EPFL

Co-electrolysis process in Aspen Plus®

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17/03/2025

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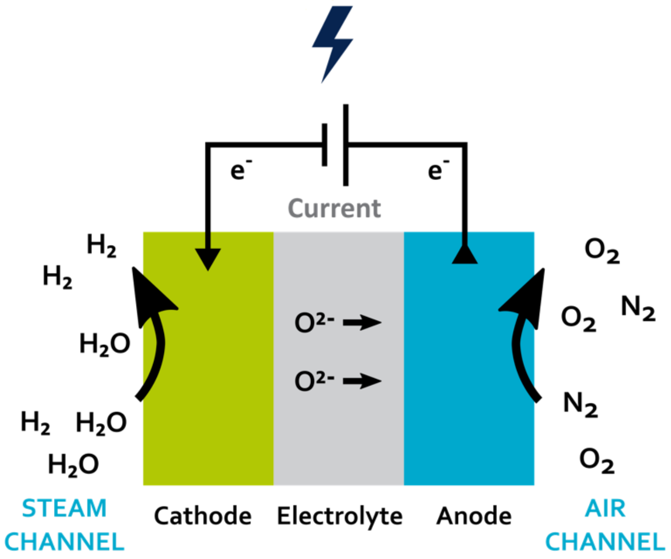
General information on Co-electrolyzer

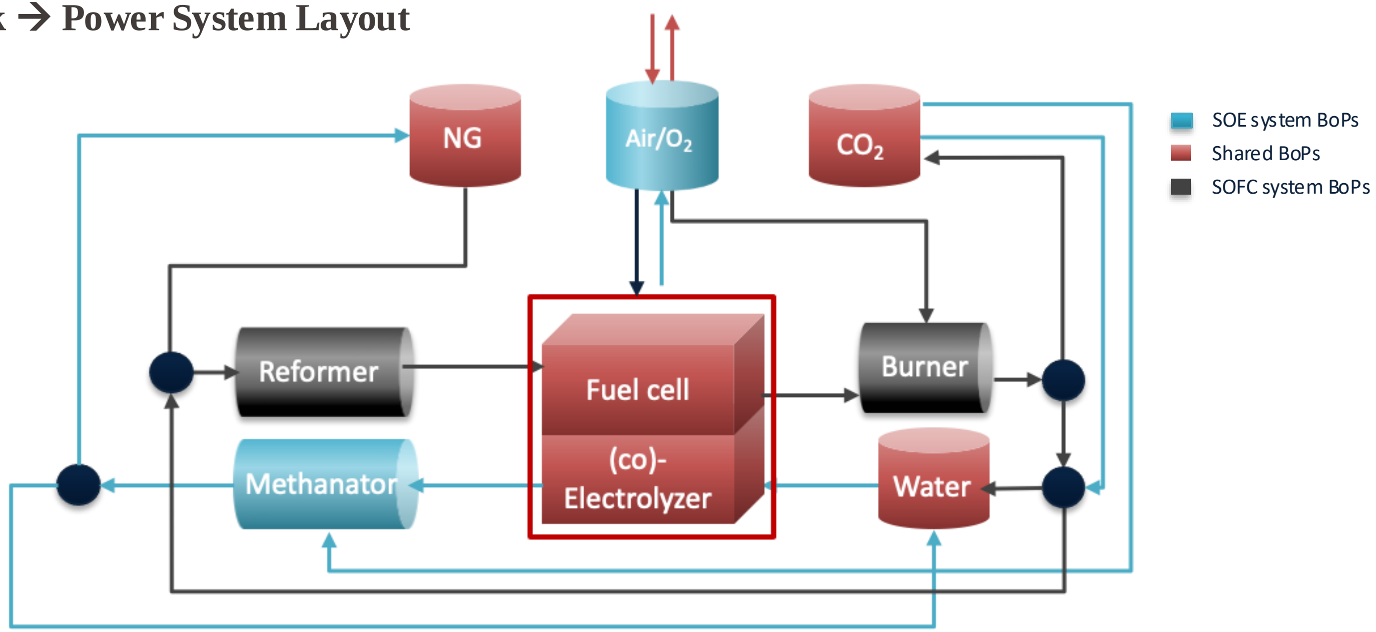
- Electrochemical reduction of H_2O and/or CO_2
- Solid Oxide Electrolyte at high temperature (> 700°C)
- High Temperature:
  - Good conversion efficiency
  - Challenges for integration
  - Necessitate clever heat integration
- Production of H_2 or Syngas and O_2 which are all 3 valuable products
- 3 operation modes:
  - Endothermic (need heat at high T)
  - **Thermoneutral (High T heat is balanced)**
  - Exothermic (outputs heat at high T)
- SOC stack is reversible (can operate in fuel cell mode as well)

Electrolyser mode



General information on Power – X – Power (rSOC)

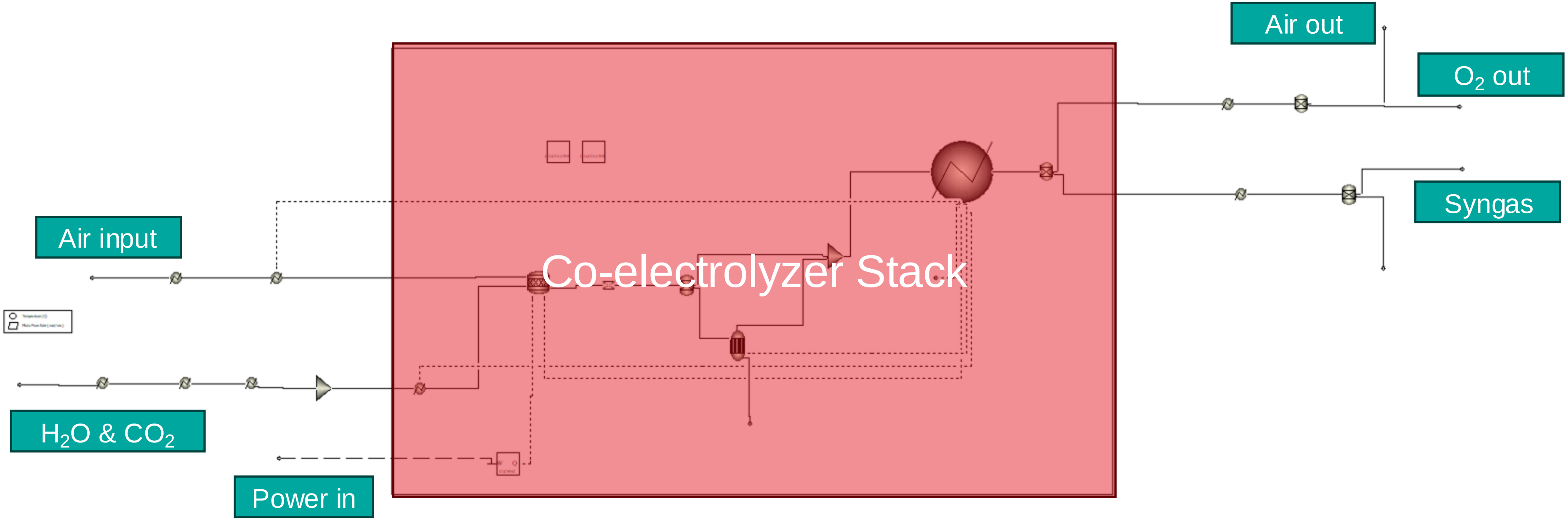
Power → NG Tank → Power System Layout



- When renewable electricity is available, methane can be produced *via* electrolyzer-methanation unit.
- When system requires electricity, it can be produced *via* reformer-fuel cell-burner unit.
- Oxy-combustion is considered in fuel cell system (to avoid presence of N_2).
- High temperature heat is available

