NOVEMBER 15TH, 2022

Modeling Grey, Blue and Green Hydrogen Production using AVEVA PRO/II Simulation

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Modeling grey, blue and green hydrogen production

Challenge

- Technip Energies (T.EN) is the market leader in the EPC of grey H_2 plants
- Classical grey hydrogen production via Steam Methane Reforming (SMR) will be complimented in the future by blue and green H_2 plants

Solution

- PRO/II is the platform that T.EN uses for the heat and material balance of our H_2 plants
- Incorporate the unit operations required for blue and green plants into our existing PRO/II models

Benefits

- Support the current and future demands for all types of hydrogen production facilities

Technip Energies At A Glance

Listed on
Euronext Paris
Stock Exchange

Headquartered in **Paris**
Registered in
The Netherlands

60+
years of operations

€6B
Full year 2020 adjusted revenue

A leading Project, Engineering & Technology company for the Energy Transition

€16.5B
Backlog at end September 2021

~15,000
Employees in 34 countries

25+
Leading proprietary technologies

450 projects
Under execution

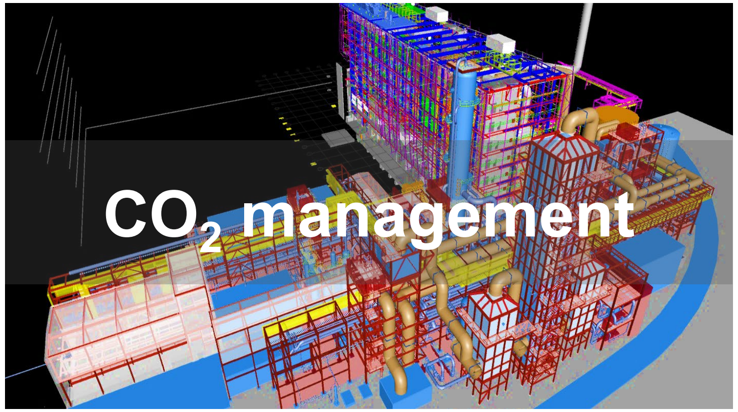
Unlocking The Energy Chains Of Tomorrow

Hydrogen

- A world leader with >270 plants delivered (>35% of installed base)
- Recognized partner of choice (Air Products, McPhy)

Sustainable chemistry

- Key proprietary technologies in biochemicals and biofuels
- Introducing circularity to conventional ethylene production
- Notable alliances such as with Neste, PLAnet



CO_2 management

- >50 references for CO_2 removal solutions
- Strategic alliance with Shell CANSOLV® on CO_2 capture

World Leader In Hydrogen

Ready For The Hydrogen Wave

270+
H_2 plants & reformer

5 to 220
MMSCFD
H_2 plants

20+
H_2 plants
120 to 220
MMSCFD

3B SCFD &
40+ plants
for
Air Products
since 1992

24+
H_2 plants with pre-reformer

9+
H_2 plants with parallel reformer

1st
Polybed PSA unit in a H_2 plant

50+
CO_2 Capture plants

- CUSTOMIZED SOLUTIONS
- SINGLE-SOURCE RESPONSIBILITY
- STATE-OF-THE-ART DESIGNS
- EXTENSIVE REFERENCE BASE

Colors Of Hydrogen

Grey

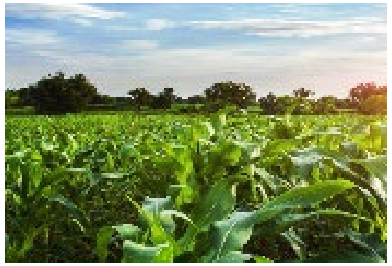
H_2 produced from fossil fuels in which CO_2 is an emission

Blue

H_2 produced from fossil fuels but CO_2 is captured

Green

H_2 produced from renewable feed stocks and often called “clean hydrogen”

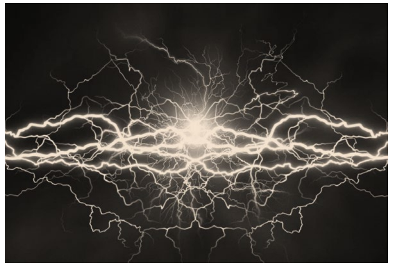


Turquoise

H_2 produced from natural gas through pyrolysis generating solid carbon as a byproduct

Pink

H_2 produced from electrolysis through nuclear energy



Reforming Basics – Reactions In PRO/II

Reforming

$CH_4 + H_2O \rightarrow 3H_2 + CO$

$CH_4 + ½\, O_2 \rightarrow 2H_2 + CO$

$CO + H_2O \rightarrow H_2 + CO_2$

$C_xH_y + 2xH_2O \rightarrow \frac{4x+y}{2}H_2 + xCO_2$

Overall endothermic reaction which takes place over nickel catalyst

4 moles of H_2 = 1 mole of CO_2

100 kg of H_2 = 546 kg CO_2

Combustion

$CH_4 + 2O_2 \rightarrow 2H_2O + CO_2$

$CO + ½\, O_2 \rightarrow CO_2$

$H_2 + ½\, O_2 \rightarrow H_2O$

Supplies the required heat of reaction using burners. Burners work on induced draft or balanced draft. Typical SMR radiant section efficiencies around 50% to 55%

Water Gas Shift (WGS)

$CO + H_2O = H_2 + CO_2$

WGS reaction is exothermic, takes place in vessels filled with catalyst

1 mole of H_2 = 1 mole of CO_2

100 kg of H_2 = 2184 kg CO_2

PRO/II Reactors

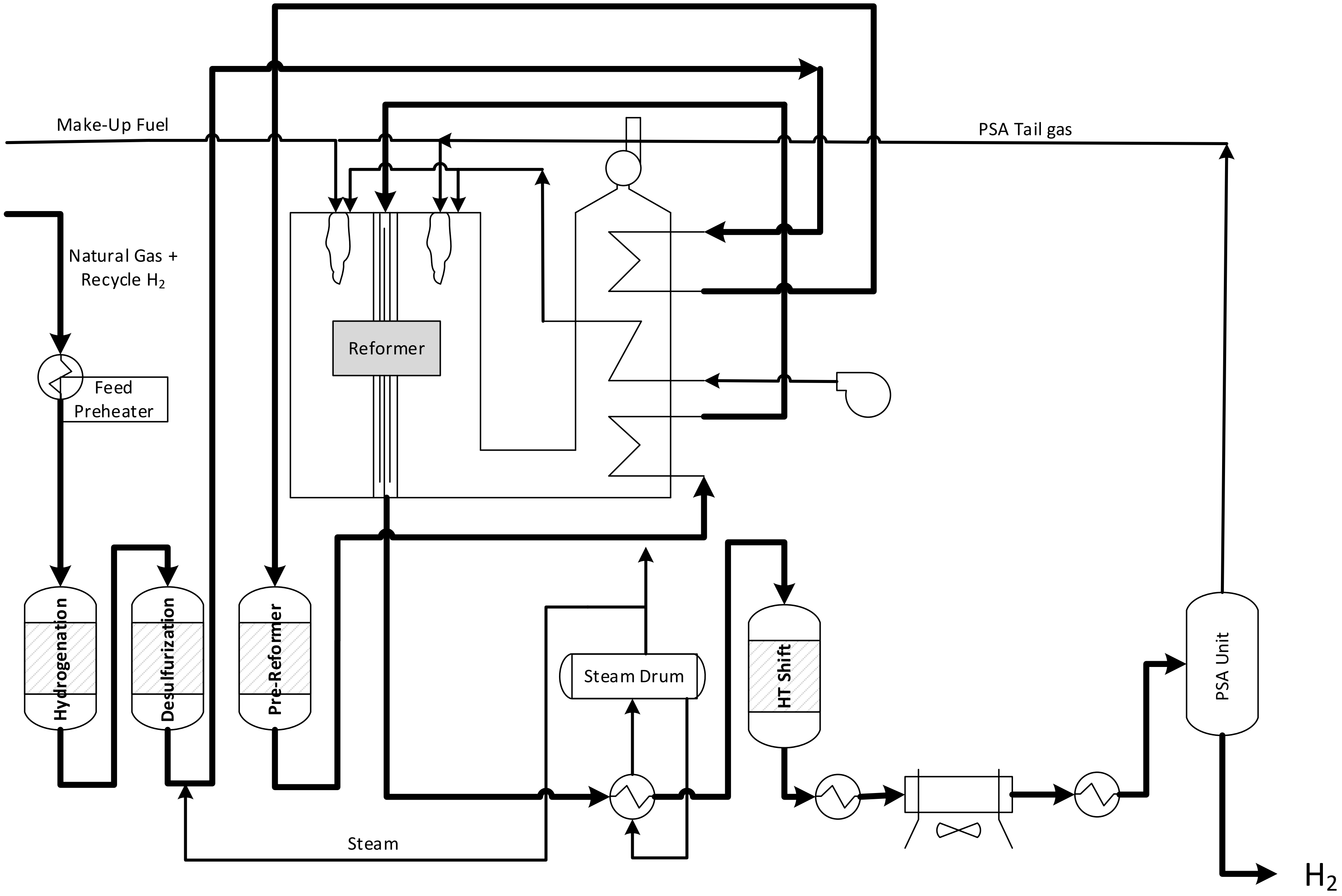
Conversion Reactor

- Hydrolysis - higher hydrocarbons to CO (prior to Equilibrium Reactor)
- Combustion
- Electrolyzer
- Methane Pyrolysis

