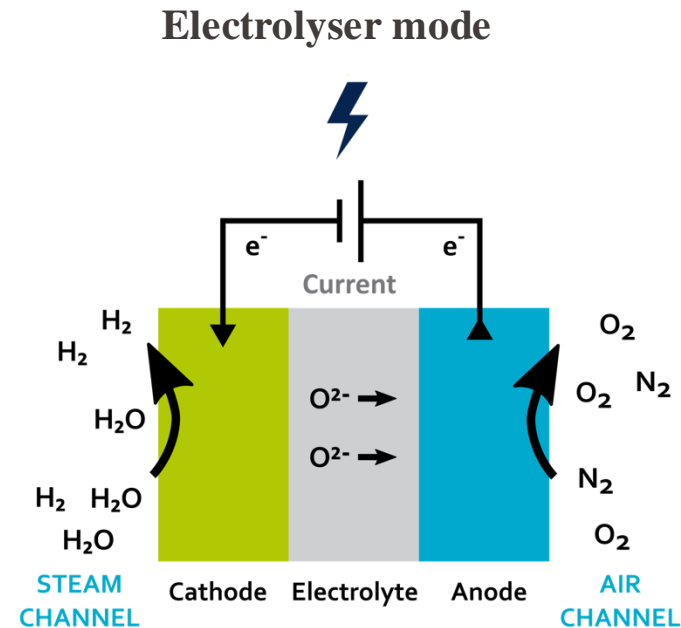
The background of the slide is an aerial photograph of the EPFL campus in Lausanne, Switzerland. The image shows various university buildings, green spaces, and a large lake (Lake Geneva) in the distance, with snow-capped mountains on the horizon under a clear sky.

Co-electrolysis process in Aspen Plus®

Arthur Waeber
Xinyi Wei

17/03/2025

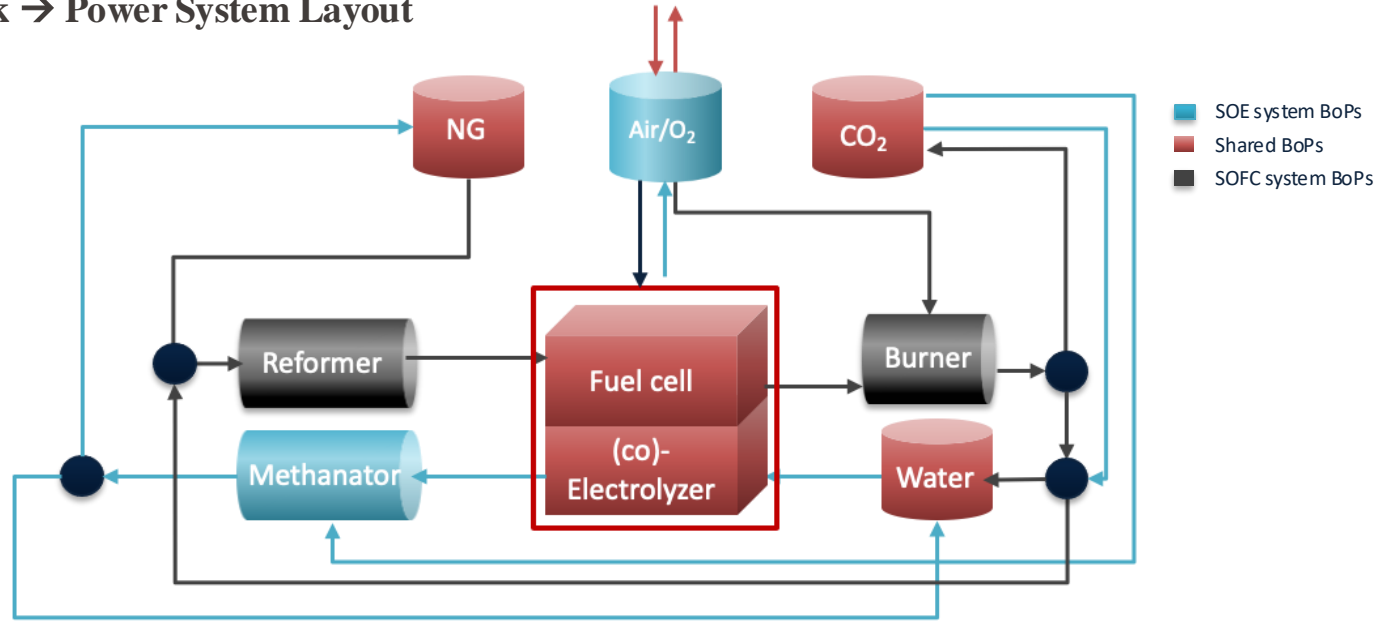
- Electrochemical reduction of H_2O and/or CO_2
- Solid Oxide Electrolyte at high temperature ($> 700^\circ\text{C}$)
- High Temperature:
 - Good conversion efficiency
 - Challenges for integration
 - Necessitate clever heat integration
- Production of H_2 or Syngas and O_2 which are all 3 valuable products
- 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)



EPFL General information on Power – X – Power (rSOC)