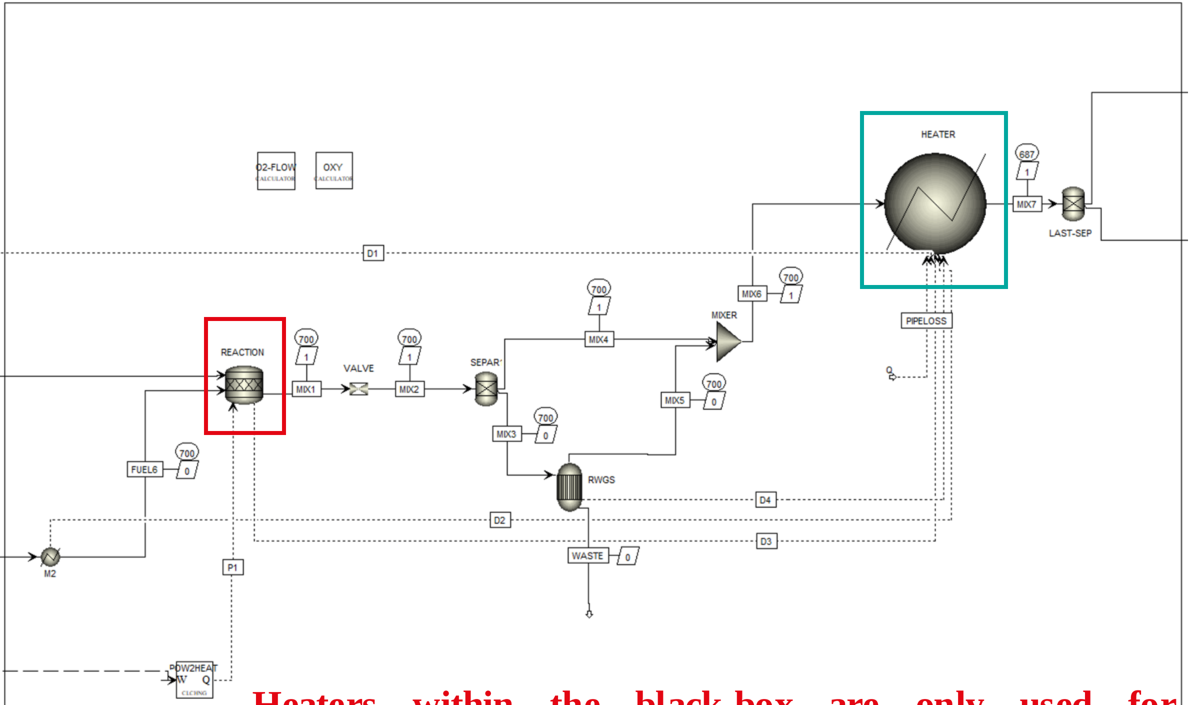
Co-electrolyzer Aspen layout

Power → H_2 / Syngas via Solid Oxide Electrolyzer (SOE)



Co-electrolyzer Aspen layout

Solid Oxide Electrolyzer (SOE) – Thermoneutral operation



Heaters within the black-box are only used for simulation, no need to include them into heat integration

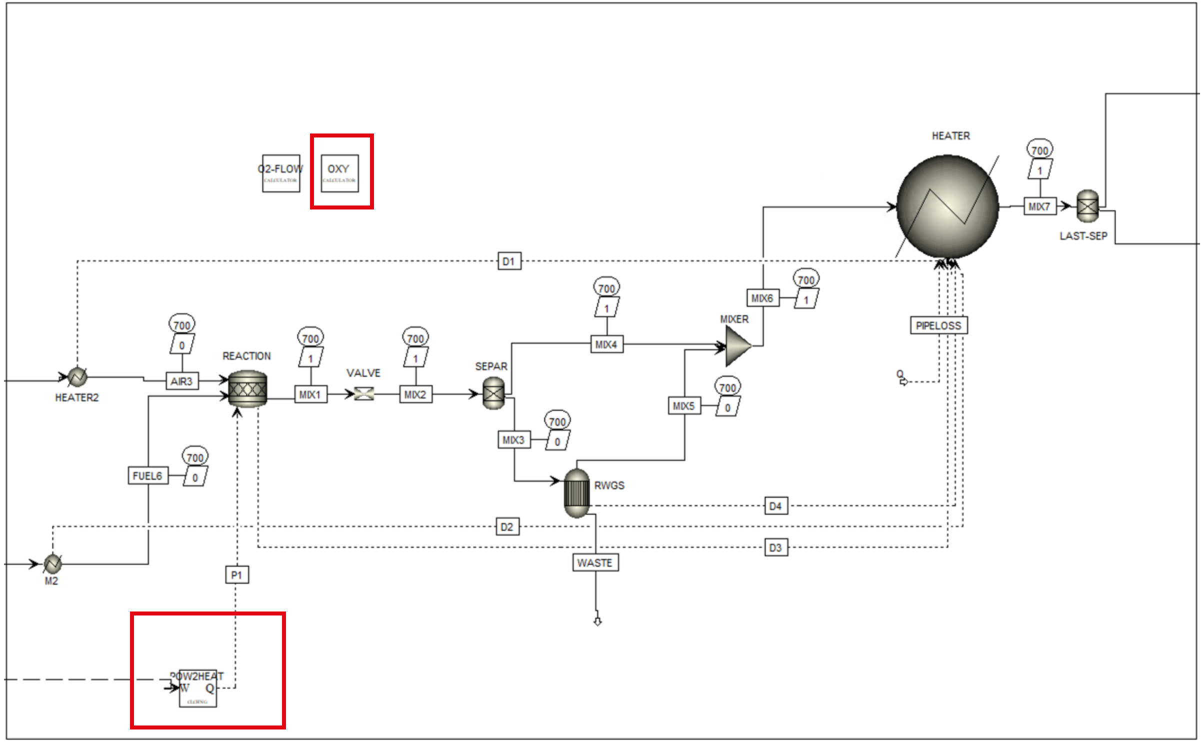
- No need to modify SOE stack model in your project.
- "REACTION" reactor contains main co-electrolysis reactions.

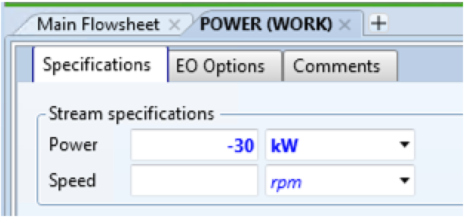
Fractional conversion	Fractional Conversion of Component	Stoichiometry
0.85	H2O	H2O --> H2(MIXED) + 0.5 O2(MIXED)
0.85	CO2	CO2 --> CO(MIXED) + 0.5 O2(MIXED)

- "HEATER" is used to count the heat within the stack.
- The HEATER will have a heat output of 0 kW (thermoneutral operation)

Co-electrolyzer Aspen layout

Solid Oxide Electrolyzer (SOE)

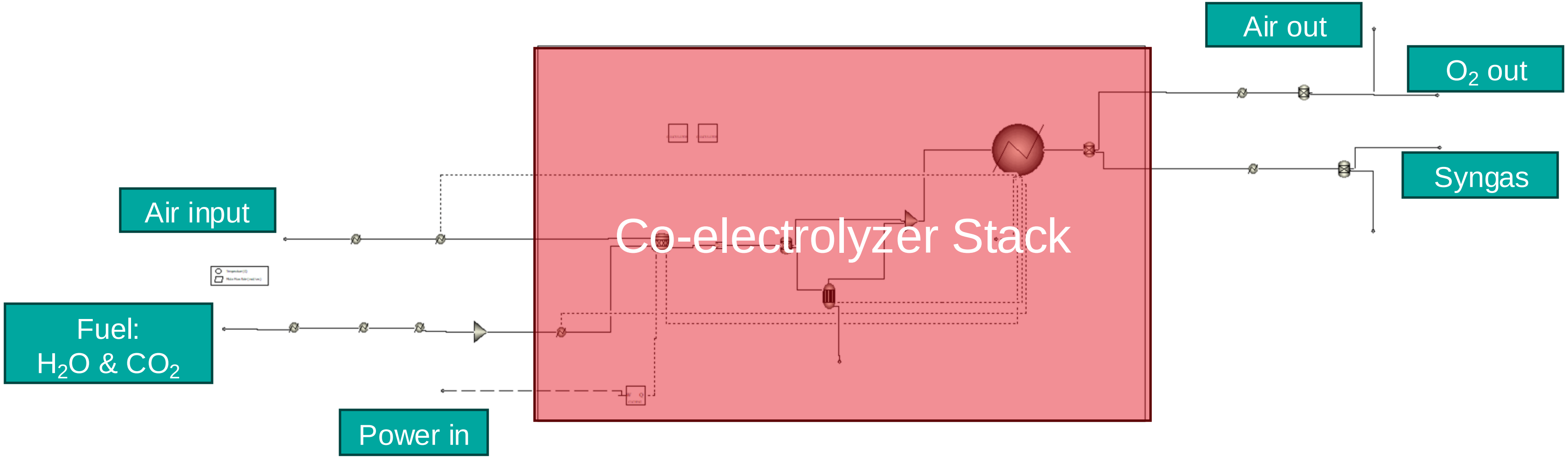




- Power input in current file is 30 kW. (negative as input)
- When you change the electrolyzer power input, the fuel flow rate "FUEL1" will be automatically updated by "OXY" calculator - **no need to change by yourself.**

Co-electrolyzer Aspen tutorial layout

1. Uniformize all up-stream temperatures (through calculator block)
2. Understand fuel heating-up process (differentiate heaters)
3. Ensure thermoneutral operation (T_SOEC_in == T_SOEC_out) through design specification
4. Apply technical constraint on O_2/Air flow through design specification
5. Define a variable to tune the H2O/CO2 ratio in the fuel. (in class)
6. Define the right stoichiometric number for further syngas usage (in class)



