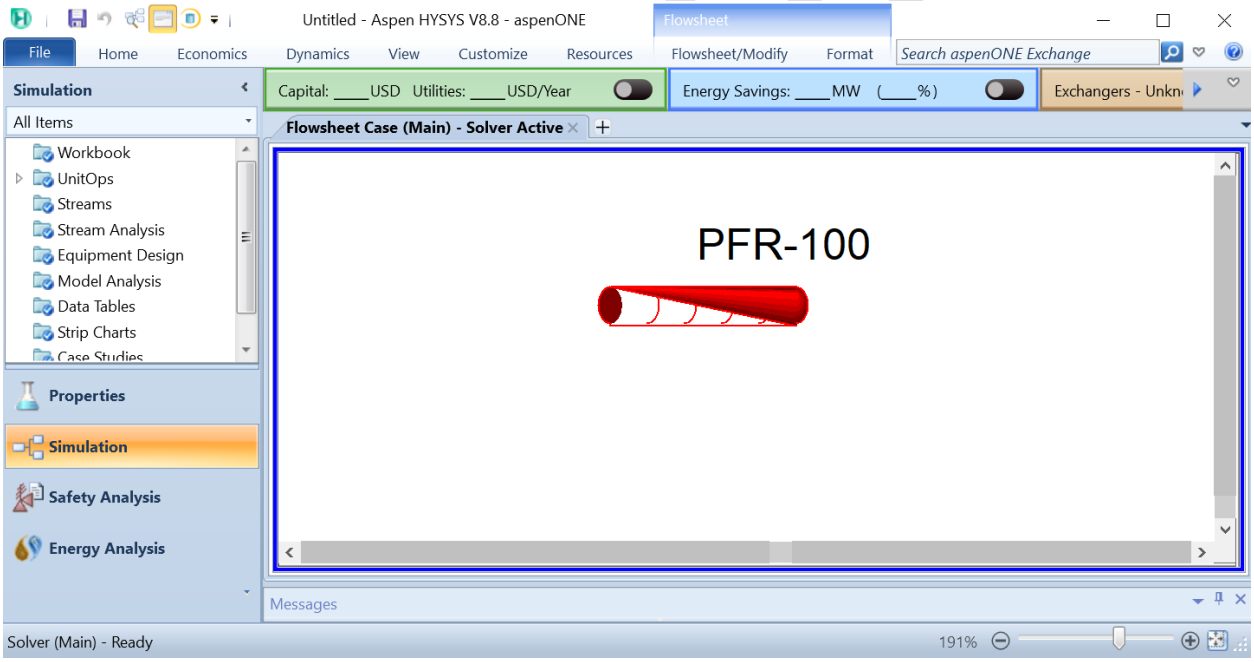

Figure 58. Add the reactor to the PFD

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

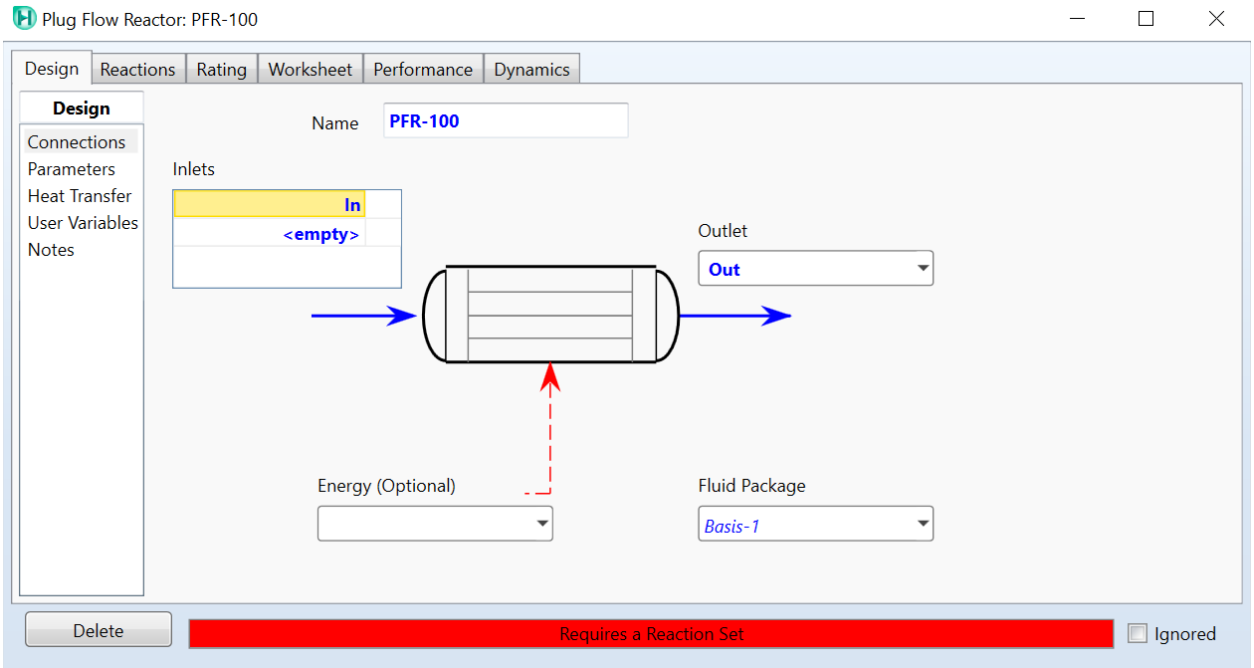

Figure 59. Setting the streams in the reactor

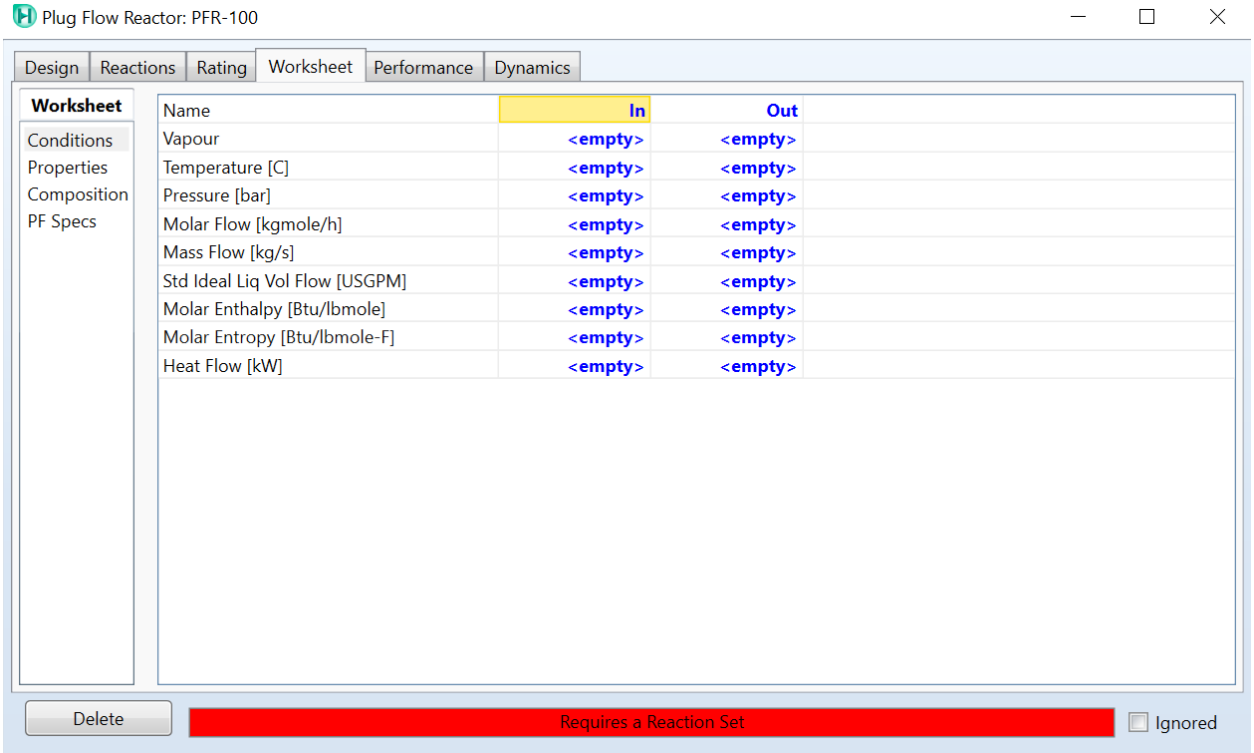

Figure 60. Insert the different parameters of the fluxes

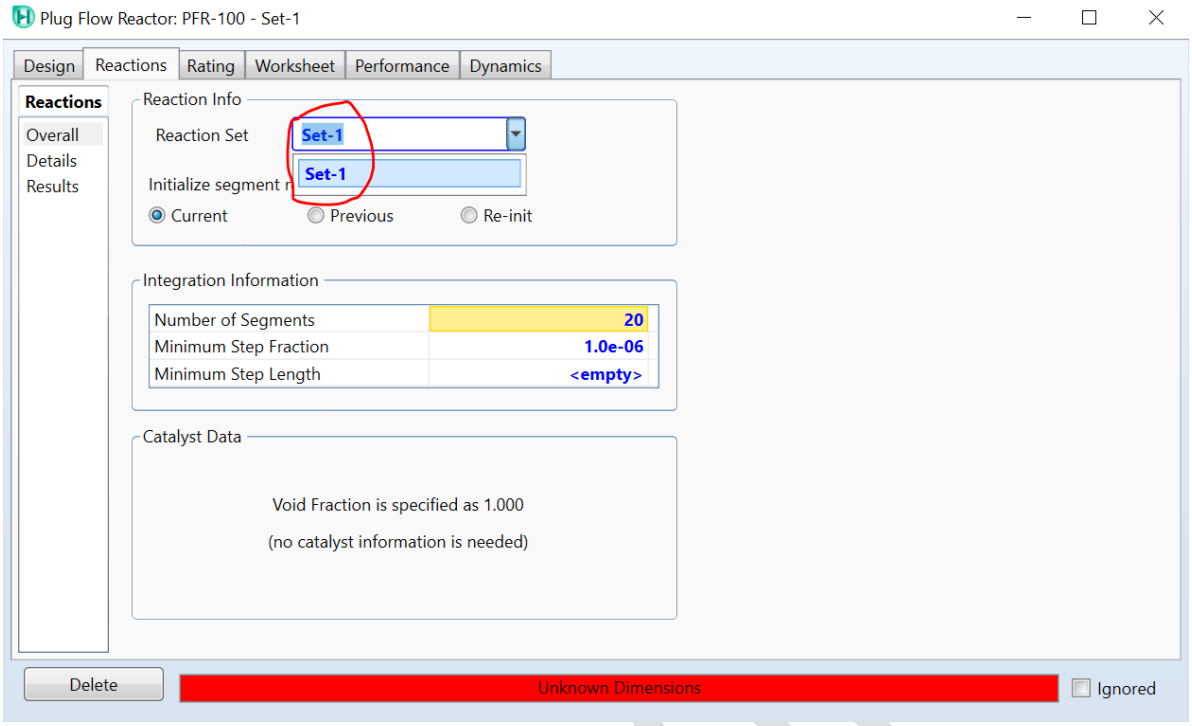

Figure 61. Adding reaction set

After adding the reaction set, it is necessary to add some associated parameters such as the length of the plug flow reactor, its diameter, and the pressure drops, in order to calculate the different related parameters, this could be discussed in details in the PW sessions.