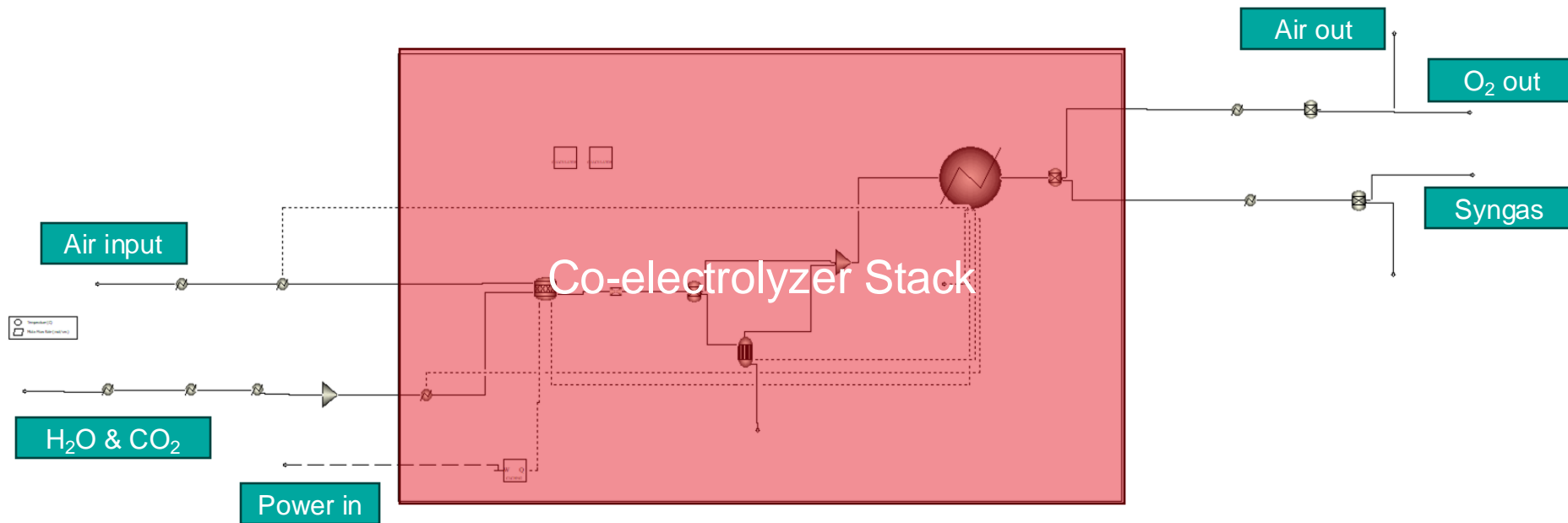
3

Power → NG Tank → Power System Layout

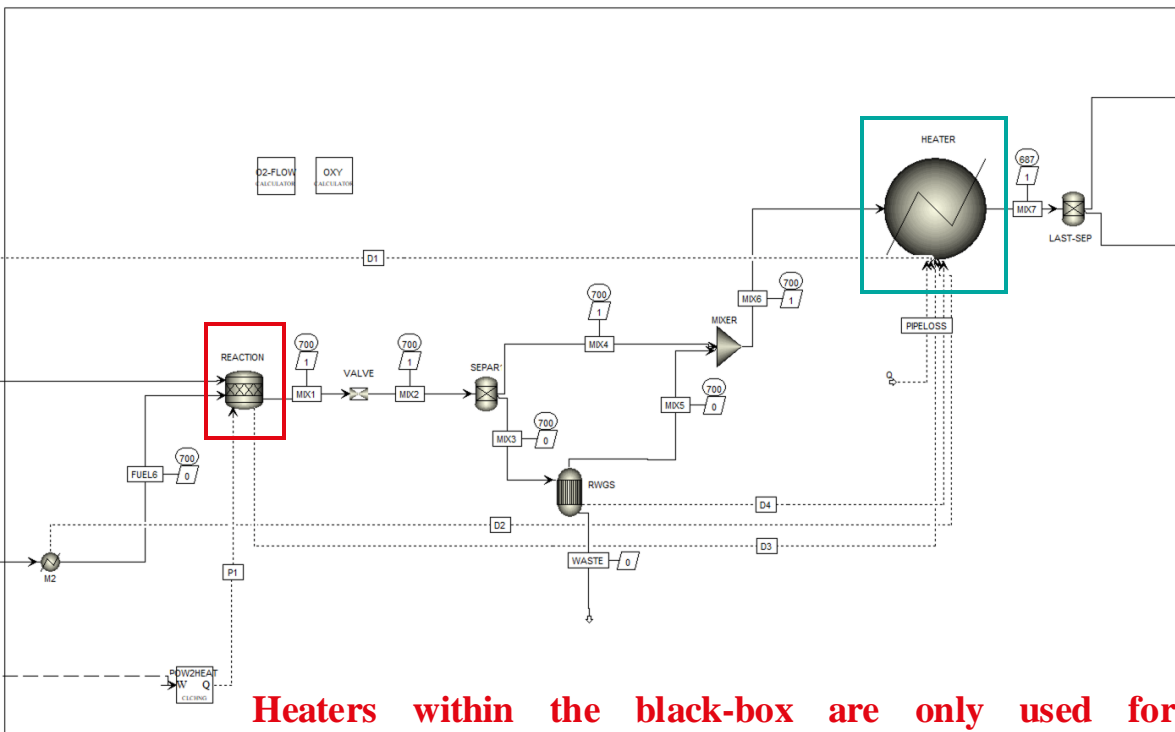


- When renewable electricity is available, methane can be produced *via* electrolyzer-methanation unit.
- When system requires electricity, it can be produced *via* reformer-fuel cell-burner unit.
- Oxy-combustion is considered in fuel cell system (to avoid presence of N₂).
- High temperature heat is available

Power \rightarrow H₂ / Syngas via Solid Oxide Electrolyzer (SOE)



Solid Oxide Electrolyzer (SOE) – Thermoneutral operation

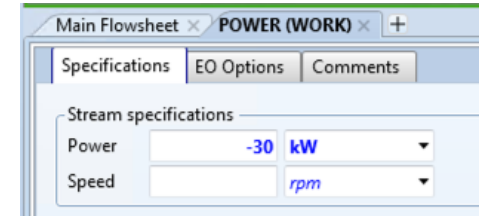
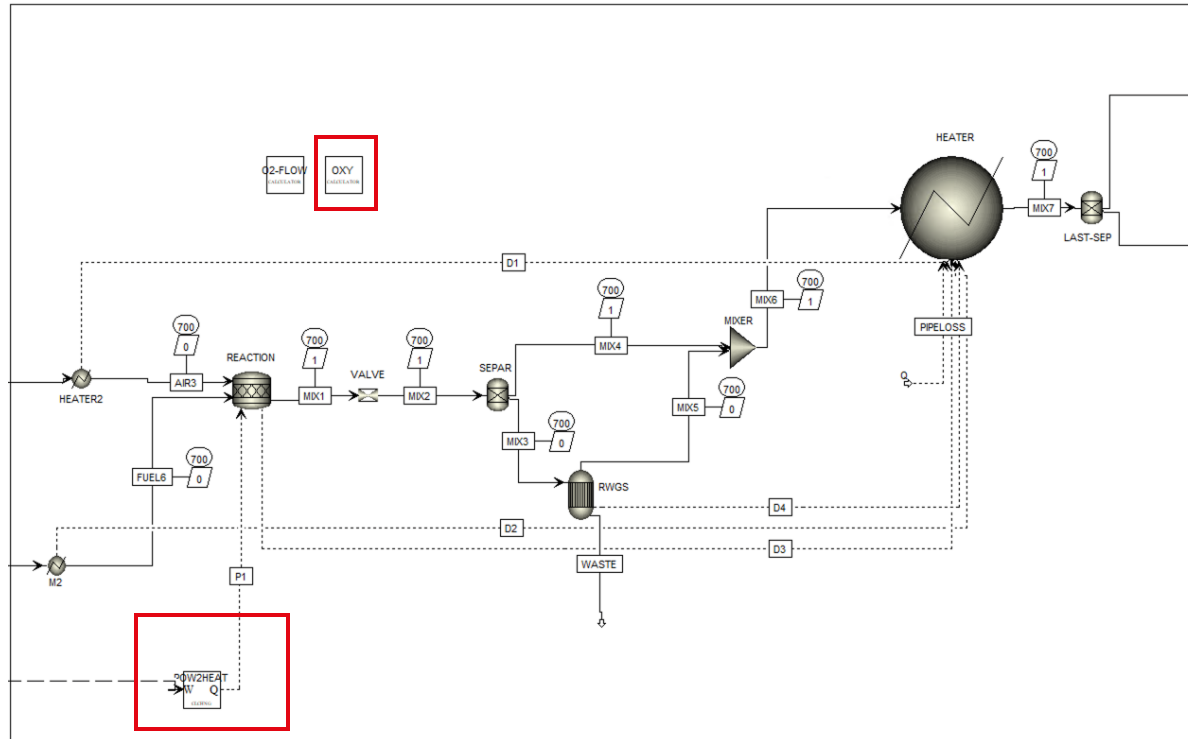


- No need to modify SOE stack model in your project.
- “REACTION” reactor contains main co-electrolysis reactions.

ativity	PSD	Component Attr.	Utility	Comments
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)		

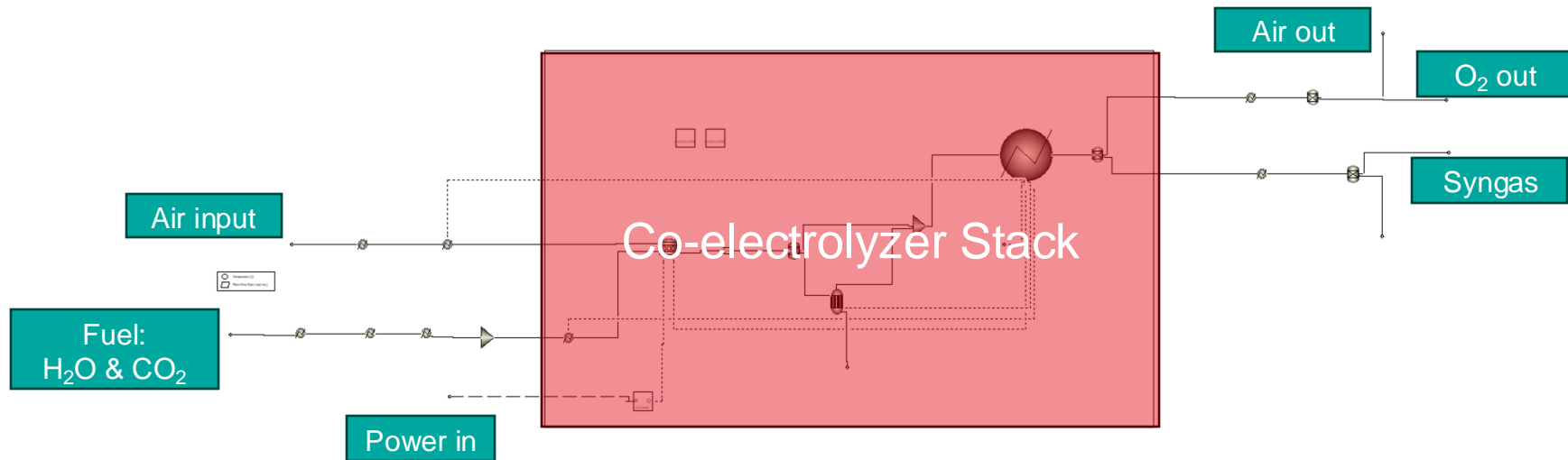
- “HEATER” is used to count the heat within the stack.
- The HEATER will have a heat output of 0 kW (thermoneutral operation)