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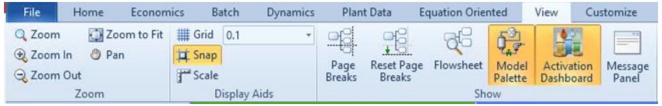
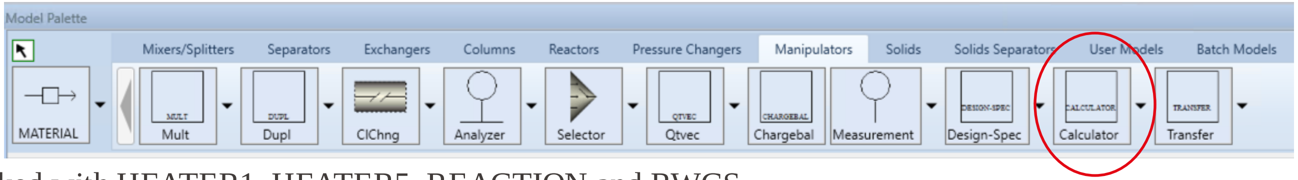
Co-electrolyzer Aspen modelling

Step 1: Set SOEC upstream components temperature into 700 °C via calculator

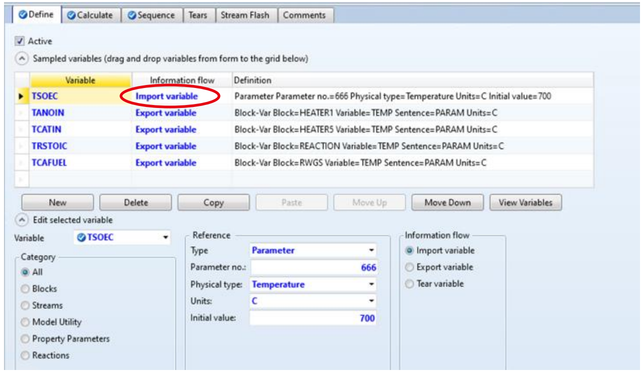
- Go to View → Model Palette

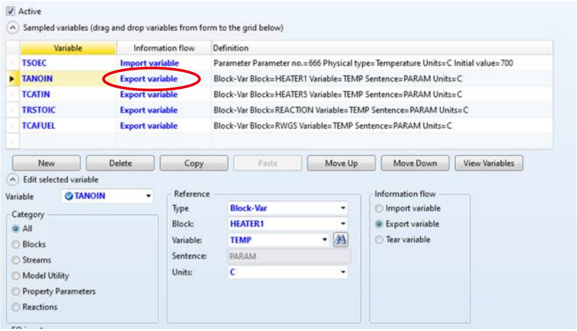


- Go to Manipulators → Calculator
  - Name calculator "SET-TSOE"



- Target: Set a parameter which is linked with HEATER1, HEATER5, REACTION and RWGS
  - Define a new **parameter** "TSOEC", select it to be the "import variable".
  - Import variable is the input from user.
  - Export variable is the output from the calculator, it gives the order to ASPEN.

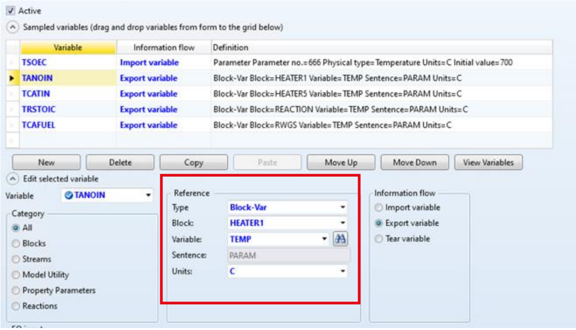




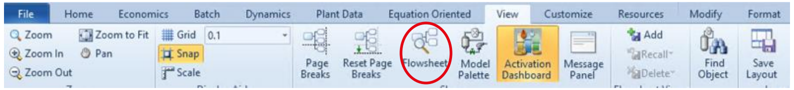
By adding this calculator, if we want to change the stack inlet T, we only need to change Parameter – "TSOEC"

Co-electrolyzer Aspen modelling

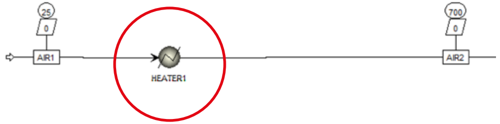
Question: What if we are not sure about “Reference”?

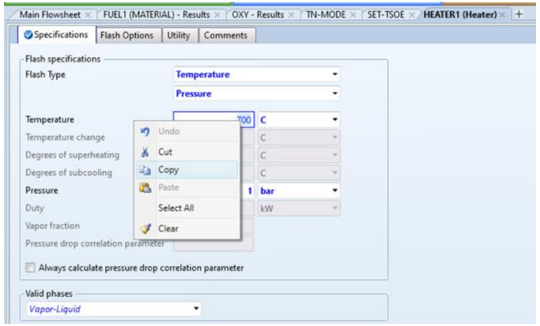


- Go to Flowsheet



- Find “HEATER1” → “Temperature” → Select value → “Copy”



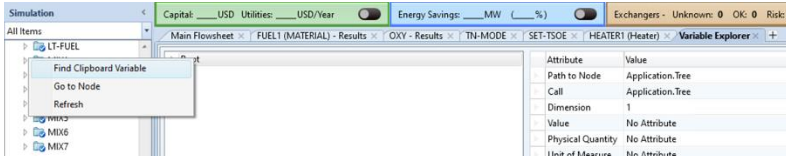


Co-electrolyzer Aspen modelling

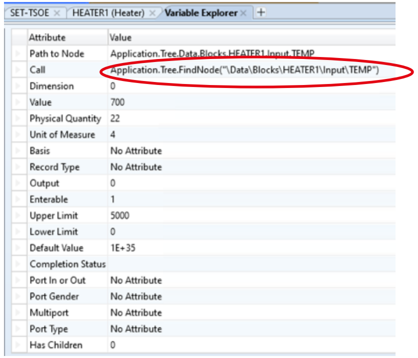
Question: What if we are not sure about “Reference”?

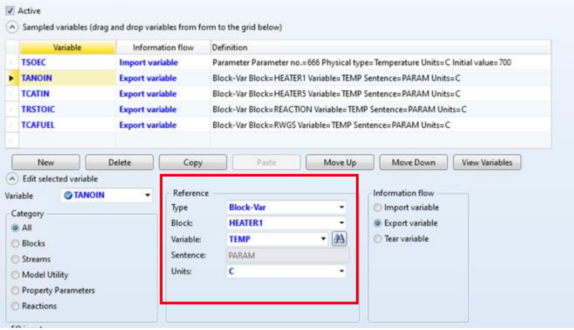
- Go to Customize → Variable Explorer

- Go to Variable Explorer → Right Click “Root” → “Find Clipboard Variable”



- “Call” → the “path” of one variable → Provide hint for “Reference”

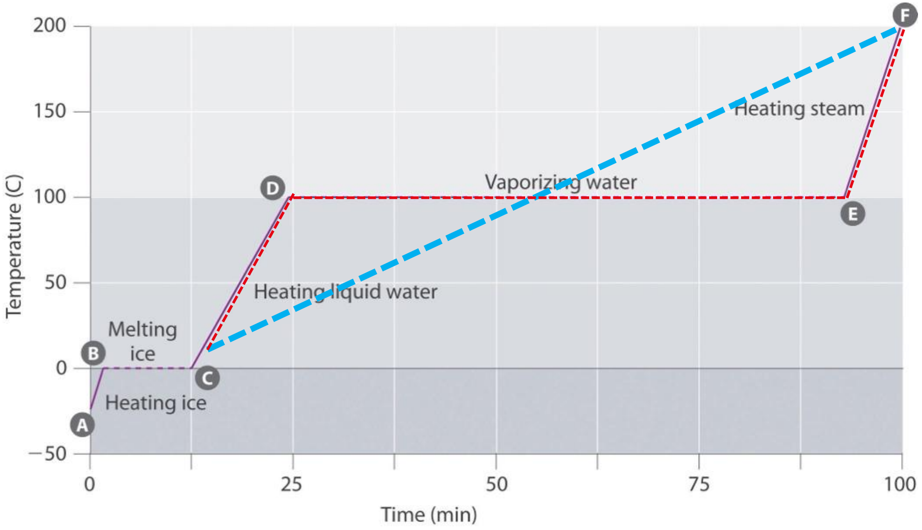




Co-electrolyzer Aspen modelling

Step 2: Set "Fuel" heating up process

- "Fuel1" contains CO_2, H_2O → How to heat it up?
  - CO_2 is easy to be heated up, as it is gas.
  - Water has three stages in heating up process: Liquid heating, evaporation, steam superheating