Equilibrium Reactor

- Methanation Reactor
  - Methane-Steam Reaction – Equilibrium Predefined in PRO/II (nice!)
    - $CH_4 + H_2O = CO + 3H_2$
    - K_{eq} = f(temperature)
  - Water-Gas Shift Reaction – Equilibrium Predefined in PRO/II (nice!)
    - $CO + H_2O = CO_2 + H_2$
    - K_{eq} = f(temperature)
- Water Gas Shift Reactor
  - WGS equilibrium controlled
  - No methane-steam reaction

Grey H_2 Plant Basic Flowsheet: SMR

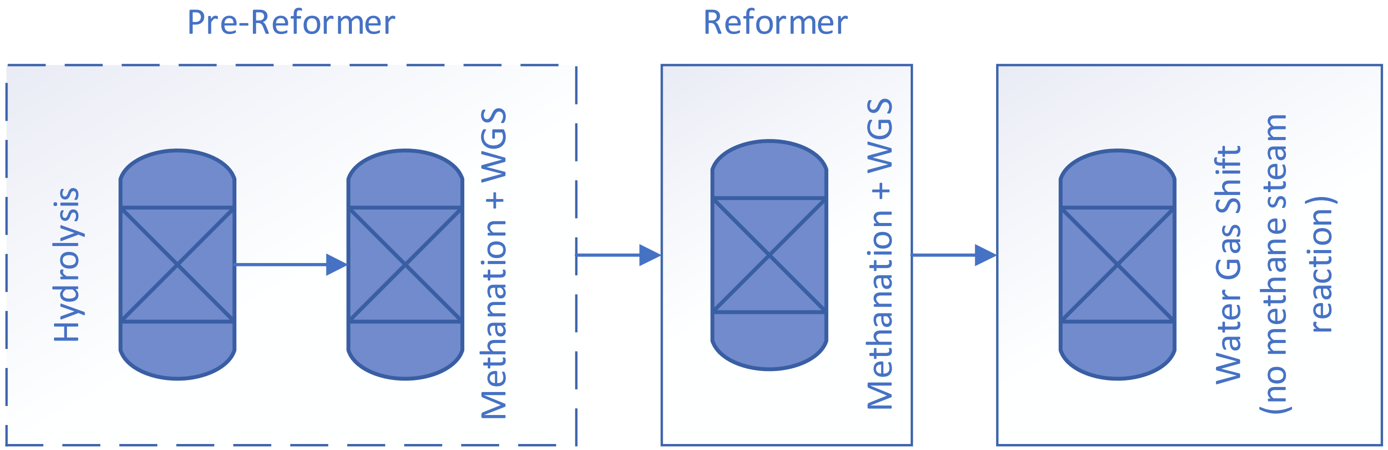


TECHNIP ENERGIES

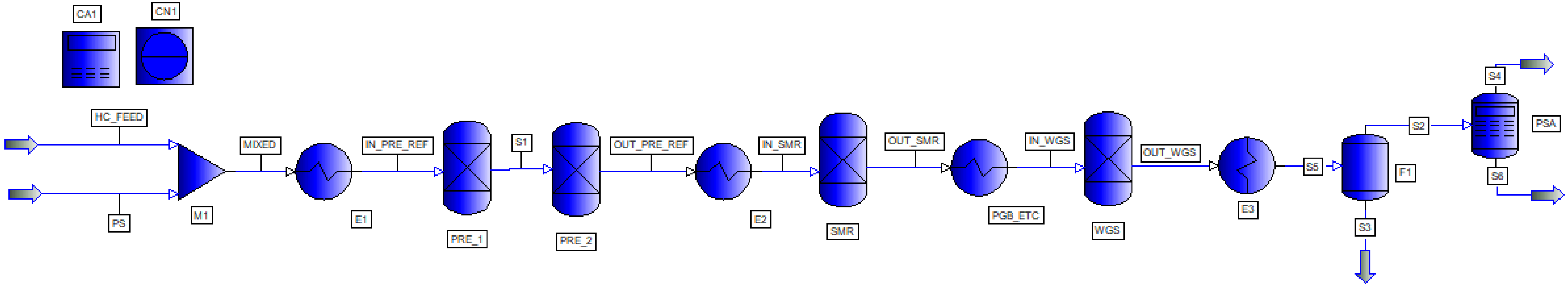
CONFIDENTIAL

SMR Reactor Sequence

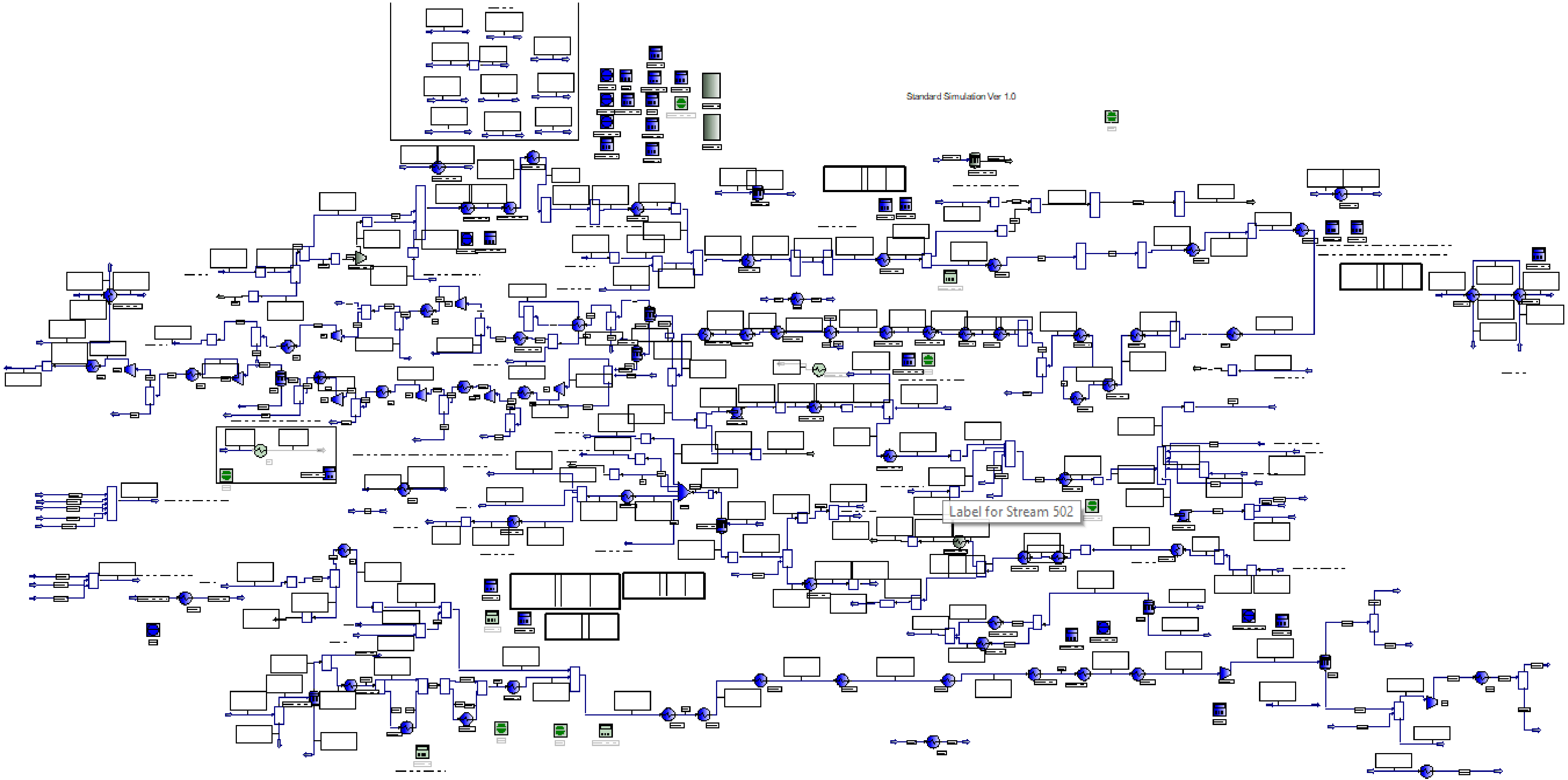
1. **Pre-Reformer will convert higher hydrocarbons to CO, CO and CH_4**
   - Model a pre-reformer in two separate adiabatic reactors in series (one actual reactor)
     - Conversion Reactor: Hydrolysis of hydrocarbons → CO
     - Equilibrium Reactor: Methane-Steam reaction + Water Gas Shift reaction
2. **SMR is modeled as a single equilibrium reactor "Methanation"**
3. **Water Gas Shift modeled as a single equilibrium reactor "Shift"**