Solid Oxide Electrolyzer (SOE)



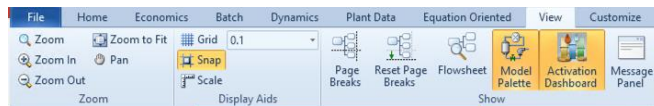
- Power input in current file is 30 kW. (negative as input)
- When you change the electrolyzer power input, the fuel flow rate “FUEL1” will be automatically updated by “OXY” calculator - **no need to change by yourself.**

1. Uniformize all up-stream temperatures (through calculator block)
2. Understand fuel heating-up process (differentiate heaters)
3. Ensure thermoneutral operation ($T_{\text{SOEC_in}} == T_{\text{SOEC_out}}$) through design specification
4. Apply technical constraint on O_2 /Air flow through design specification
5. Define a variable to tune the $\text{H}_2\text{O}/\text{CO}_2$ ratio in the fuel. (in class)
6. Define the right stoichiometric number for further syngas usage (in class)



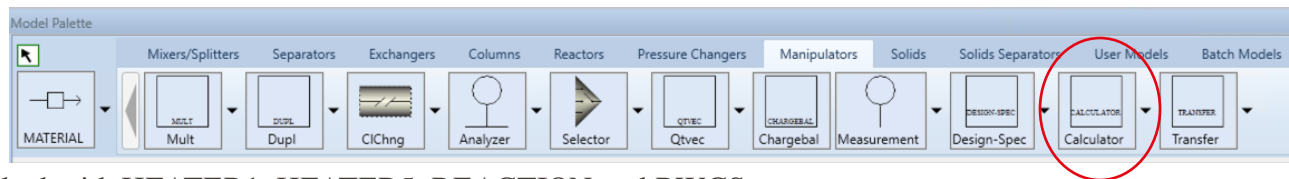
Step 1: Set SOEC upstream components temperature into 700 °C via calculator

➤ Go to View → Model Palette



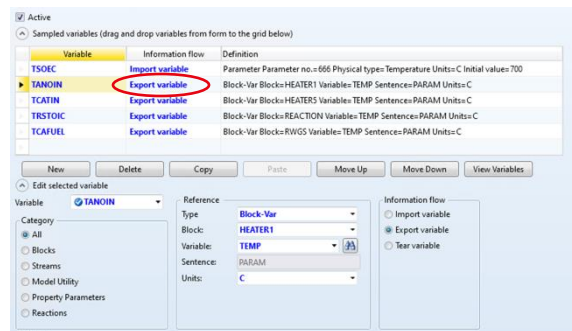
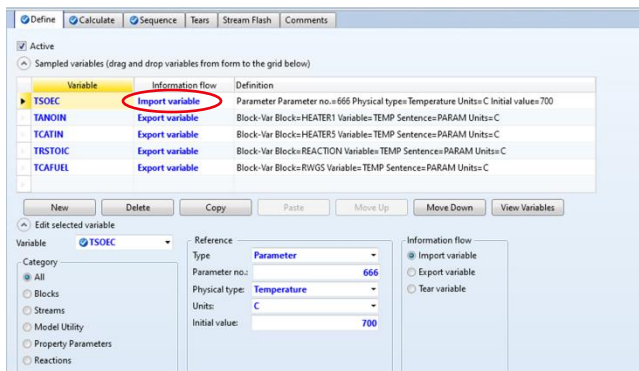
➤ Go to Manipulators → Calculator

- Name calculator “SET-TSOE”



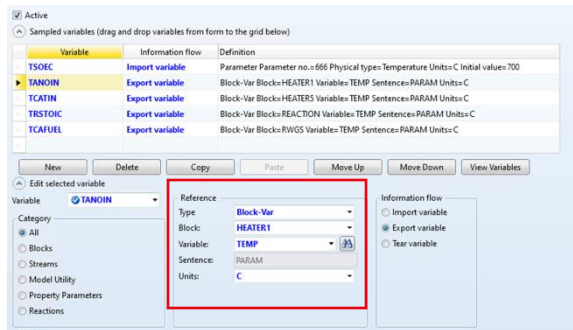
➤ Target: Set a parameter which is linked with HEATER1, HEATER5, REACTION and RWGS

- Define a new **parameter** “TSOEC”, select it to be the “import variable”.
- Export variable is the output from the calculator, it gives the order to ASPEN.
- Import variable is the input from user.

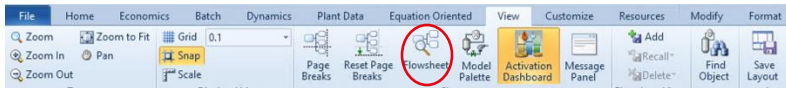


By adding this calculator, if we want to change the stack inlet T, we only need to change Parameter – “TSOEC”

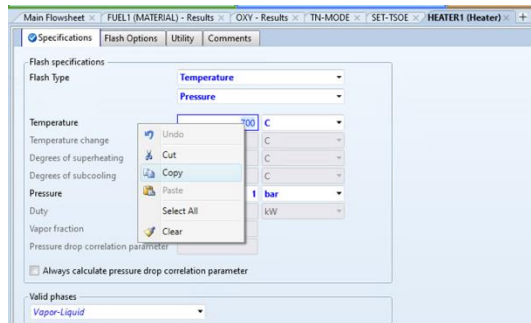
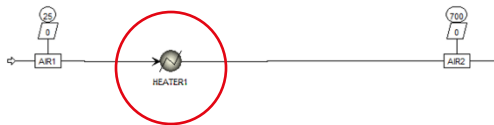
Question: What if we are not sure about “Reference”?



➤ Go to Flowsheet

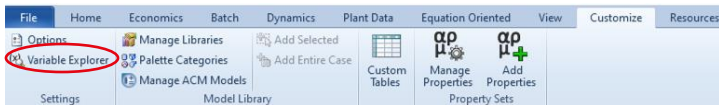


➤ Find “HEATER1” → “Temperature” → Select value → “Copy”

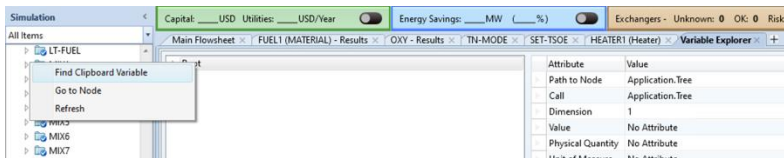


Question: What if we are not sure about “Reference”?