If only 1 heater was used:

inlet T, outlet T and average cp → linear interpolation

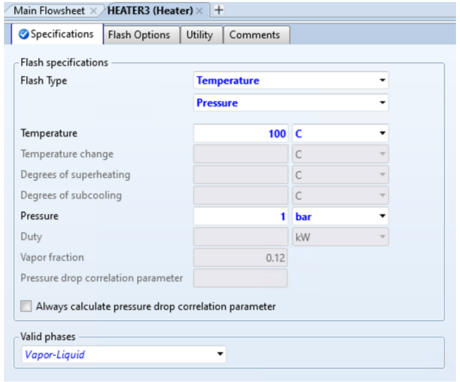
3 Three heaters:

To capture each stage temperature changing and the duties

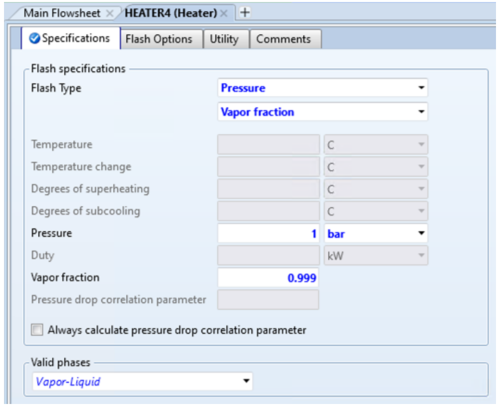
Co-electrolyzer Aspen modelling

Step 2: Set “Fuel” heating up process

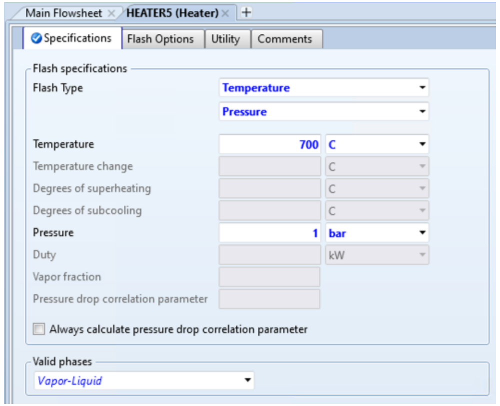
- If “Fuel1” only contains H_2O
  - HEATER3



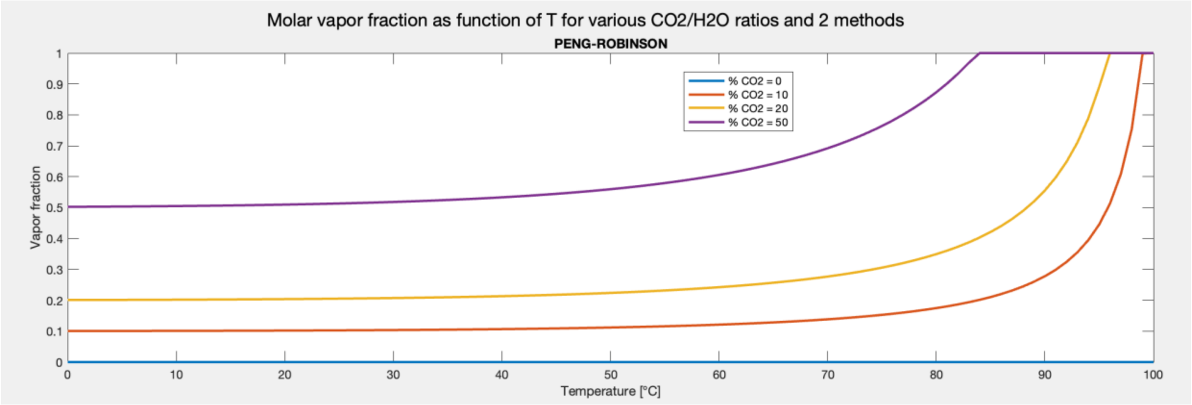
- HEATER4



- HEATER5



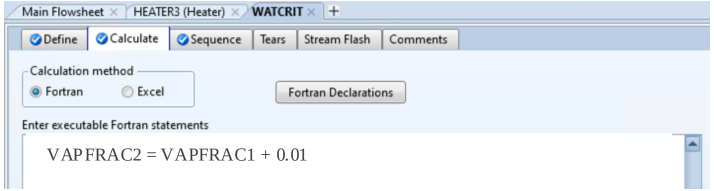
- If “Fuel1” contains both H_2O and CO_2 → “HEATER3” needs to be updated → Boiling point of H_2O will change as the pressure change

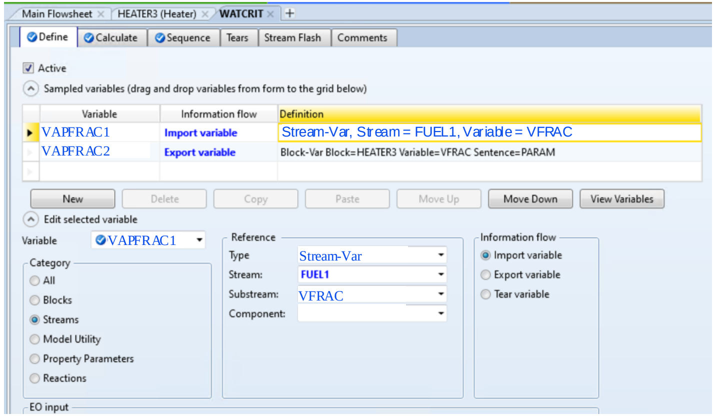


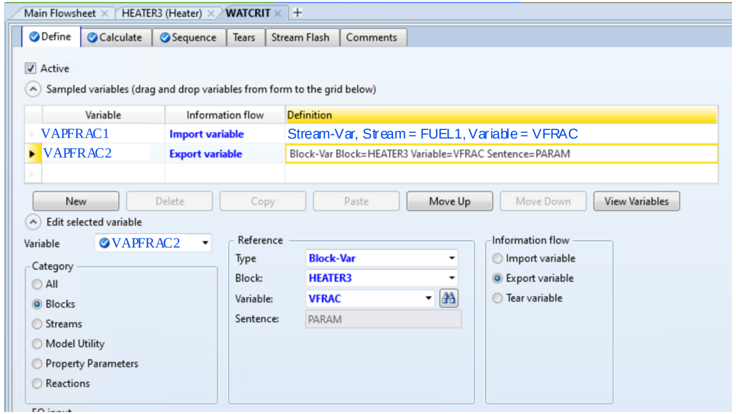
Co-electrolyzer Aspen modelling

Step 2: Set “Fuel” heating up process

- ➢ After “HEATER3”, H_2O is going to evaporate further → stream “FUEL2” vapor fraction shall be slightly higher than “FUEL1”
- ➢ Add a calculator, name it as “WATCRIT”
  - Import “FUEL1” vapor mole fraction as “VAPFRAC1”
  - Export “HEATER3” vapor fraction as “VAPFRAC2”
  - “HEATER3” vapor fraction = “FUEL1” vapor mole fraction + 0.01



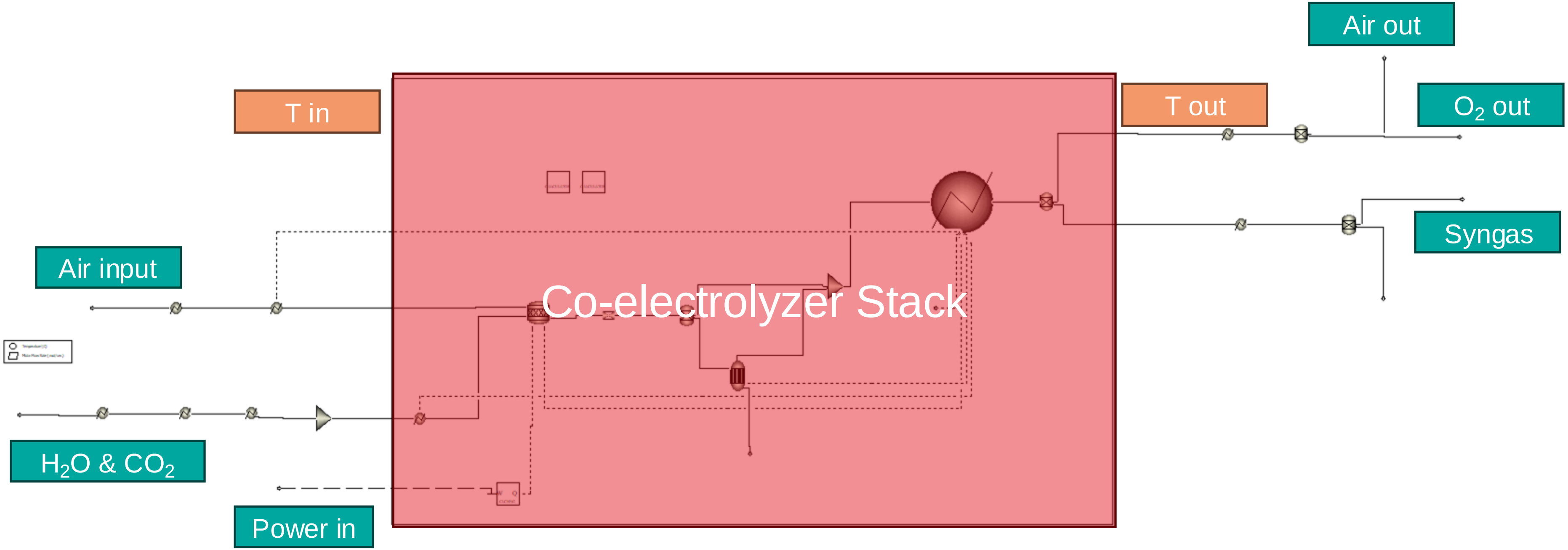




- Note: “HEATER3” shall have pressure and vapor fraction as the specifications, otherwise, calculator CAN NOT give order