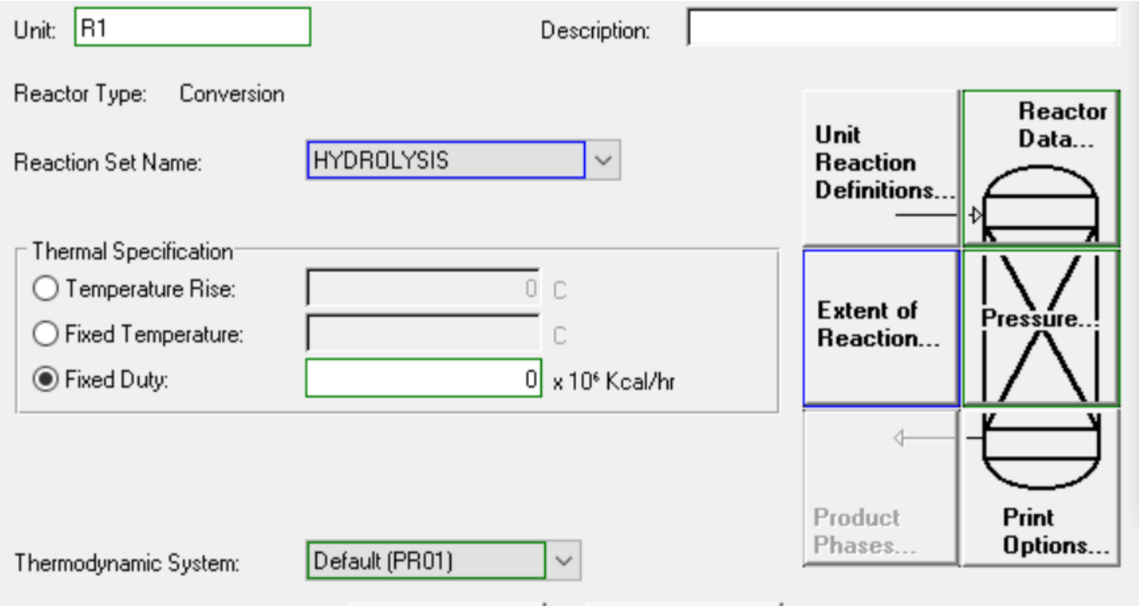
PRO/II - Grey SMR H_2 Plant Overview - Simplified



Blue H_2 SMR – Complex Simulation



Hydrolysis in PRO/II: Conversion Reactor



Unit: R1

Description:

Reactor Type: Conversion

Reaction Set Name: HYDROLYSIS

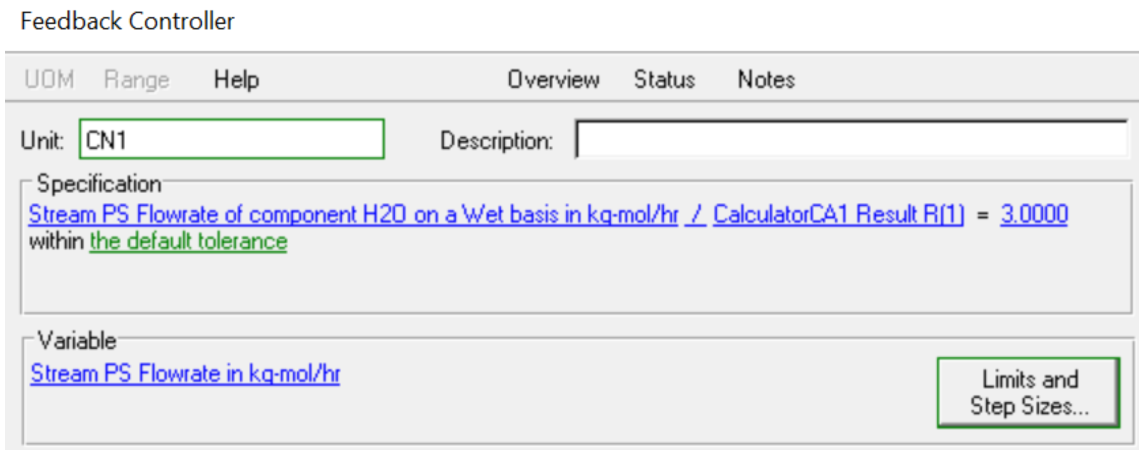
Thermal Specification

○ Temperature Rise: 0 C

○ Fixed Temperature: C

● Fixed Duty: 0 $\times 10^6$ Kcal/hr

Thermodynamic System: Default (PR01)



Feedback Controller

Unit: CN1

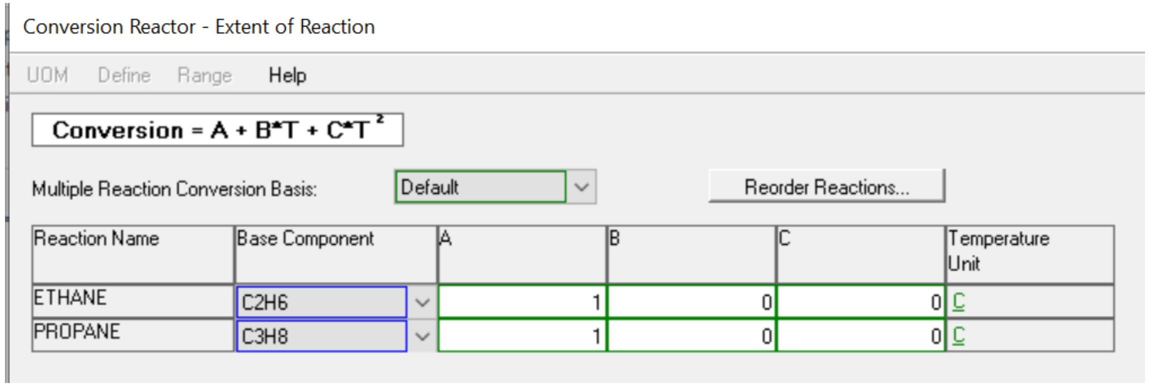
Description:

Specification

Stream PS Flowrate of component H2O on a Wet basis in kg-mol/hr / CalculatorCA1 Result R(1) = 3.0000 within the default tolerance

Variable

Stream PS Flowrate in kg-mol/hr



Conversion Reactor - Extent of Reaction

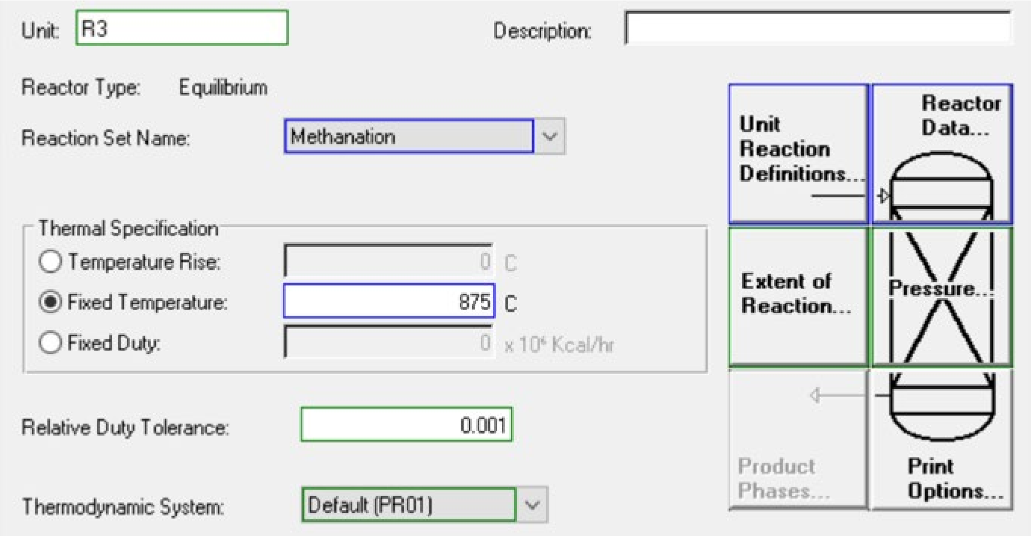
$\text{Conversion} = A + B*T + C*T^2$

Multiple Reaction Conversion Basis: Default

Reaction Name	Base Component	A	B	C	Temperature Unit
ETHANE	C2H6	1	0	0	C
PROPANE	C3H8	1	0	0	C

- Used for step 1 of the Pre-Reformer

Methanation in PRO/II : Equilibrium Reactor



Unit: R3

Description:

Reactor Type: Equilibrium

Reaction Set Name: Methanation

Thermal Specification

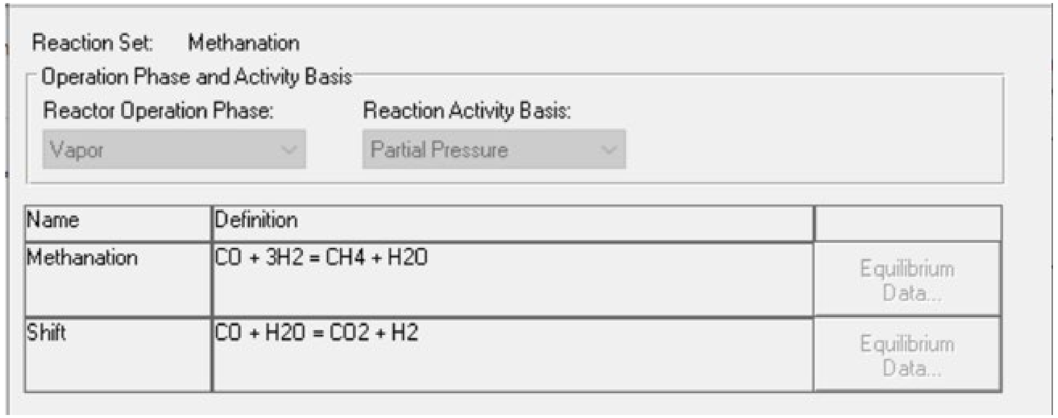
○ Temperature Rise: 0 C

● Fixed Temperature: 875 C

○ Fixed Duty: 0 x 10⁶ Kcal/hr

Relative Duty Tolerance: 0.001

Thermodynamic System: Default (PR01)