- Go to Customize → Variable Explorer

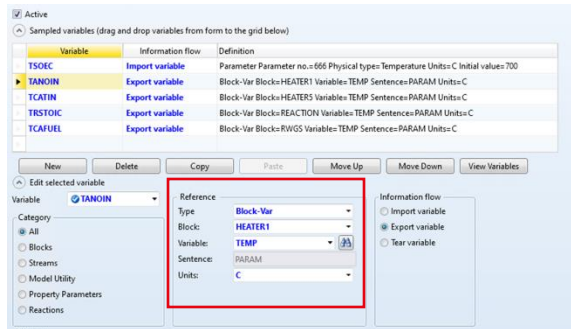


- Go to Variable Explorer → Right Click “Root” → “Find Clipboard Variable”



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

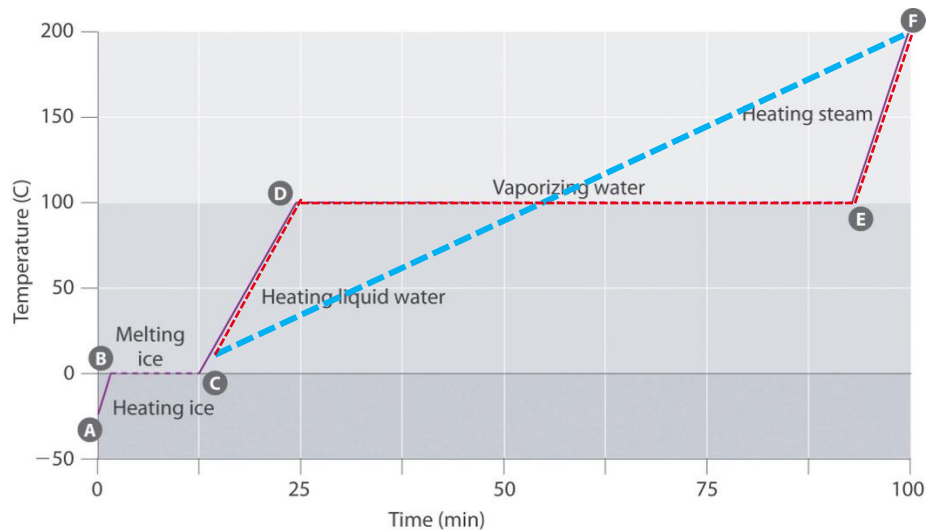
Attribute	Value
Path to Node	Application.Tree.Data.Blocks.HEATER1.Input.TEMP
Call	Application.Tree.FindNode("Data.Blocks.HEATER1.Input.TEMP")
Dimension	0
Value	700
Physical Quantity	22
Unit of Measure	4
Basis	No Attribute
Record Type	No Attribute
Output	0
Enterable	1
Upper Limit	5000
Lower Limit	0
Default Value	1E+35
Completion Status	
Port In or Out	No Attribute
Port Gender	No Attribute
Multipoint	No Attribute
Port Type	No Attribute
Has Children	0



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

Step 2: Set “Fuel” heating up process

- If “Fuel1” only contains H_2O

- HEATER3

Main Flowsheet > HEATER3 (Heater) > +

Specifications Flash Options Utility Comments

Flash specifications

Flash Type: Temperature

Temperature: 100 C

Temperature change: C

Degrees of superheating: C

Degrees of subcooling: C

Pressure: 1 bar

Duty: kW

Vapor fraction: 0.12

Pressure drop correlation parameter:

☐ Always calculate pressure drop correlation parameter

Valid phases: Vapor-Liquid

- If “Fuel1” contains both H_2O and $\text{CO}_2 \rightarrow$ “HEATER3” needs to be updated \rightarrow Boiling point of H_2O will change as the pressure change

- HEATER4

Main Flowsheet > HEATER4 (Heater) > +

Specifications Flash Options Utility Comments

Flash specifications

Flash Type: Pressure

Vapor fraction:

Temperature: C

Temperature change: C

Degrees of superheating: C

Degrees of subcooling: C

Pressure: 1 bar

Duty: kW

Vapor fraction: 0.999

Pressure drop correlation parameter:

☐ Always calculate pressure drop correlation parameter

Valid phases: Vapor-Liquid

- HEATER5

Main Flowsheet > HEATER5 (Heater) > +

Specifications Flash Options Utility Comments

Flash specifications

Flash Type: Temperature

Temperature: 700 C

Temperature change: C

Degrees of superheating: C

Degrees of subcooling: C

Pressure: 1 bar

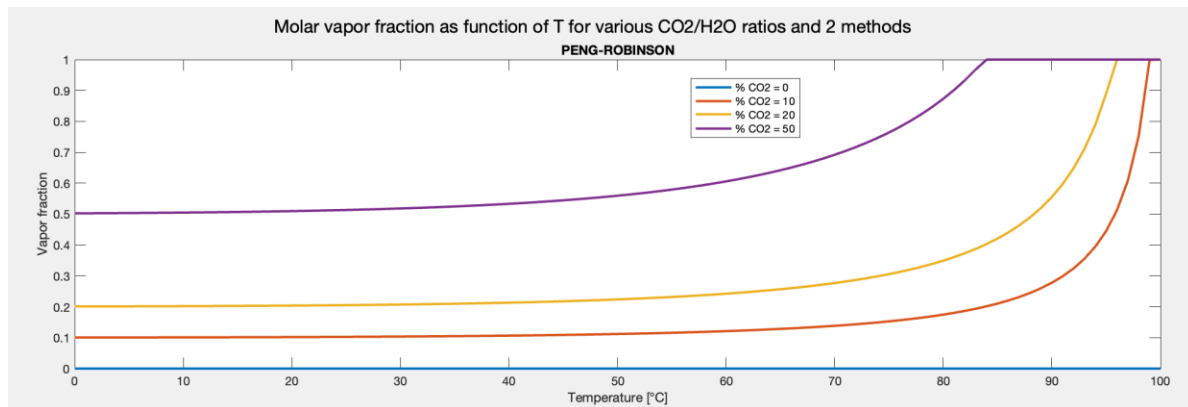
Duty: kW

Vapor fraction:

Pressure drop correlation parameter:

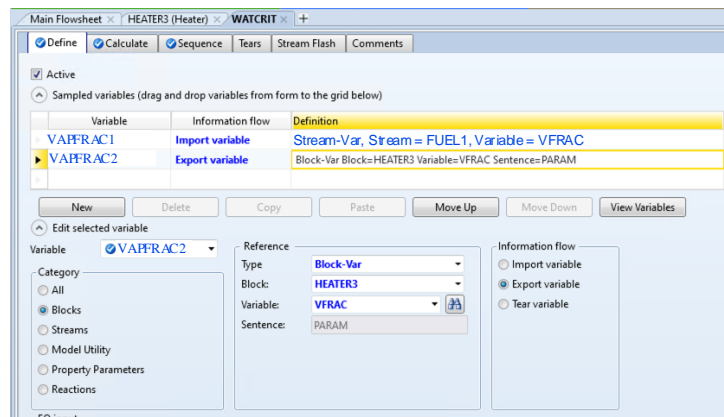
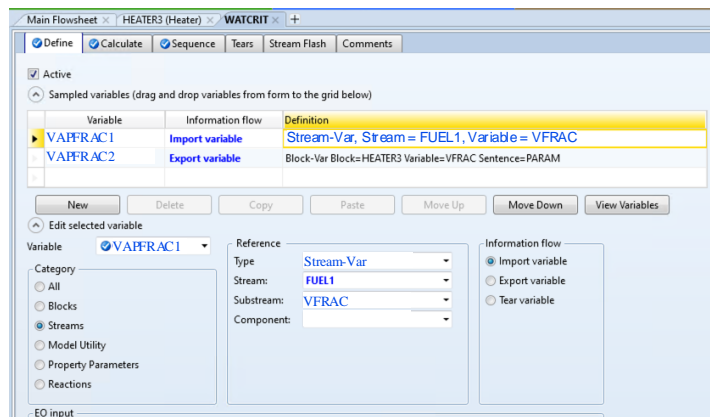
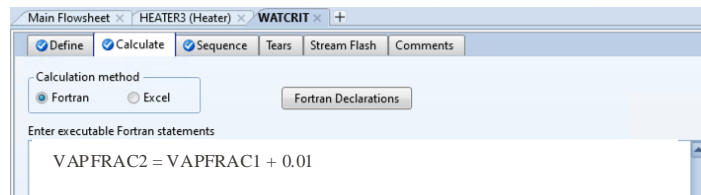
☐ Always calculate pressure drop correlation parameter