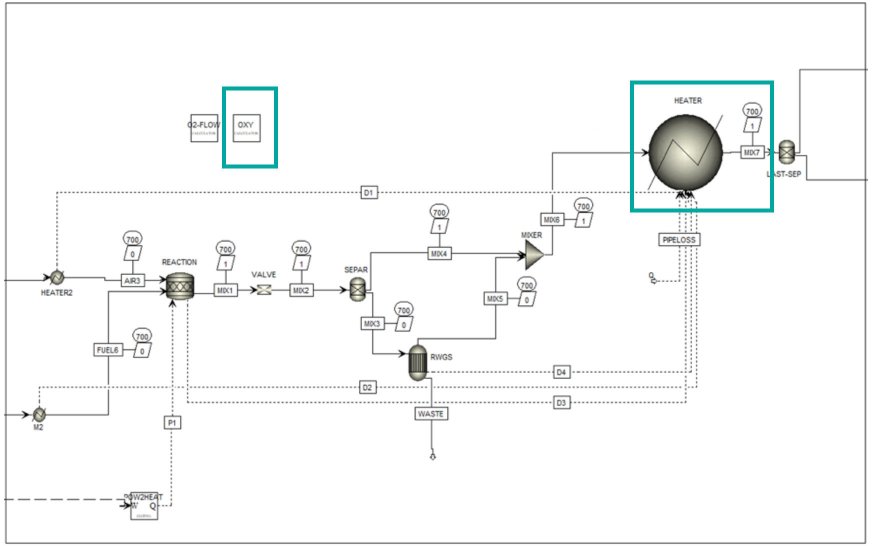
Co-electrolyzer Aspen layout

Step 3: operate in thermoneutral mode, dictated by the operating voltage applied

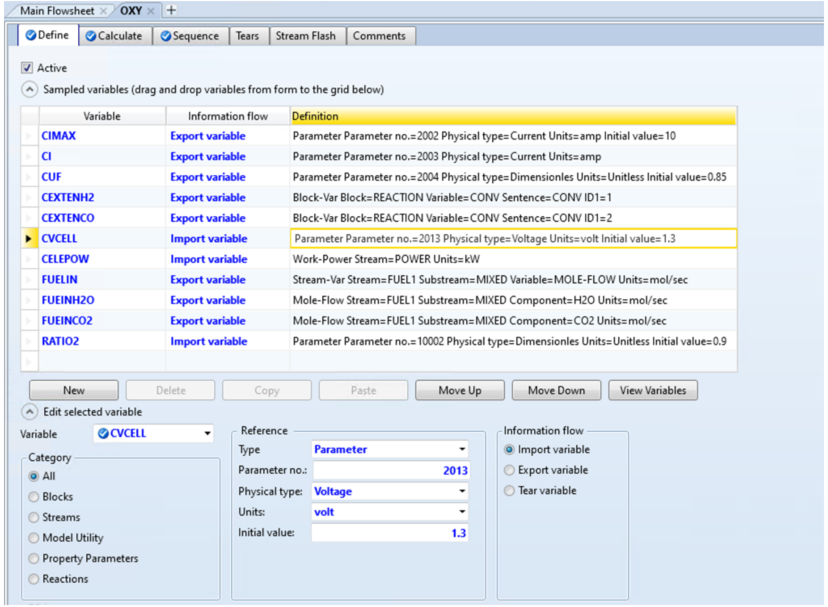


Co-electrolyzer Aspen layout

Solid Oxide Electrolyzer (SOE)



- ➢ "CVCELL" IN "OXY" calculator is an **"Import variable"**, it is used as a **parameter** to influence SOE outlet T – "MIX7".

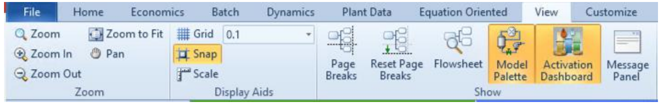


- ➢ We have defined a calculator for the inlet T of SOE, how about the outlet T of SOE?
- ➢ "HEATER" is used to count all the heat within the stack and calculate the outlet T of SOE.

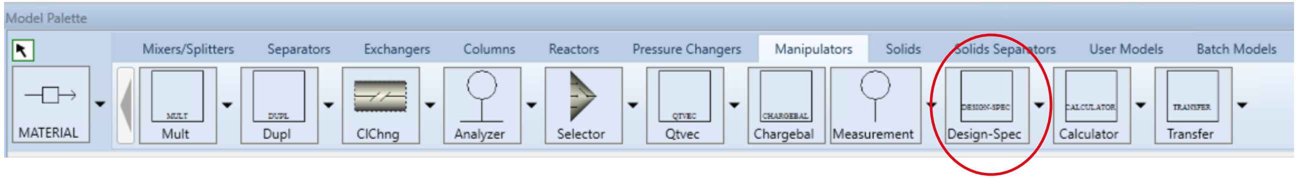
Co-electrolyzer Aspen modelling

Step 3: Create a design specification block, which is able to make SOE inlet T = SOE outlet T

- Go to View → Model Palette



- Go to Manipulators → Design-Spec
  - Name it as "TN-MODE"



- Target: "MIX7" temperature = "FUEL4" temperature, by varying "CVCELL"
  - "FUEL4" temperature is fixed by the previous calculator
  - "MIX7" temperature is calculated by using "CVCELL" parameter value
  - The temperature difference of these two streams shall be 0 by varying CVCELL value

Co-electrolyzer Aspen modelling

Step 3: Create a design specification block, which is able to make SOE inlet T = SOE outlet T

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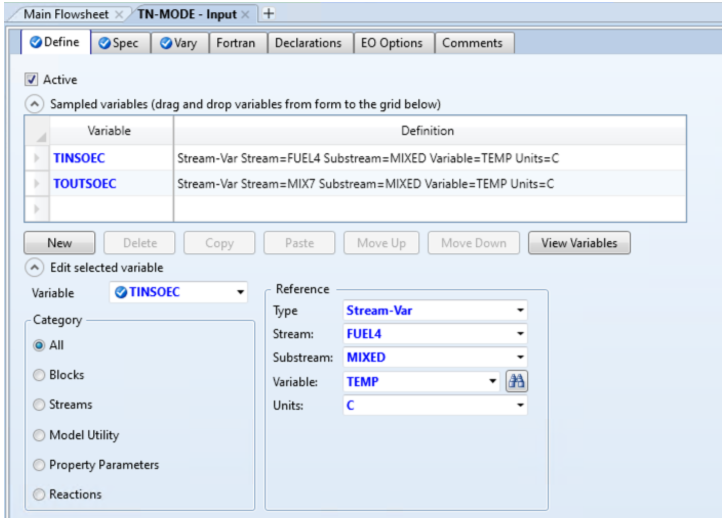
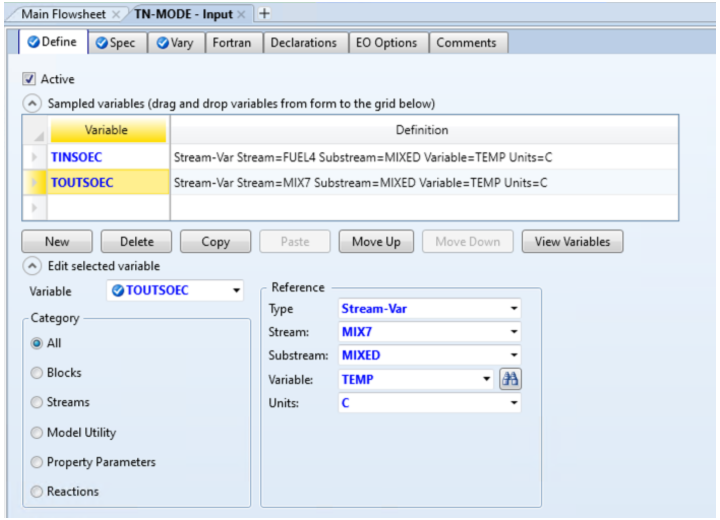
- Define SOEC inlet T