Reaction Set: Methanation

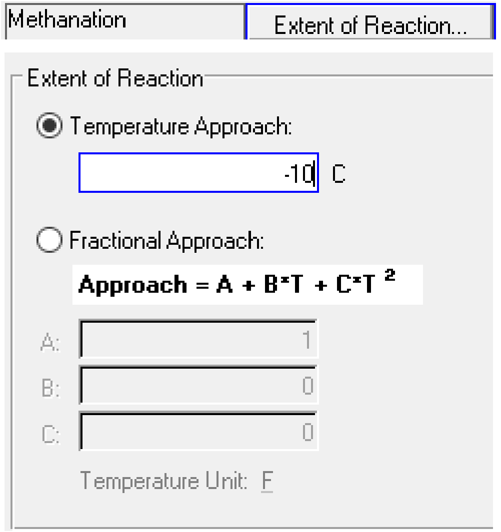
Operation Phase and Activity Basis

Reactor Operation Phase: Vapor

Reaction Activity Basis: Partial Pressure

Name	Definition	
Methanation	CO + 3H2 = CH4 + H2O	Equilibrium Data...
Shift	CO + H2O = CO2 + H2	Equilibrium Data...

- Used for Pre-Reformer (step 2), Steam-Methane Reformer (SMR), Autothermal Reformer (ATR)
- Predefined methanation reaction
- Methanation and water gas shift reactions take place simultaneously



Methanation

Extent of Reaction

● Temperature Approach: -10 C

○ Fractional Approach:

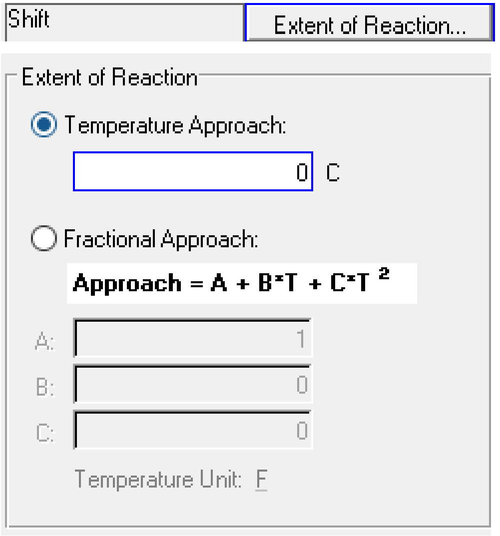
Approach = A + B*T + C*T ²

A: 1

B: 0

C: 0

Temperature Unit: F



Shift

Extent of Reaction

● Temperature Approach: 0 C

○ Fractional Approach:

Approach = A + B*T + C*T ²

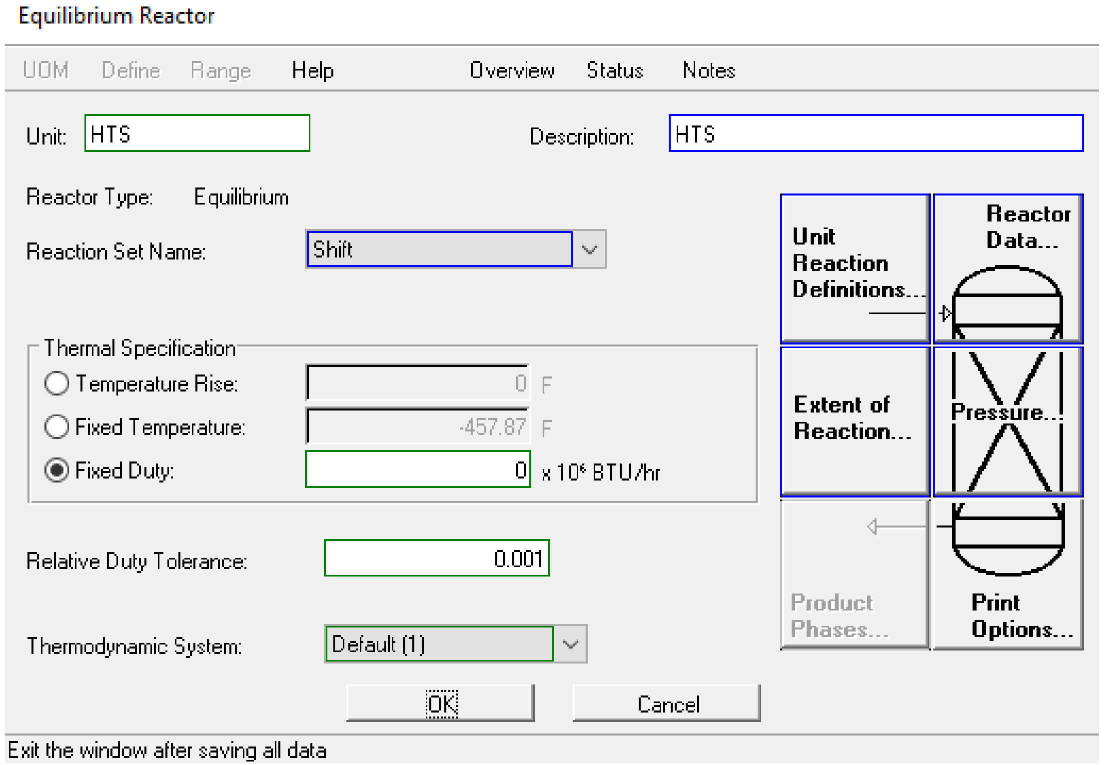
A: 1

B: 0

C: 0

Temperature Unit: F

Water Gas Shift in PRO/II : Equilibrium Reactor



Equilibrium Reactor

Unit: HTS

Description: HTS

Reactor Type: Equilibrium

Reaction Set Name: Shift

Thermal Specification

○ Temperature Rise: 0 F

○ Fixed Temperature: -457.87 F

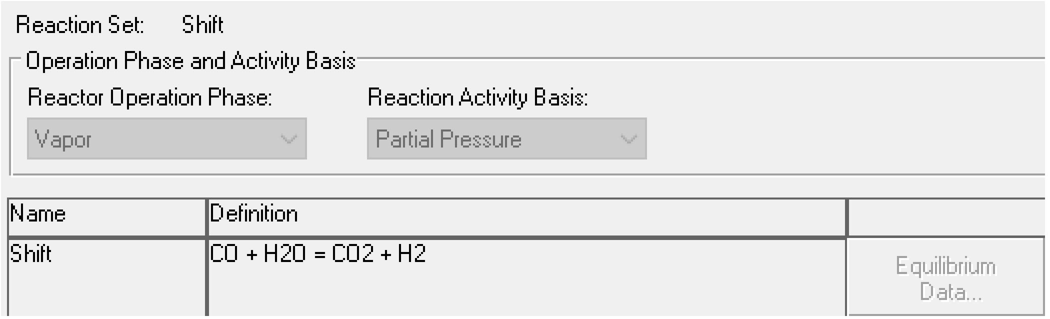
● Fixed Duty: 0 x 10^6 BTU/hr

Relative Duty Tolerance: 0.001

Thermodynamic System: Default (1)

Exit the window after saving all data

- Predefined shift reaction
- Only water gas shift reaction takes place



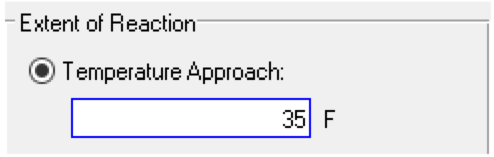
Reaction Set: Shift

Operation Phase and Activity Basis

Reactor Operation Phase: Vapor

Reaction Activity Basis: Partial Pressure

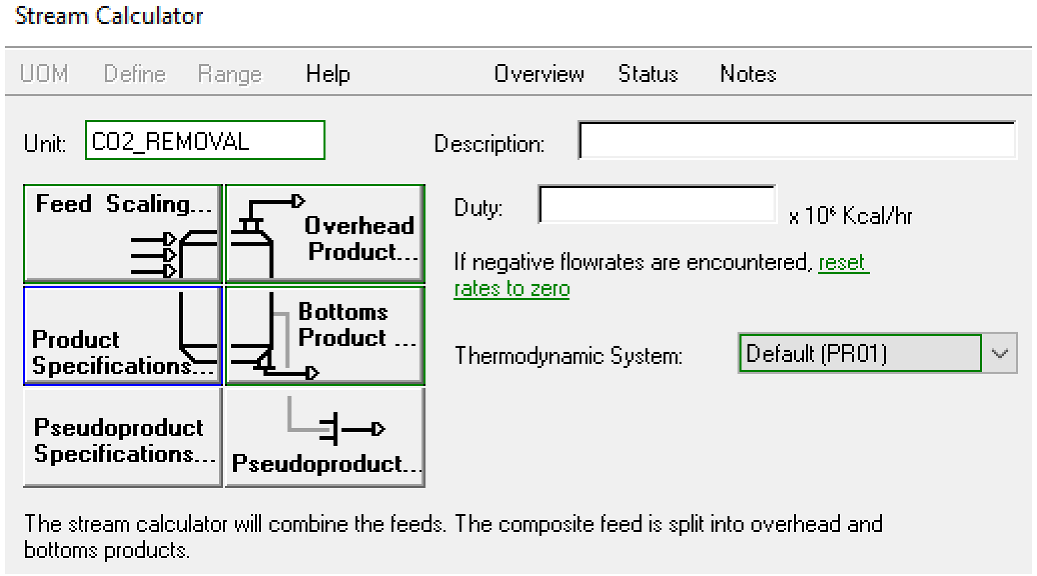
Name	Definition
Shift	CO + H2O = CO2 + H2