Valid phases: Vapor-Liquid



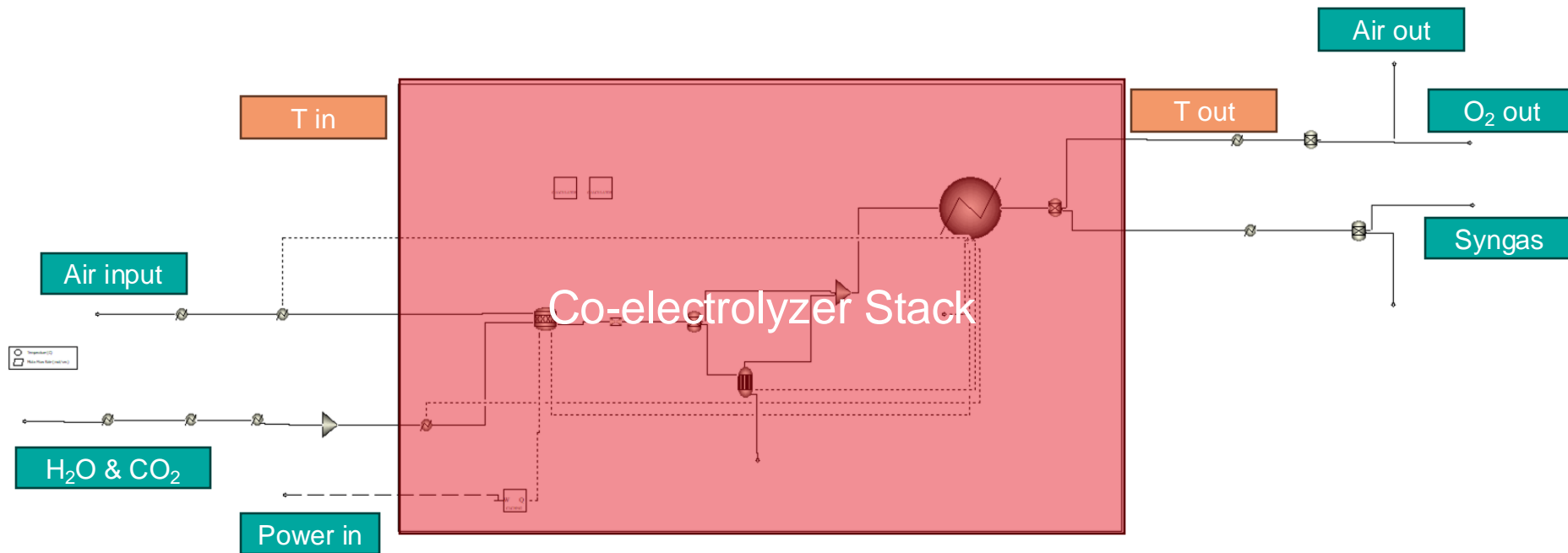
Step 2: Set “Fuel” heating up process

- After “HEATER3”, H₂O is going to evaporate further → stream “FUEL2” vapor fraction shall be slightly higher than “FUEL1”
- Add a calculator, name it as “WATCHRIT”
 - Import “FUEL1” vapor mole fraction as “VAPFRAC1”
 - Export “HEATER3” vapor fraction as “VAPFRAC2”
 - “HEATER3” vapor fraction = “FUEL1” vapor mole fraction + 0.01

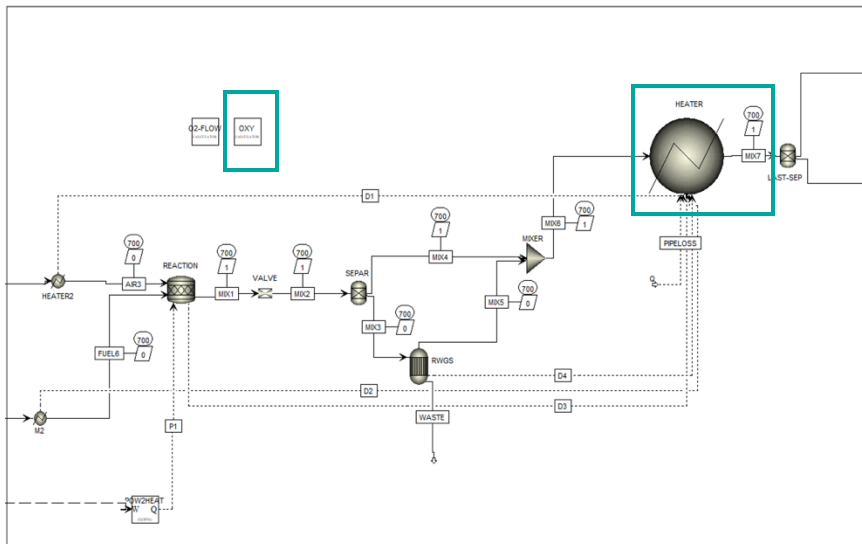


- Note: “HEATER3” shall have pressure and vapor fraction as the specifications, otherwise, calculator CAN NOT give order

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



Solid Oxide Electrolyzer (SOE)



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

Main Flowsheet x OXY x +

Define Calculate Sequence Tears Stream Flash Comments

☒ Active

Sampled variables (drag and drop variables from form to the grid below)

Variable	Information flow	Definition
CIMAX	Export variable	Parameter Parameter no.=2002 Physical type=Current Units=amp Initial value=10
CI	Export variable	Parameter Parameter no.=2003 Physical type=Current Units=amp
CUF	Export variable	Parameter Parameter no.=2004 Physical type=Dimensionless Units=Unitless Initial value=0.85
CEXTENH2	Export variable	Block-Var Block=REACTION Variables=CONV Sentences=CONV ID1=1
CEXTENCO	Export variable	Block-Var Block=REACTION Variables=CONV Sentences=CONV ID1=2
CVCELL	Import variable	Parameter Parameter no.=2013 Physical type=Voltage Units=volt Initial value=1.3
CELEPOW	Import variable	Work-Power Stream=POWER Units=kW
FUELIN	Export variable	Stream-Var Stream=FUEL1 Substream=MIXED Variable=MOLE-FLOW Units=mol/sec
FUEINH2O	Export variable	Mole-Flow Stream=FUEL1 Substream=MIXED Component=H2O Units=mol/sec
FUEINCO2	Export variable	Mole-Flow Stream=FUEL1 Substream=MIXED Component=CO2 Units=mol/sec
RATIO2	Import variable	Parameter Parameter no.=10002 Physical type=Dimensionless Units=Unitless Initial value=0.9

New Delete Copy Paste Move Up Move Down View Variables

Edit selected variable

Variable: CVCELL

Category: All

Reference

Type: Parameter

Parameter no.: 2013

Physical type: Voltage

Units: volt

Initial value: 1.3

Information flow

☒ Import variable

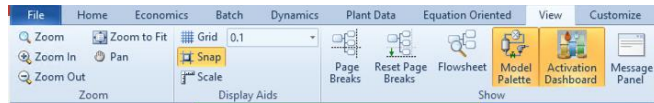
☐ Export variable

☐ Tear variable

- 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.

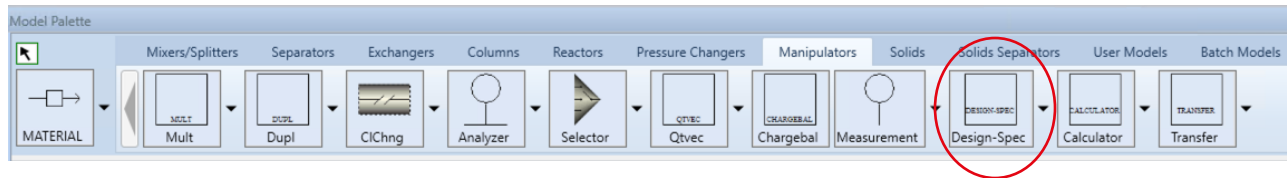
Step 3: Create a design specification block, which is able to make SOE inlet T = SOE outlet T

- 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

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

➤ 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

• Define SOEC inlet T

The screenshot shows the Aspen Plus 'Main Flowsheet' window with the 'TN-MODE - Input' tab selected. The 'Define' button is active. A table lists sampled variables:

Variable	Definition
TINSOEC	Stream-Var Stream=FUEL4 Substream=MIXED Variable=TEMP Units=C
TOUTSOEC	Stream-Var Stream=MIX7 Substream=MIXED Variable=TEMP Units=C

Below the table, the 'Edit selected variable' section is shown for the variable 'TINSOEC'. The 'Reference' section has the following settings:

- Type: Stream-Var
- Stream: FUEL4
- Substream: MIXED
- Variable: TEMP
- Units: C