- Define SOEC outlet T



Co-electrolyzer Aspen modelling

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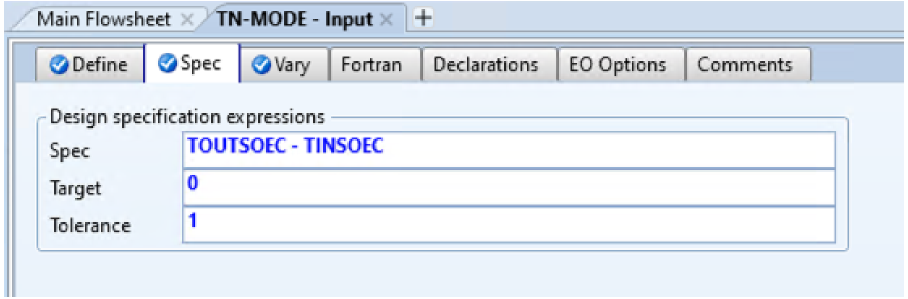
- Set target/objective of this design **specification**



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Co-electrolyzer Aspen modelling

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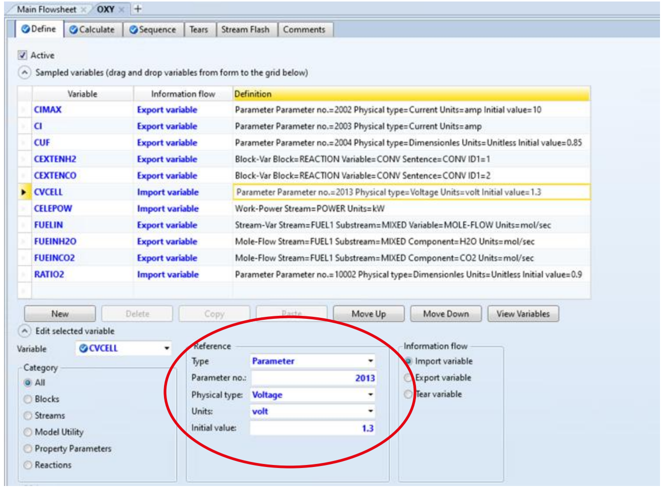
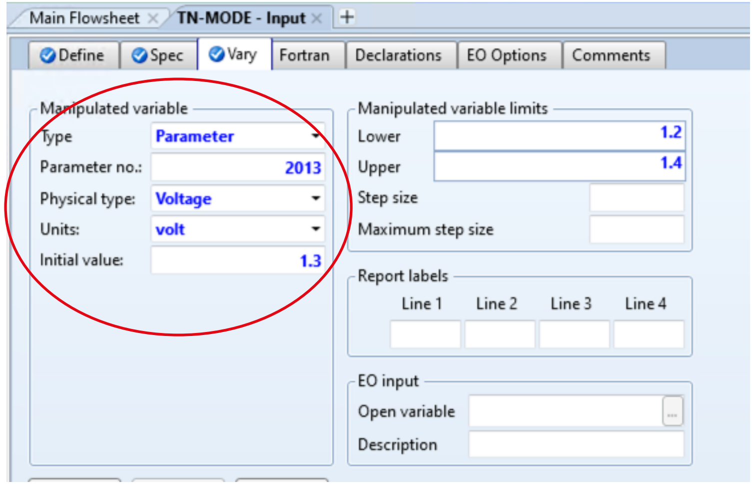


- By **varying** parameter "CVCELL", set lower and upper bound



Co-electrolyzer Aspen modelling

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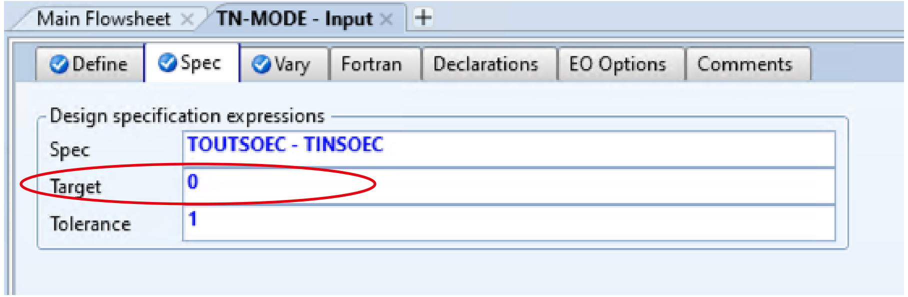
- "MIX7" temperature is calculated by using "CVCELL" parameter value
- The temperature difference of these two streams shall be 0 by varying CVCELL value

➢ SOE normally can be operated in the thermal neutral mode → T in = T out

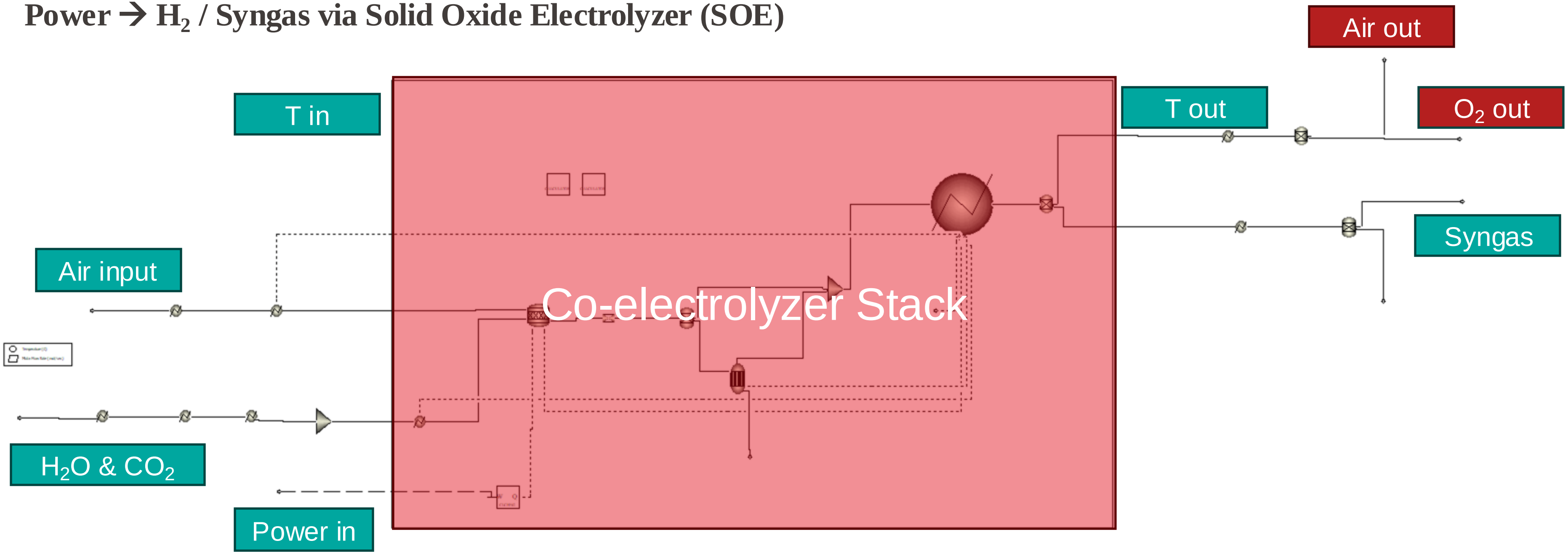
- T in > T out, it is called as endothermic mode
- T in < T out, it is called as exothermic mode

Rule: Maximum temperature difference between inlet and outlet of SOE shall be smaller than 100C



Co-electrolyzer Aspen layout

Power → H_2 / Syngas via Solid Oxide Electrolyzer (SOE)



- ✓ For SOE, fuel flow rate is automatically calculated by **Power input**
- ✓ For SOE, O_2 mole fraction normally shall be smaller than 0.3, to prevent any material degradation and oxidation

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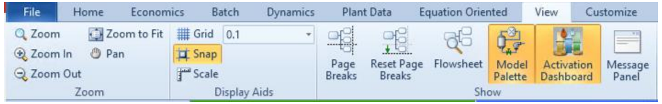
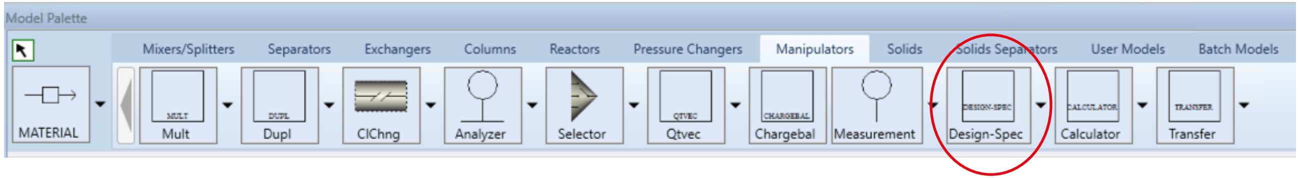
Co-electrolyzer Aspen modelling