Extent of Reaction

● Temperature Approach: 35 F

PSA and CO_2 Removal in PRO/II : Stream Calculator



Unit: CO2_REMOVAL

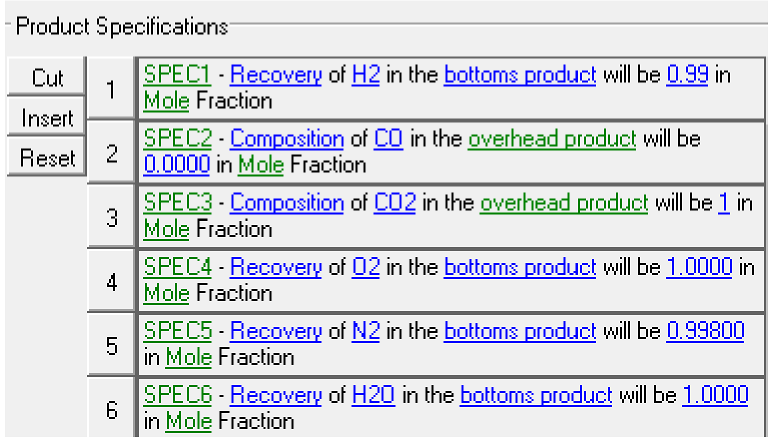
Description:

Duty: x 10⁶ Kcal/hr

If negative flowrates are encountered, reset rates to zero

Thermodynamic System: Default (PR01)

The stream calculator will combine the feeds. The composite feed is split into overhead and bottoms products.



1 SPEC1 - Recovery of H2 in the bottoms product will be 0.99 in Mole Fraction

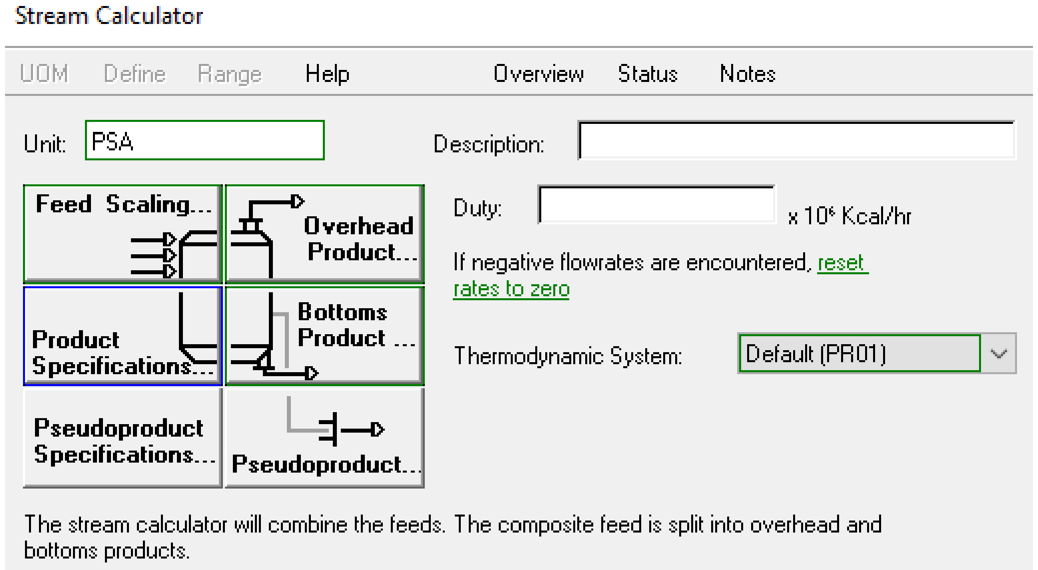
2 SPEC2 - Composition of CO in the overhead product will be 0.0000 in Mole Fraction

3 SPEC3 - Composition of CO2 in the overhead product will be 1 in Mole Fraction

4 SPEC4 - Recovery of O2 in the bottoms product will be 1.0000 in Mole Fraction

5 SPEC5 - Recovery of N2 in the bottoms product will be 0.99800 in Mole Fraction

6 SPEC6 - Recovery of H2O in the bottoms product will be 1.0000 in Mole Fraction



Unit: PSA

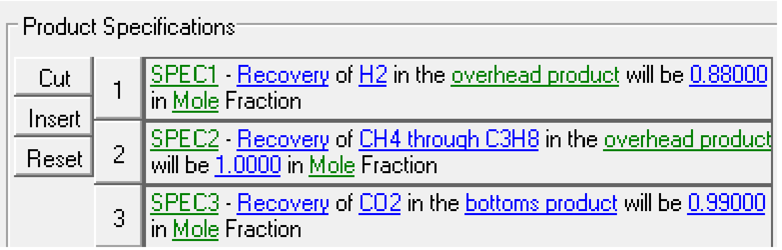
Description:

Duty: x 10⁶ Kcal/hr

If negative flowrates are encountered, reset rates to zero

Thermodynamic System: Default (PR01)

The stream calculator will combine the feeds. The composite feed is split into overhead and bottoms products.



1 SPEC1 - Recovery of H2 in the overhead product will be 0.88000 in Mole Fraction

2 SPEC2 - Recovery of CH4 through C3H8 in the overhead product will be 1.0000 in Mole Fraction

3 SPEC3 - Recovery of CO2 in the bottoms product will be 0.99000 in Mole Fraction

Route To Blue Hydrogen

Steam Methane Reformer

- Reduction in fired duty using
  - Pre-reformer
  - Air Preheaters
  - Lower S/C
  - Advanced heat recovery cycles
- Using Technip Energies proprietary equipment
  - EARTH®
  - Technip Parallel Reformer® (TPR®)
- Improves energy efficiencies while reducing CO_2 footprint

Auto Thermal Reformer

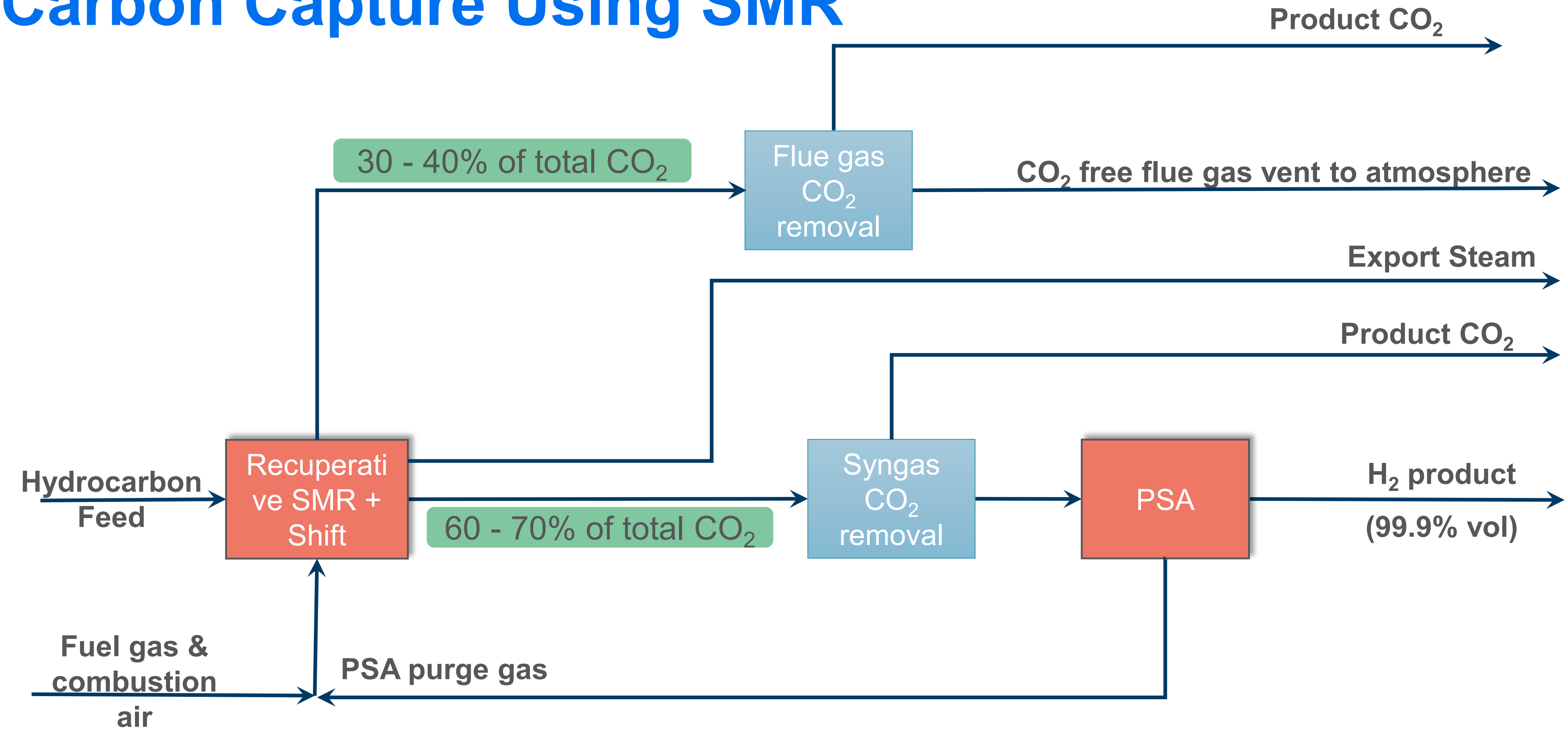
- Traditionally used for ammonia, methanol, GTL, HyCO, DRI plants
- Now relevant to blue hydrogen plants
- Syngas has lower H_2:CO ratios
- Minimal flue gas emissions (Fired heater for feed preheat required)
- Requires an Air Separation Unit (ASU) which can be energy and capital intensive, possible application of green electricity.