• Define SOEC outlet T

The screenshot shows the Aspen Plus 'Main Flowsheet' window with the 'TN-MODE - Input' tab selected. The 'Define' button is active. A table lists sampled variables:

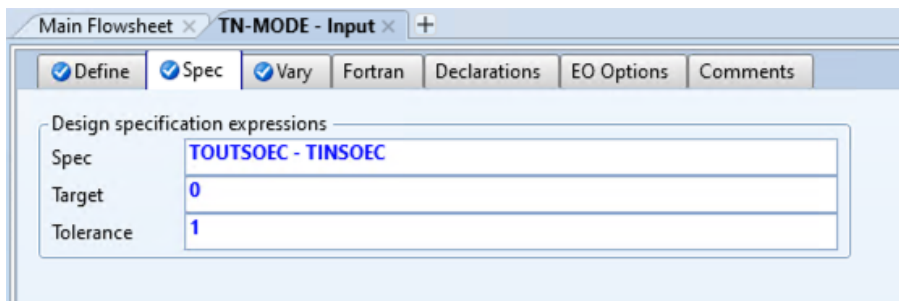
Variable	Definition
TINSOEC	Stream-Var Stream=FUEL4 Substream=MIXED Variable=TEMP Units=C
TOUTSOEC	Stream-Var Stream=MIX7 Substream=MIXED Variable=TEMP Units=C

Below the table, the 'Edit selected variable' section is shown for the variable 'TOUTSOEC'. The 'Reference' section has the following settings:

- Type: Stream-Var
- Stream: MIX7
- Substream: MIXED
- Variable: TEMP
- Units: C

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

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

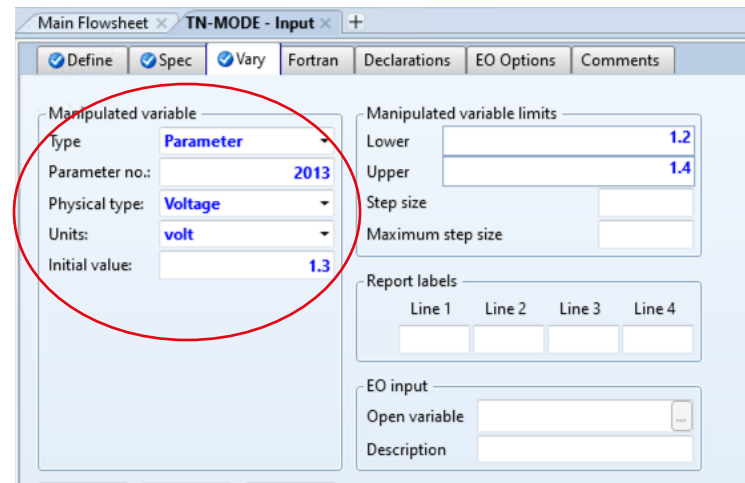
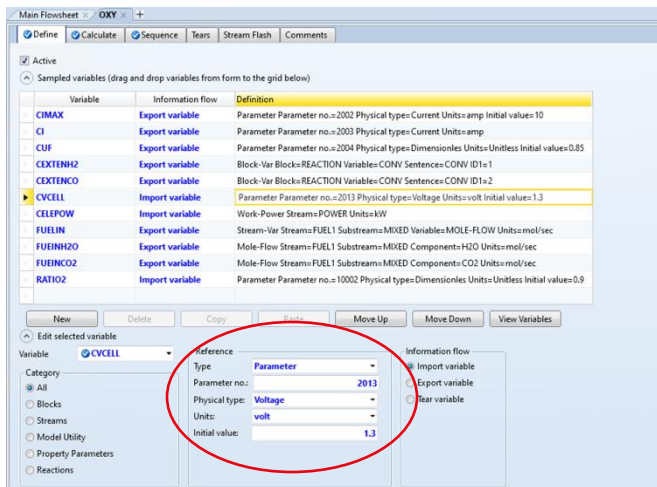


Step 3: Create a design specification block, which is able to make SOE inlet T = SOE outlet T

➤ 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

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



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

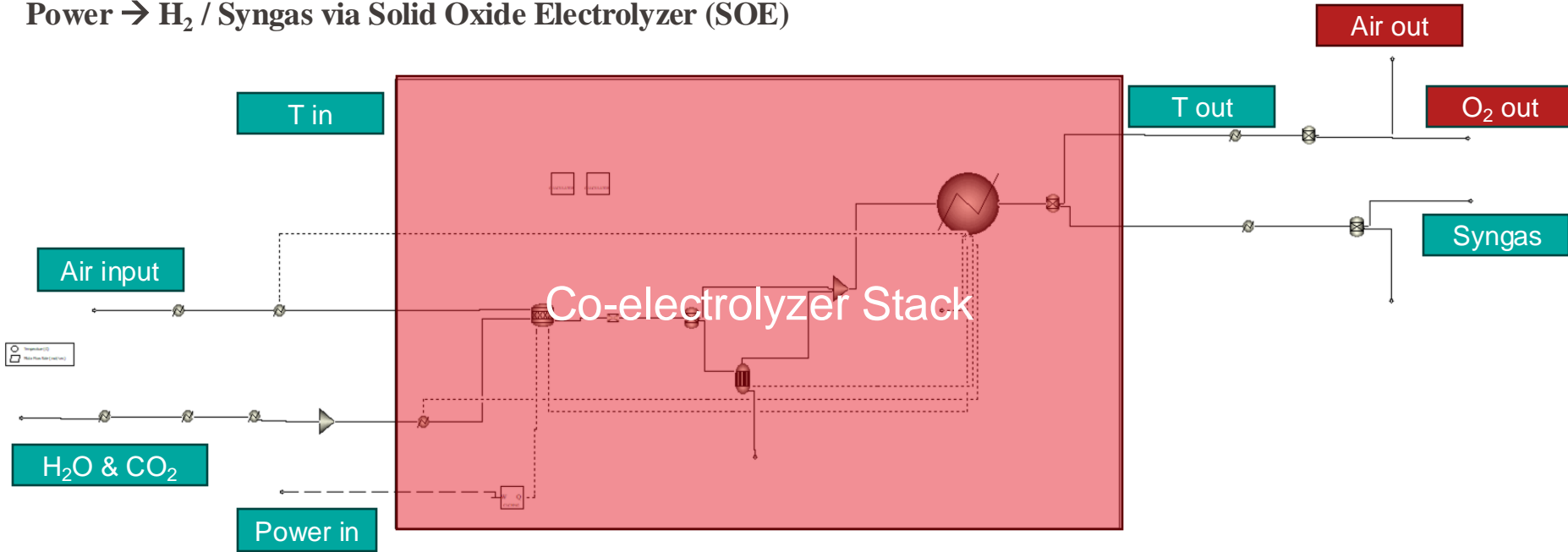
- Target: “MIX7” temperature = “FUEL4” temperature, by varying “CVCELL”
 - “FUEL4” temperature is fixed by the previous calculator
 - “MIX7” temperature is calculated by using “CVCELL” parameter value
 - The temperature difference of these two streams shall be 0 by varying CVCELL value
- SOE normally can be operated in the thermal neutral mode $\rightarrow T_{in} = T_{out}$
 - $T_{in} > T_{out}$, 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

The screenshot shows the 'Design specification expressions' dialog box for the 'TN-MODE - Input' block. The 'Spec' field contains the expression 'TOUTSOEC - TINSOEC'. The 'Target' field is circled in red and contains the value '0'. The 'Tolerance' field contains the value '1'. The dialog box has tabs for 'Define', 'Spec', 'Vary', 'Fortran', 'Declarations', 'EO Options', and 'Comments', with 'Spec' currently selected.