Step 4: Create a design specification block, define the air flow rate input

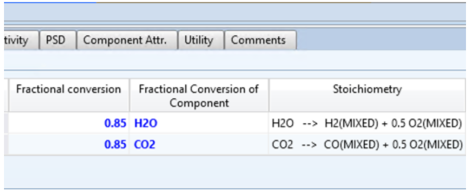
- Go to View → Model Palette



- Go to Manipulators → Design-Spec
  - Name it as "COSOEAIR"



Power input → *Fuel flow rate* → *Syngas flow rate* / *O_2 production flow rate*



Fractional conversion	Fractional Conversion of Component	Stoichiometry
0.85	H2O	H2O --> H2(MIXED) + 0.5 O2(MIXED)
0.85	CO2	CO2 --> CO(MIXED) + 0.5 O2(MIXED)

- Target: "AIR-OUT" O_2 mole fraction = 0.3
  - If there is no air flow input, then the O_2 mole fraction is 1, which is dangerous for stack material, and also it is not SAFE!
  - "AIR1" mole flow rate can be adjusted, to reach this target, as it contains N_2 and it can dilute the concentration of O_2

Co-electrolyzer Aspen modelling

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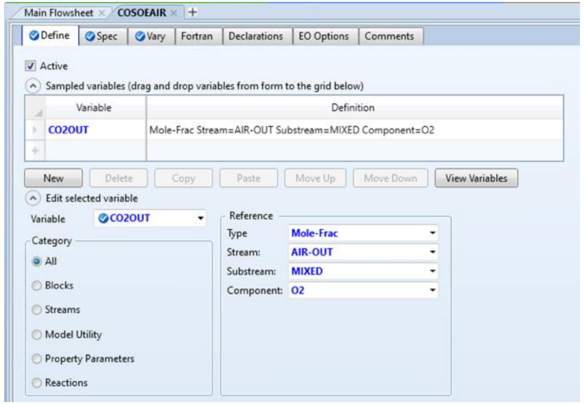
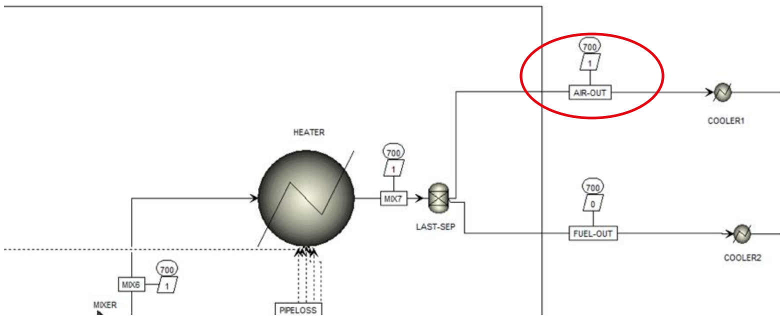
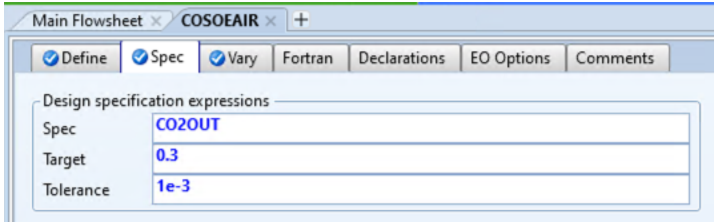


- Define your target and specification: "AIR-OUT" O_2 mole fraction = 0.3





Co-electrolyzer Aspen modelling

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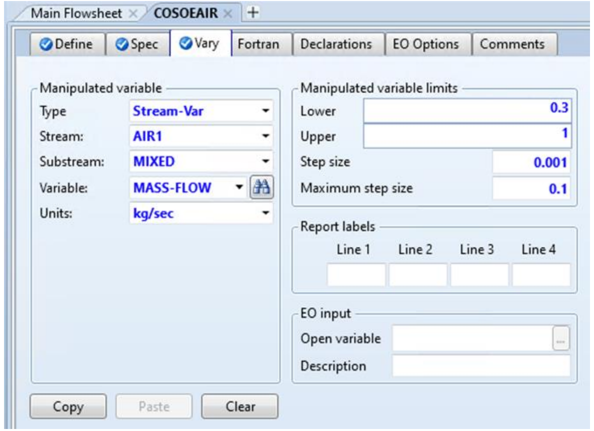
❑ **<u>Varying</u>** "AIR1" mass flow rate, to achieve your target and specification: "AIR-OUT" O_2 mole fraction = 0.3



Note: If you are sure about the lower and upper limits, you can put a very big range, but it will increase the calculation time.

Co-electrolyzer Aspen modelling

Step 4: Create a design specification block, define the air flow rate input

➢ Target: "AIR-OUT" O_2 mole fraction = 0.3

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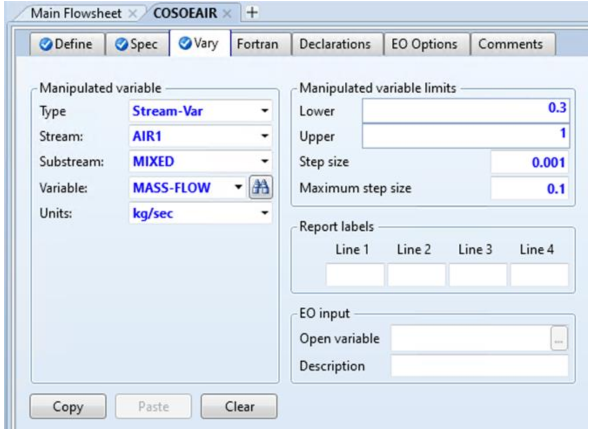
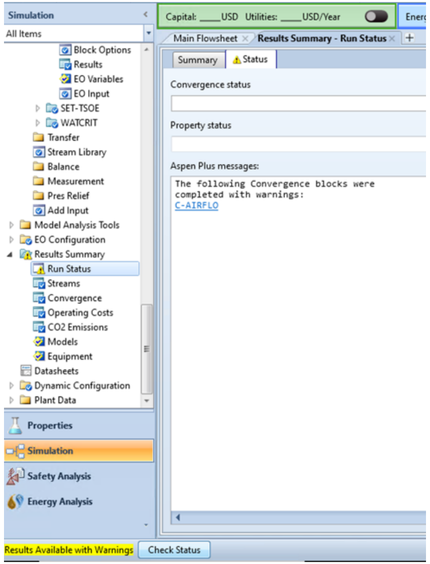
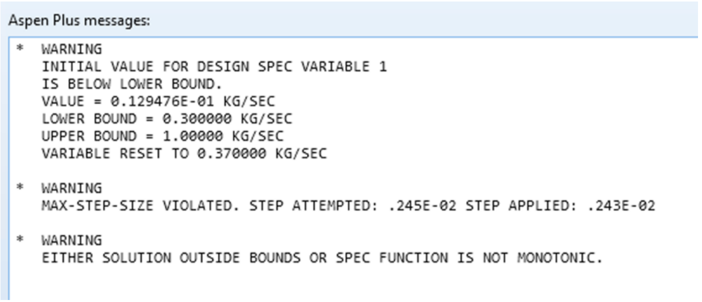




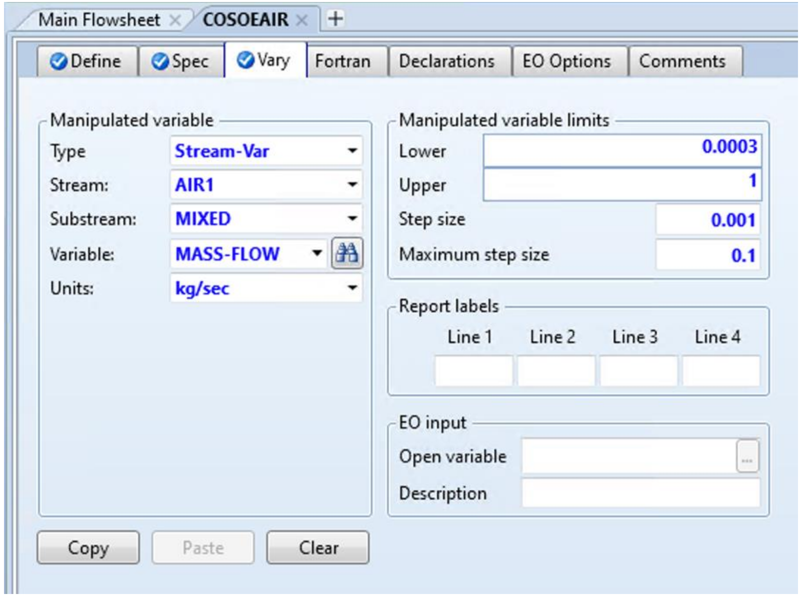


Co-electrolyzer Aspen modelling

Step 4: Create a design specification block, define the air flow rate input

- Target: “AIR-OUT” O_2 mole fraction = 0.3
  - If there is no air flow input, then the O_2 mole fraction is 1, which is dangerous for stack material, and also it is not SAFE!
  - “AIR1” mole flow rate can be adjusted, to reach this target, as it contains N_2 and it can dilute the concentration of O_2

❑ **<u>Varying</u>** ”AIR1” mass flow rate, to achieve your target and specification: “AIR-OUT” O_2 mole fraction = 0.3



If you are not sure about the lower and upper limits, you can set it as a big range, but it can increase the calculation time.