Carbon Capture

- Use of solvents to capture CO_2 from
  - Syngas
  - Flue gas
- Removal of CO_2 from syngas substantially easier than removal from flue gas
- Other CO_2 removal technologies applicable such as membrane, cryogenic capture.

Co-Generation via integration of gas turbine or steam turbine possible for all options.

Carbon Capture Using SMR



Product CO_2

30 - 40% of total CO_2

Flue gas CO_2 removal

CO_2 free flue gas vent to atmosphere

Export Steam

Product CO_2

Hydrocarbon Feed

Recuperative SMR + Shift

60 - 70% of total CO_2

Syngas CO_2 removal

PSA

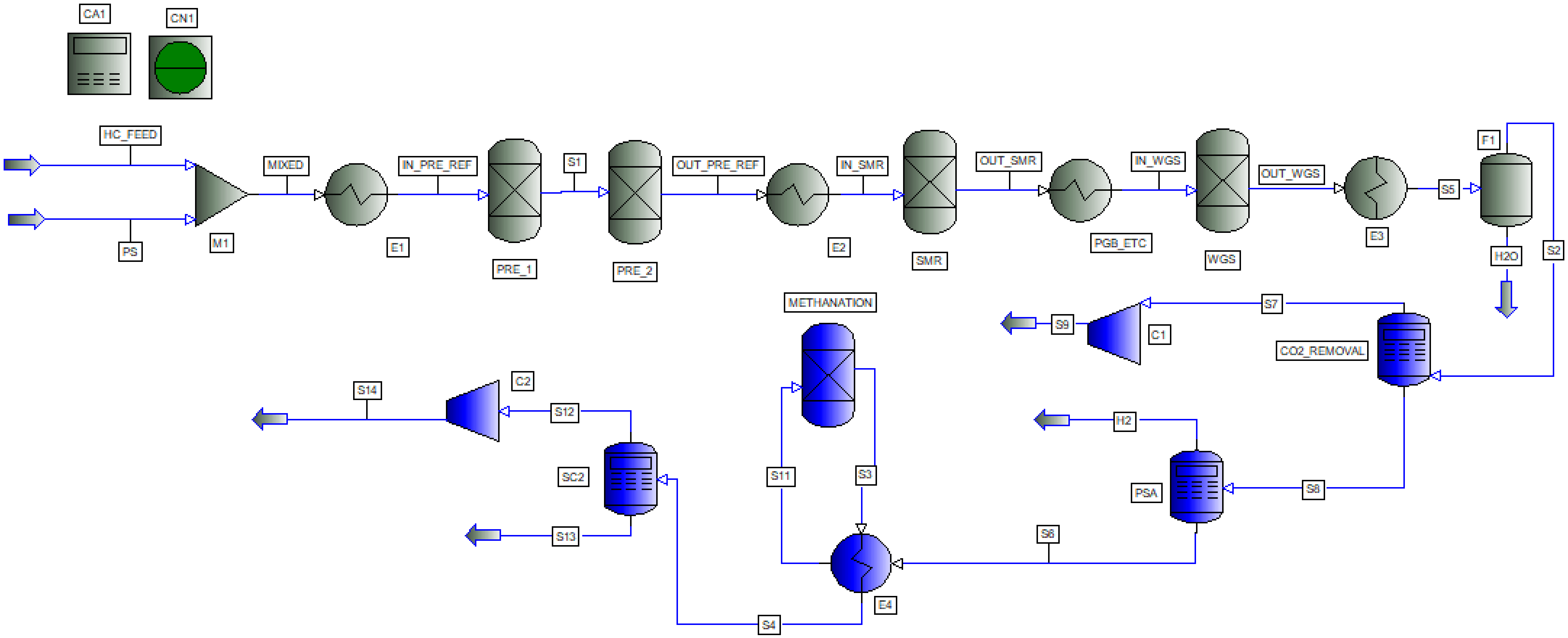
H_2 product (99.9% vol)

Fuel gas & combustion air

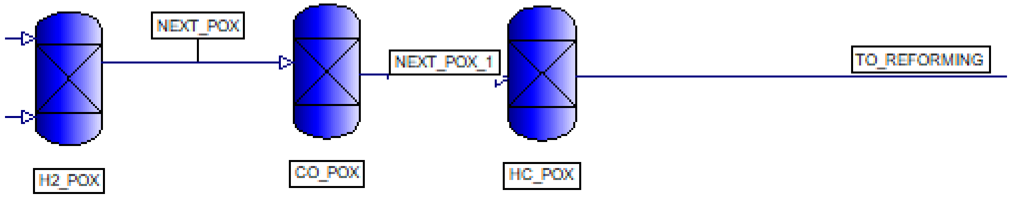
PSA purge gas

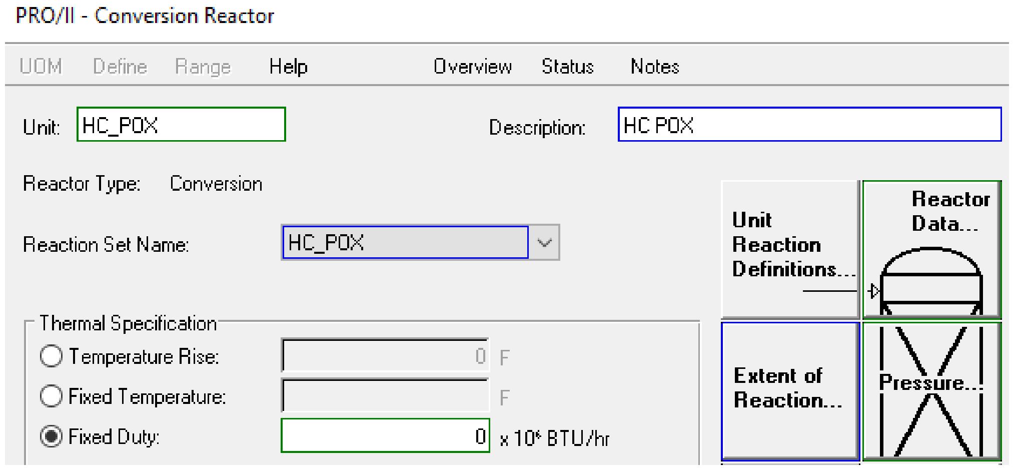
Carbon emission index << 1 kg CO_2 / kg H_2