Design specification expressions	
Spec	TOUTSOEC - TINSOEC
Target	0
Tolerance	1

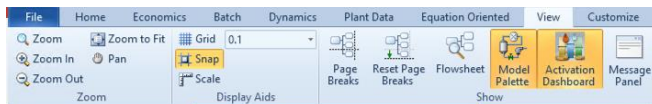
Power \rightarrow H_2 / Syngas via Solid Oxide Electrolyzer (SOE)



- ✓ For SOE, fuel flow rate is automatically calculated by **Power input**
- ✓ For SOE, O₂ mole fraction normally shall be smaller than 0.3, to prevent any material degradation and oxidation

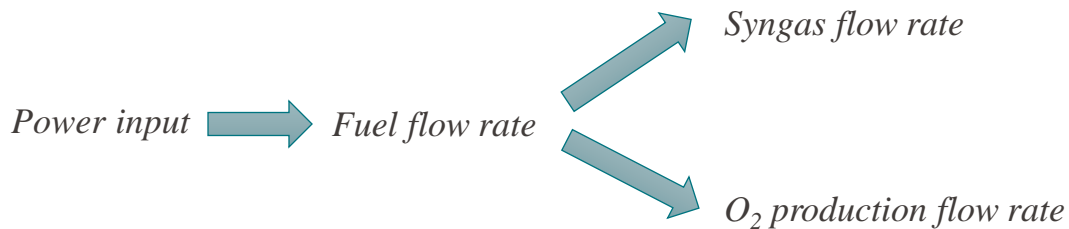
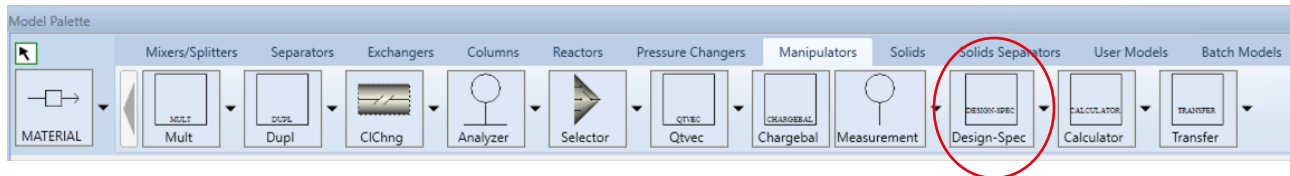
Step 4: Create a design specification block, define the air flow rate input

➤ Go to View → Model Palette



➤ Go to Manipulators → Design-Spec

- Name it as “COSOEAIR”



Activity	PSD	Component Attr.	Utility	Comments
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” O₂ mole fraction = 0.3

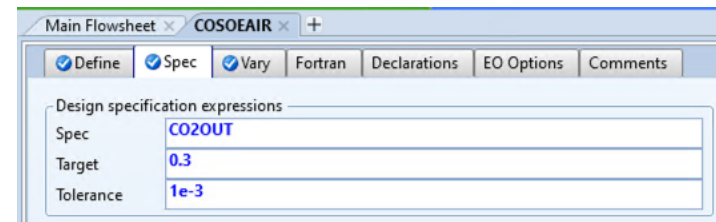
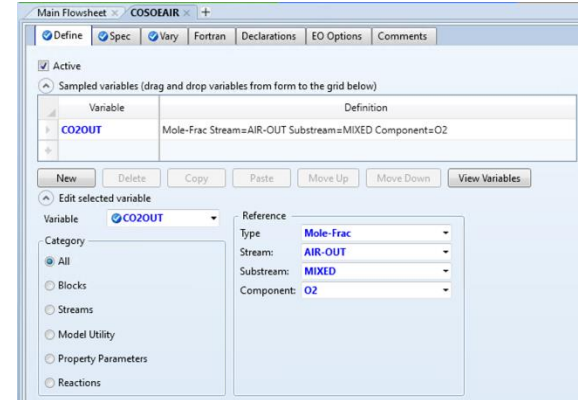
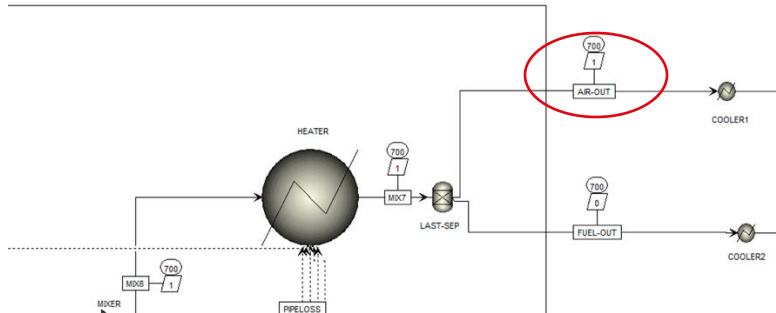
- If there is no air flow input, then the O₂ mole fraction is 1, which is dangerous for stack material, and also it is not SAFE!
- “AIR1” mole flow rate can be adjusted, to reach this target, as it contains N₂ and it can dilute the concentration of O₂

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

□ **Define** your target and specification: “AIR-OUT” O_2 mole fraction = 0.3

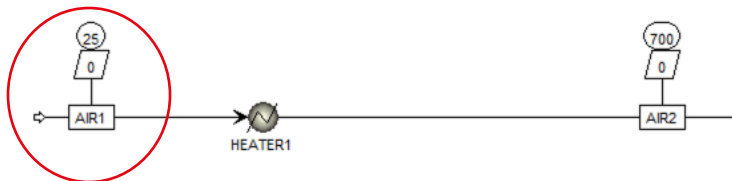


Step 4: Create a design specification block, define the air flow rate input

➤ 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

□ Varying “AIR1” mass flow rate, to achieve your target and specification: “AIR-OUT” O_2 mole fraction = 0.3



The screenshot shows the 'Vary' dialog box in Aspen Plus for the 'COSOEAIR' flowsheet. The 'Manipulated variable' section is configured as follows:

- Type: Stream-Var
- Stream: AIR1
- Substream: MIXED
- Variable: MASS-FLOW
- Units: kg/sec

The 'Manipulated variable limits' section is configured as follows:

- Lower: 0.3
- Upper: 1
- Step size: 0.001
- Maximum step size: 0.1

The 'Report labels' section shows four empty boxes for Line 1, Line 2, Line 3, and Line 4.

The 'EO input' section has an 'Open variable' field and a 'Description' field.

Buttons at the bottom include Copy, Paste, and Clear.

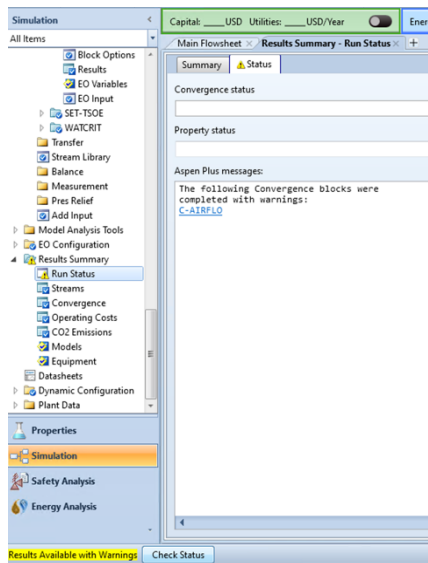
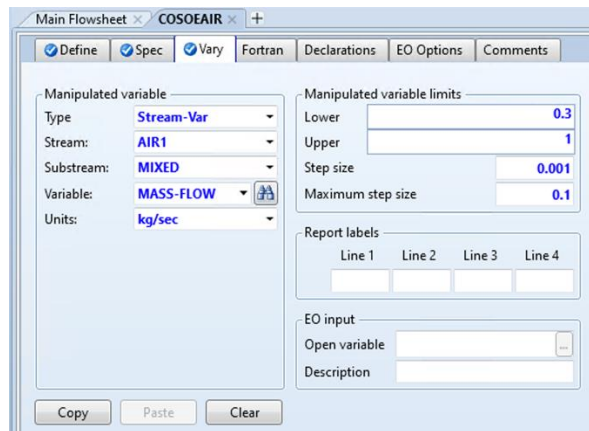
Note: If you are sure about the lower and upper limits, you can put a very big range, but it will increase the calculation time.