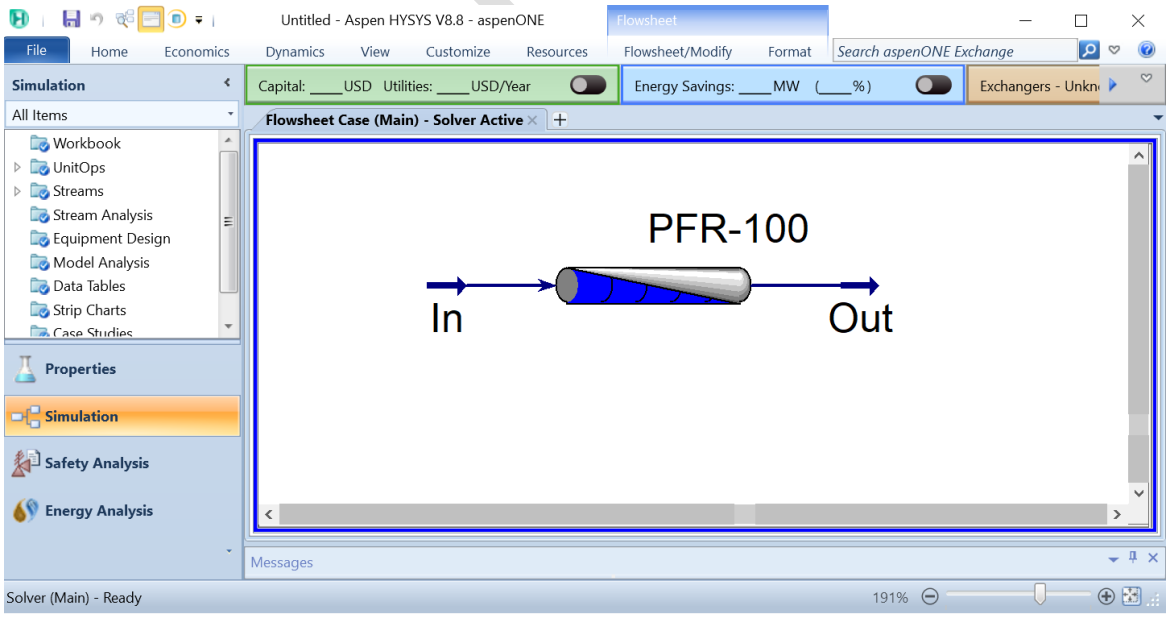

Figure 62. Getting the results

These steps offer a simplified guide to simulating catalytic reactors using Aspen HYSYS. Keep in mind that the specifics can vary based on the particular reactor and catalytic reactions you are working with. Aspen HYSYS serves as a valuable tool for understanding and optimizing the performance of catalytic reactors, ensuring that chemical processes are carried out efficiently and cost-effectively in various industries.

However, more details will be discussed and be practiced in the PW sessions, in which numerous examples of this type of reactor will be studied.

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Alexandre C. Dimian, Costin Sorin Bildea, Chemical Process Design: Computer-Aided Case Studies, John Wiley & Sons, Apr 2008 - 527 pages.

Computer-aided Industrial Process Design: The ASPEN Project: Functional Specifications for ASPEN, Sixth Quarterly Progress Report, Department of Chemical Engineering and Energy Laboratory, Massachusetts Institute of Technology Cambridge.

Juma Haydary, Chemical Process Design and Simulation: Aspen Plus and Aspen Hysys Applications, Willey, ISBN: 978-1-119-08911-7, January 2019, 448 Pages.

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