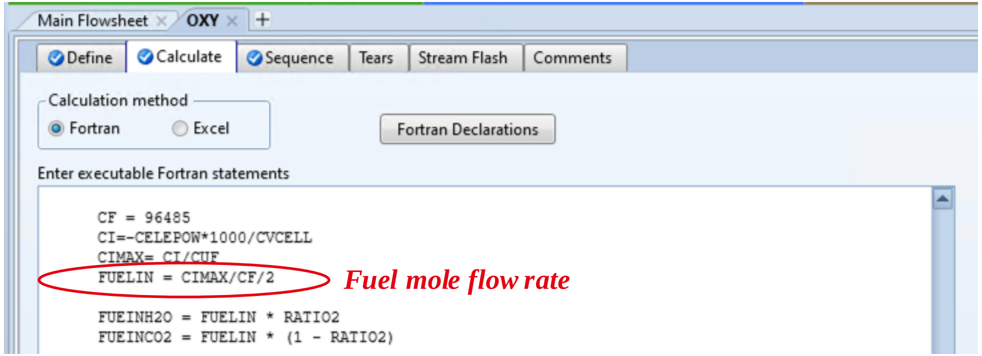
Now you can change the power input, the fuel and air flow rate can be calculated automatically!!

EPFL

Co-electrolyzer Aspen modelling

Step 5: Create a design specification block, define "FUEL1" H_2O and CO_2 mole fraction

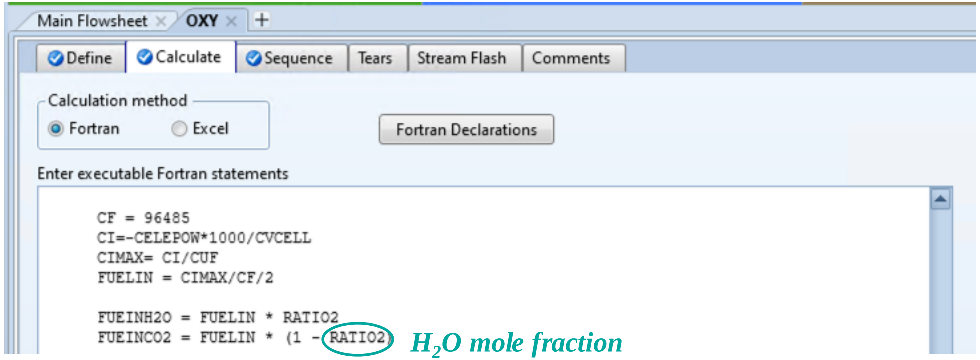
- "FUEL1" mole flow rate is automatically calculated by SOE power input ---- In "OXY" block



Fuel mole flow rate

How about the mole fraction of H2O and CO2?

- In "OXY" block, input parameter "RATIO2" is considered as the H_2O mole fraction of fuel input "FUEL1"



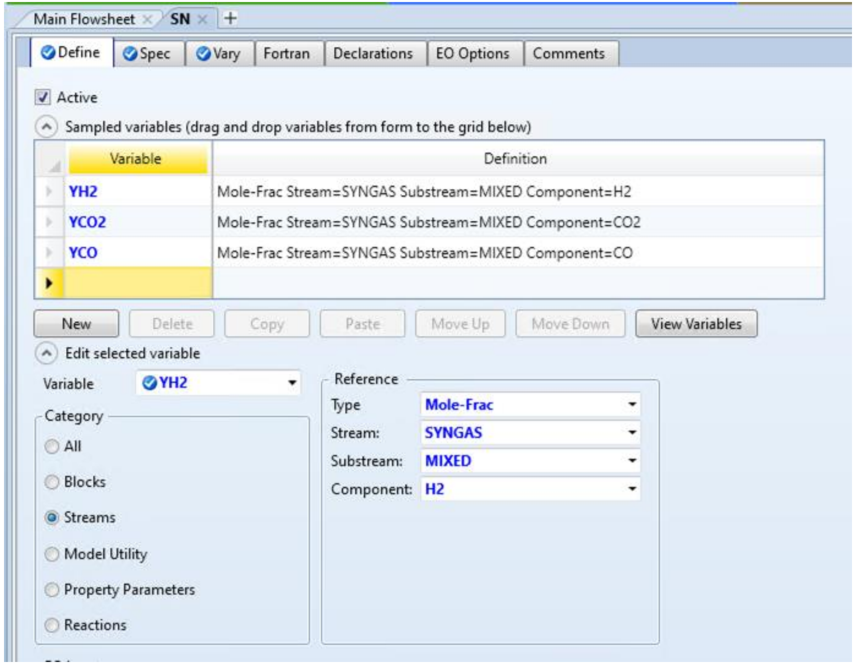
H_2O mole fraction

Co-electrolyzer Aspen modelling

Step 5: Create a design specification block, define "FUEL1" H_2O and CO_2 mole fraction

$$\mathrm{SN} = \frac{y_{\mathrm{H_2}} - y_{\mathrm{CO_2}}}{y_{\mathrm{CO}} + y_{\mathrm{CO_2}}}$$

- Requirement: "SYNGAS" SN = 3, by varying parameter "RATIO2"
- **Define** all the information that you need to calculate SN

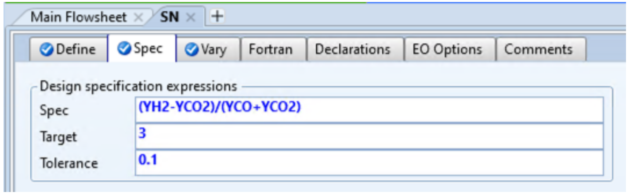


Co-electrolyzer Aspen modelling

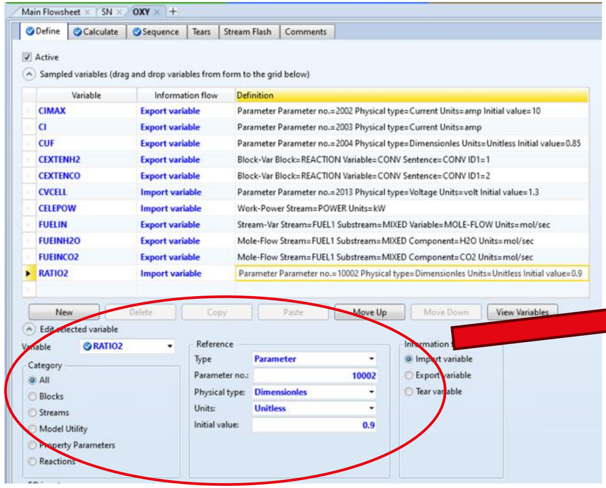
Step 5: Create a design specification block, define "FUEL1" H_2O and CO_2 mole fraction

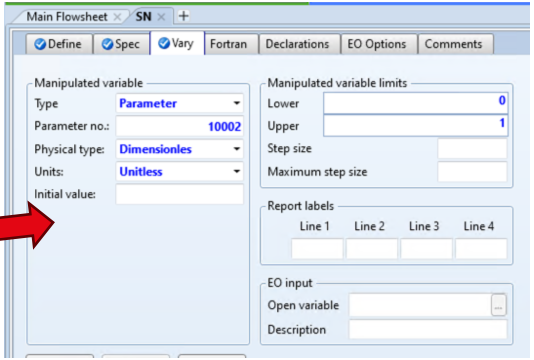
$$\mathrm{SN} = \frac{y_{H_2} - y_{CO_2}}{y_{CO} + y_{CO_2}}$$

- **Define** how to calculate SN in specification



- **Varying** "RATIO2", to reach this target





Summary of learning outcomes

- Calculator and Design Spec implementation in ASPEN
- Understand “Import variable” and “Export variable”.
- Use “Variable explorer” to find the “path” of variable
- Water needs three heaters to be heated up to the right temperature
- “Power” is the input that you can change, in order to achieve the syngas flow rate
- If you have the “warning message”, please read the status, to understand where is the error.