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

□ Varying “AIR1” mass flow rate, to achieve your target and specification: “AIR-OUT” O_2 mole fraction = 0.3



Aspen Plus messages:

- * WARNING
INITIAL VALUE FOR DESIGN SPEC VARIABLE 1
IS BELOW LOWER BOUND.
VALUE = 0.129476E-01 KG/SEC
LOWER BOUND = 0.300000 KG/SEC
UPPER BOUND = 1.00000 KG/SEC
VARIABLE RESET TO 0.370000 KG/SEC
- * WARNING
MAX-STEP-SIZE VIOLATED. STEP ATTEMPTED: .245E-02 STEP APPLIED: .243E-02
- * WARNING
EITHER SOLUTION OUTSIDE BOUNDS OR SPEC FUNCTION IS NOT MONOTONIC.

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

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

Main Flowsheet x COSOEAIR x +

Define Spec Vary Fortran Declarations EO Options Comments

Manipulated variable

Type: Stream-Var

Stream: AIR1

Substream: MIXED

Variable: MASS-FLOW

Units: kg/sec

Manipulated variable limits

Lower: 0.0003

Upper: 1

Step size: 0.001

Maximum step size: 0.1

Report labels

Line 1 Line 2 Line 3 Line 4

EO input

Open variable

Description

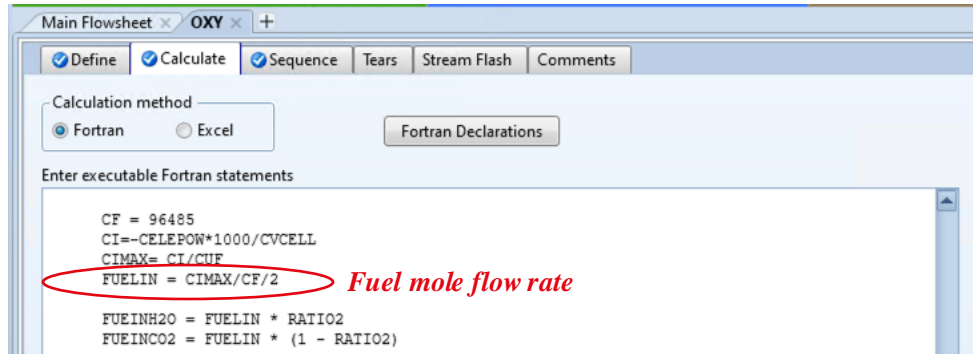
Copy Paste Clear

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!!

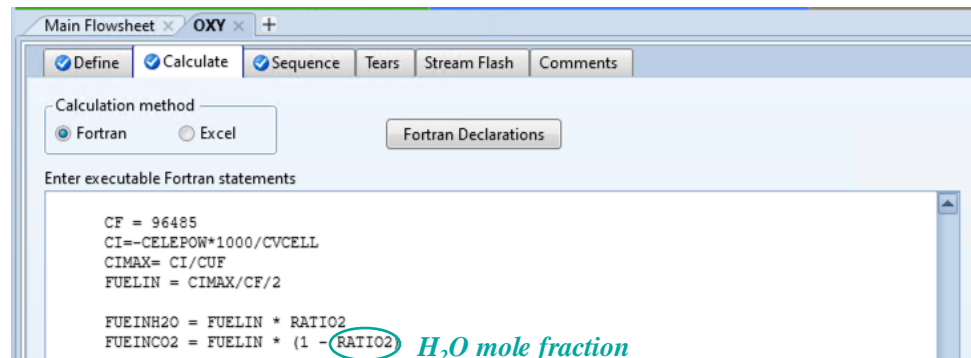
Step 5: Create a design specification block, define “FUEL1” H₂O and CO₂ mole fraction

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



How about the mole fraction of H₂O and CO₂?

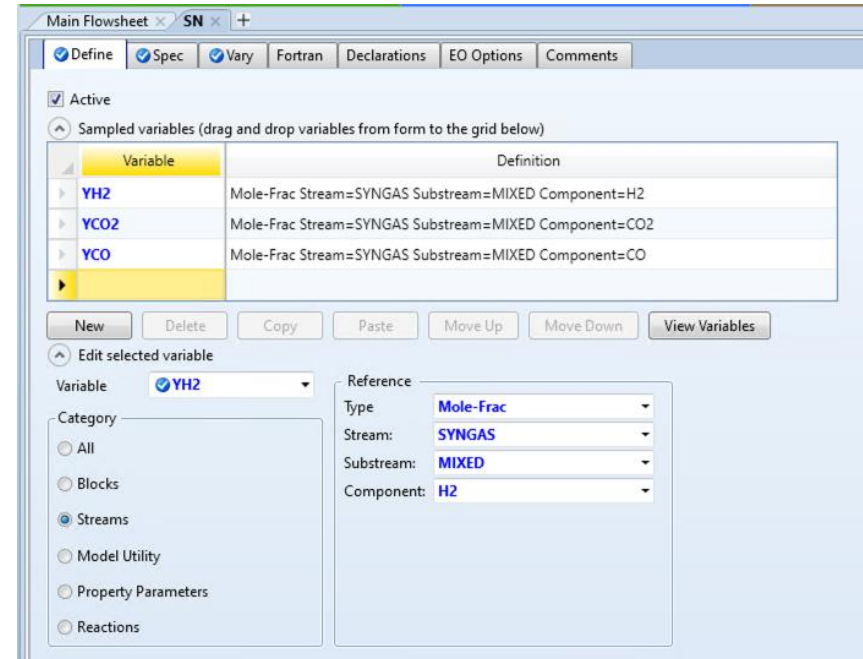
- In “OXY” block, input parameter “RATIO2” is considered as the H₂O mole fraction of fuel input “FUEL1”



Step 5: Create a design specification block, define “FUEL1” H₂O and CO₂ mole fraction

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

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



Step 5: Create a design specification block, define “FUEL1” H₂O and CO₂ mole fraction

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

➤ Define how to calculate SN in specification

Main Flowsheet × SN × +

Define Spec Vary Fortran Declarations EO Options Comments

Design specification expressions

Spec: (YH2-YCO2)/(YCO+YCO2)

Target: 3

Tolerance: 0.1

➤ Varying “RATIO2”, to reach this target

Main Flowsheet × SN × OXY × +

Define Calculate Sequence Tears Stream Flash Comments

Active

Sampled variables (drag and drop variables from form to the grid below)

Variable	Information flow	Definition
CIMAX	Export variable	Parameter Parameter no.=2002 Physical type=Current Units=amp Initial value=10
CI	Export variable	Parameter Parameter no.=2003 Physical type=Current Units=amp
CUF	Export variable	Parameter Parameter no.=2004 Physical type=Dimensionless Units=Unitless Initial value=0.85
CEXTNH2	Export variable	Block-Var Block=REACTION Variables=CONV Sentences=CONV ID=1
CEXTNCO	Export variable	Block-Var Block=REACTION Variables=CONV Sentences=CONV ID=2
CVCELL	Import variable	Parameter Parameter no.=2013 Physical type=Voltage Units=volt Initial value=1.3
CELEPOW	Import variable	Work-Power Streams=POWER Units=kW
FUELIN	Export variable	Stream-Var Stream=FUEL1 Substreams=MIXED Variable=MOLE-FLOW Units=mol/sec
FUEINH2O	Export variable	Mole-Flow Stream=FUEL1 Substreams=MIXED Components=H2O Units=mol/sec
FUEINCO2	Export variable	Mole-Flow Stream=FUEL1 Substreams=MIXED Components=CO2 Units=mol/sec
RATIO2	Import variable	Parameter Parameter no.=10002 Physical type=Dimensionless Units=Unitless Initial value=0.9

New Delete Copy Paste Move Up Move Down View Variables

Variable: RATIO2

Category: All

Reference: Parameter

Parameter no.: 10002

Physical type: Dimensionless

Units: Unitless

Initial value: 0.9

Main Flowsheet × SN × +

Define Spec Vary Fortran Declarations EO Options Comments

Manipulated variable

Type: Parameter

Parameter no.: 10002

Physical type: Dimensionless

Units: Unitless

Initial value: 0.9

Manipulated variable limits

Lower: 0

Upper: 1

Step size:

Maximum step size:

Report labels

Line 1 Line 2 Line 3 Line 4

EO input

Open variable:

Description:

- 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.