Reactor Sequence For Blue SMR H_2 Plant



ATR for Blue H_2 (Step 1): Conversion Reactor





Unit: HC_POX

Description: HC POX

Reactor Type: Conversion

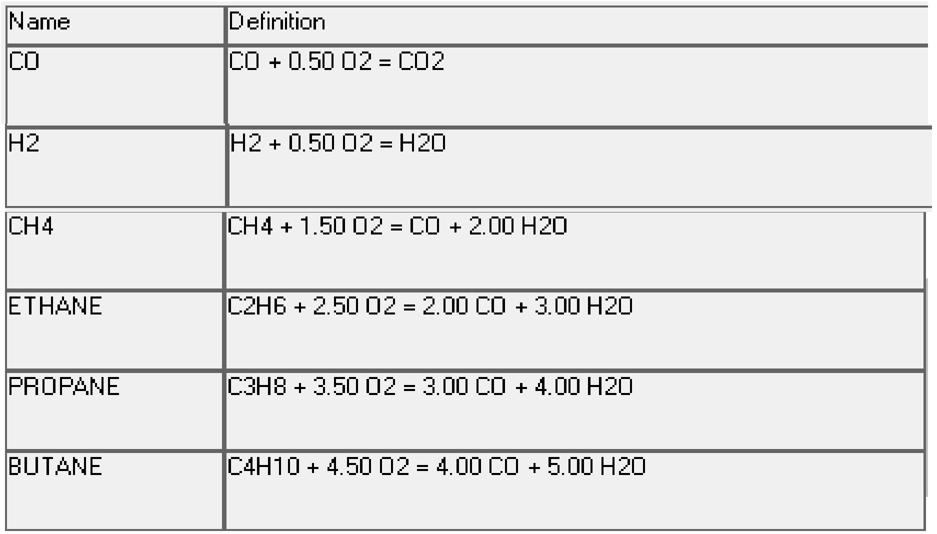
Reaction Set Name: HC_POX

Thermal Specification

○ Temperature Rise: 0 F

○ Fixed Temperature: F

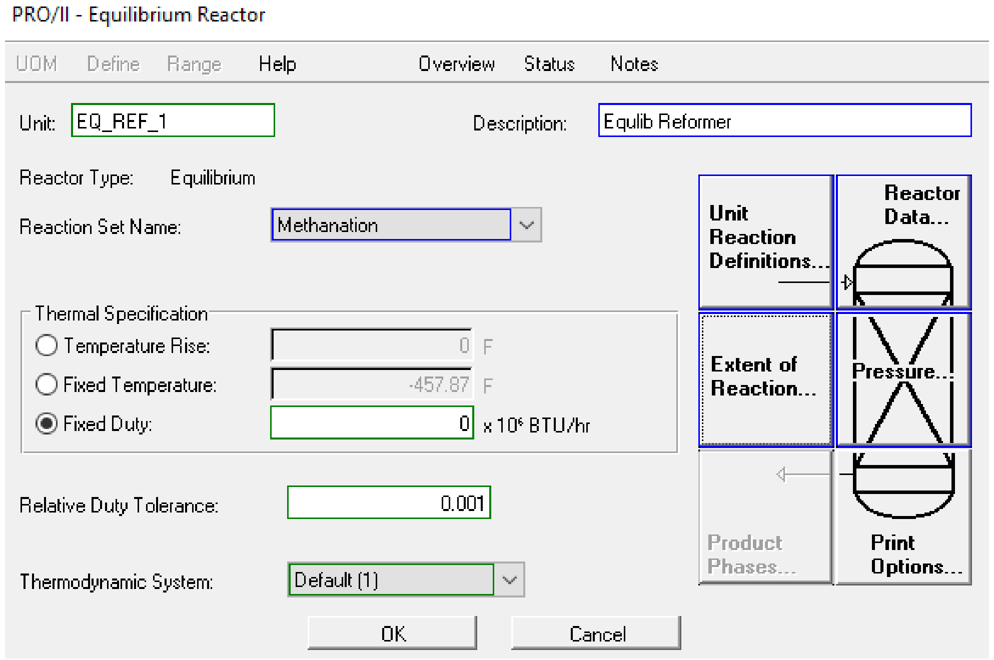
● Fixed Duty: 0 x 10⁶ BTU/hr



Name	Definition
CO	CO + 0.50 O2 = CO2
H2	H2 + 0.50 O2 = H2O
CH4	CH4 + 1.50 O2 = CO + 2.00 H2O
ETHANE	C2H6 + 2.50 O2 = 2.00 CO + 3.00 H2O
PROPANE	C3H8 + 3.50 O2 = 3.00 CO + 4.00 H2O
BUTANE	C4H10 + 4.50 O2 = 4.00 CO + 5.00 H2O

- Partial oxidation of H_2, CO and hydrocarbons

ATR for Blue H_2 (Step 2): Equilibrium Reactor



Unit: EQ_REF_1

Description: Equlib Reformer

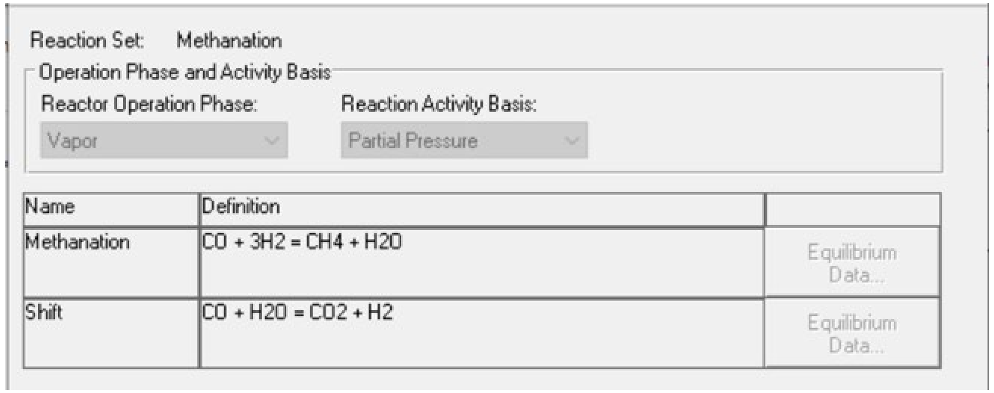
Reactor Type: Equilibrium

Reaction Set Name: Methanation

Thermal Specification
- ○ Temperature Rise: 0 F
- ○ Fixed Temperature: -457.87 F
- ● Fixed Duty: 0 x 10⁶ BTU/hr

Relative Duty Tolerance: 0.001

Thermodynamic System: Default (1)



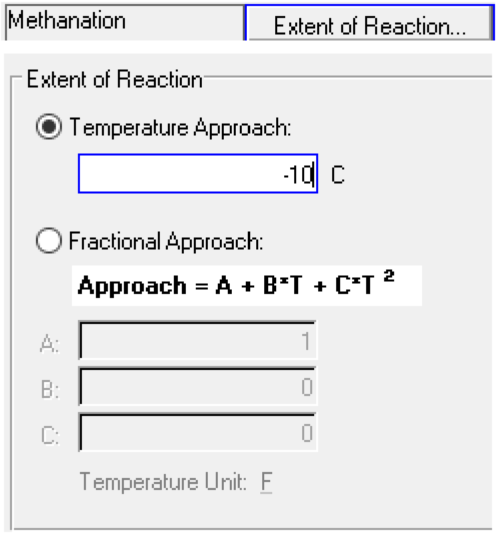
Reaction Set: Methanation

Operation Phase and Activity Basis

Reactor Operation Phase: Vapor

Reaction Activity Basis: Partial Pressure

Name	Definition	
Methanation	CO + 3H2 = CH4 + H2O	Equilibrium Data...
Shift	CO + H2O = CO2 + H2	Equilibrium Data...



Extent of Reaction
- ● Temperature Approach: -10 C
- ○ Fractional Approach:

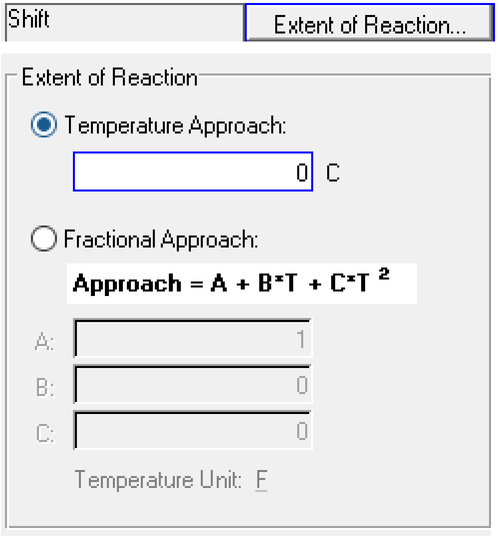
Approach = A + B*T + C*T ²

A: 1

B: 0

C: 0

Temperature Unit: F



Extent of Reaction
- ● Temperature Approach: 0 C
- ○ Fractional Approach:

Approach = A + B*T + C*T ²

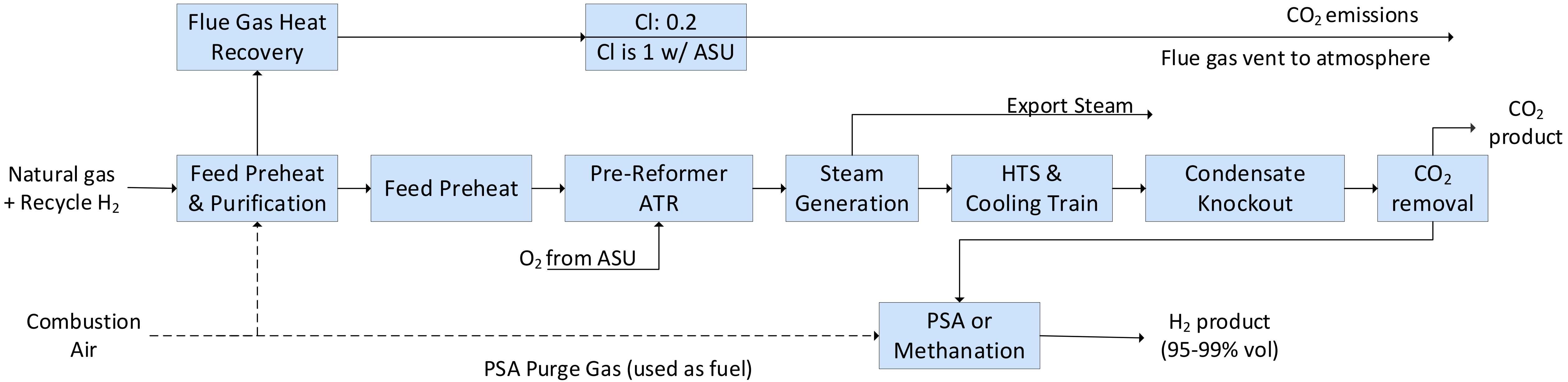
A: 1

B: 0

C: 0

Temperature Unit: F

ATR for blue H_2



Flue Gas Heat Recovery

Cl: 0.2
Cl is 1 w/ ASU

CO_2 emissions

Flue gas vent to atmosphere

Export Steam

CO_2 product

Natural gas + Recycle H_2

Feed Preheat & Purification

Feed Preheat

Pre-Reformer ATR

Steam Generation

HTS & Cooling Train

Condensate Knockout

CO_2 removal

O_2 from ASU

Combustion Air

PSA or Methanation

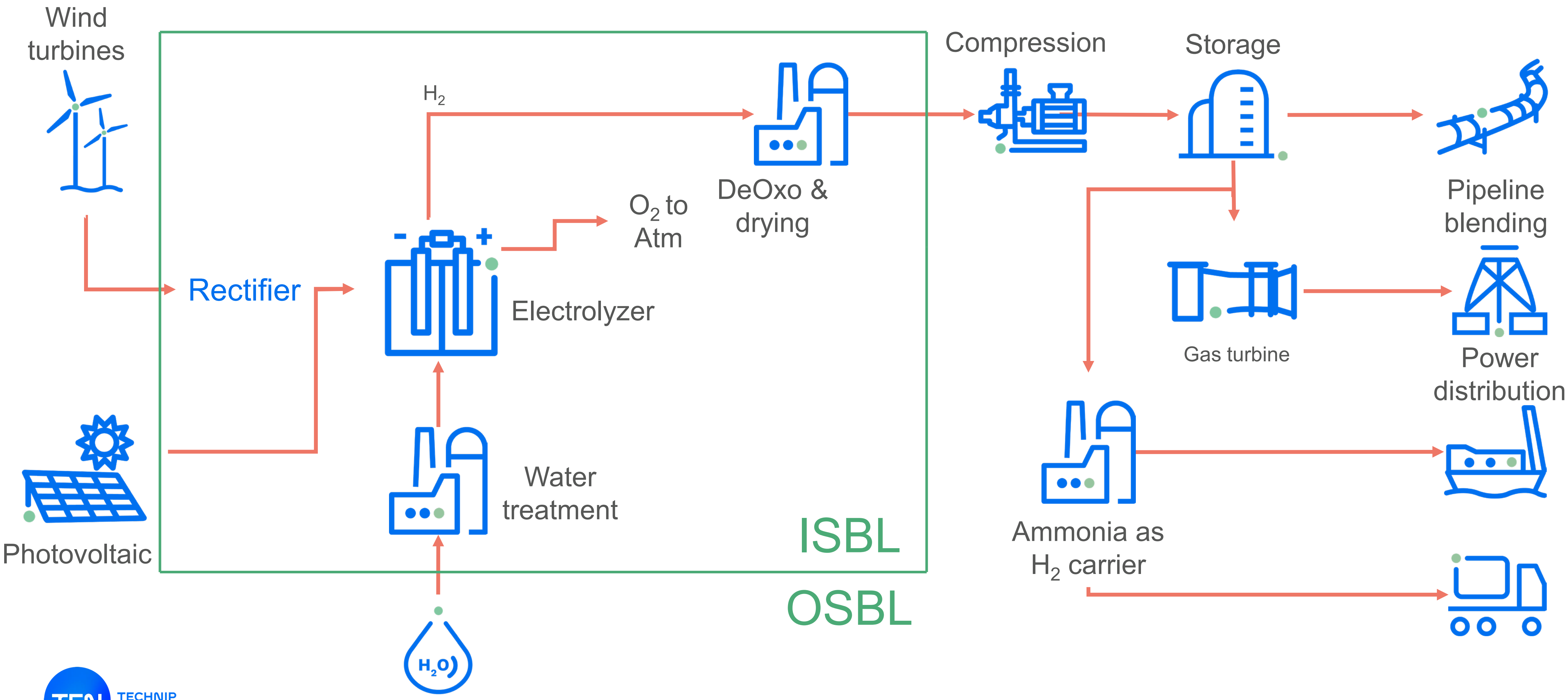
H_2 product (95-99% vol)

PSA Purge Gas (used as fuel)

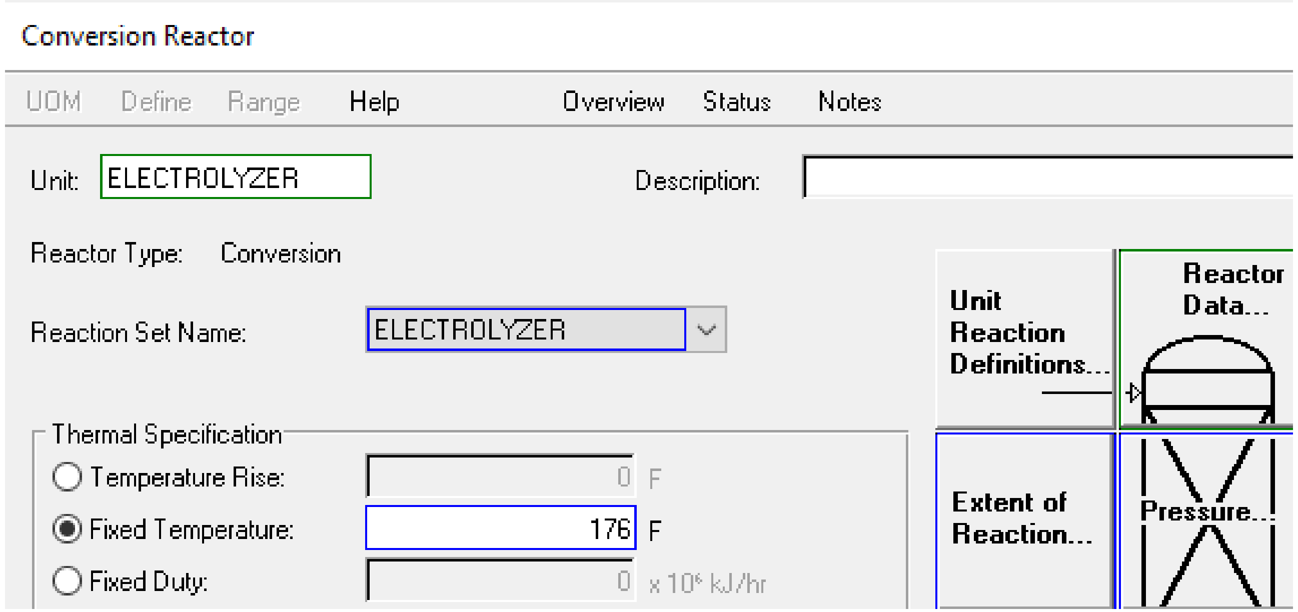
Hydrogen can be used as a fuel in fired heater

Green Hydrogen

ISBL / OSBL scope



Electrolyzer in PRO/II: Conversion Reactor



Unit: ELECTROLYZER

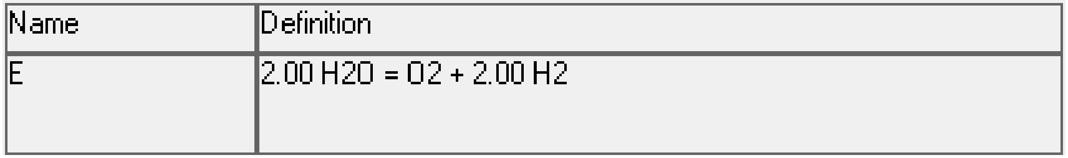
Description:

Reactor Type: Conversion

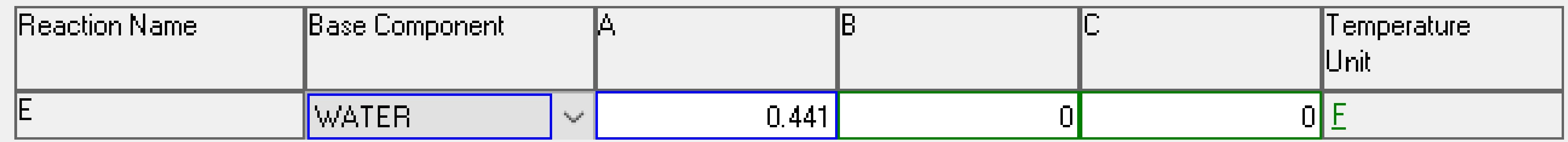
Reaction Set Name: ELECTROLYZER

Thermal Specification

- ○ Temperature Rise: 0 F
- ● Fixed Temperature: 176 F
- ○ Fixed Duty: 0 $\times 10^6$ kJ/hr



Name	Definition
E	$2.00\ H_2O = O_2 + 2.00\ H_2$



Reaction Name	Base Component	A	B	C	Temperature Unit
E	WATER	0.441	0	0	F

New Ways To Make An Old Molecule

Examples of alternate feedstocks for hydrogen production

- Electrolysis of Water
- Steam Reforming of Non-Fossil Feeds
  - Refined products
    - Ethanol
    - Synthetic natural gas
  - Partially processed materials
    - Vegetable oils
    - Biogas
    - Bio oil from fast pyrolysis
- Gasification of Non-Fossil Feeds
  - Raw bio-sourced feeds such as biomass
  - Municipal Solid Waste
- Cracking
  - Ammonia, Natural Gas

Sustainable Chemistry

Questions?

Please wait for the microphone.

State your name and company.

Please remember to…

Navigate to this session in the mobile app to complete the survey.

Thank you!

in linkedin.com/company/aveva

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ABOUT AVEVA

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Over 20,000 enterprises in over 100 countries rely on AVEVA to help them deliver life's essentials: safe and reliable energy, food, medicines, infrastructure and more. By connecting people with trusted information and AI-enriched insights, AVEVA enables teams to engineer efficiently and optimize operations, driving growth and sustainability.

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