AVEVA PI WORLD

Sustainable Process Design using AVEVA™ Process Simulation

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Agenda

1. What is AVEVA Process Simulation?
2. Greenhouse Gas Emissions
3. Hydrogen Production
4. Renewable Energy
5. Takeaways

Introduction to AVEVA Process Simulation

Reduce Total Ownership Cost and Engineering Hours

AVEVA Process Simulation – Driving Digital Transformation

Designed from the ground up, delivering the process digital twin, to the next generation of engineers

Designed from the Ground Up

- Multi-core
- Continuously saved for cloud
- Role-based user interface
- Open model writing

Delivering the Process Digital Twin

- Design, Rating and Dynamic modes
- Libraries for different assets
- One single model for the entire asset lifecycle

To the Next Generation of Process Engineers

- Groundbreaking ease of use
- Instantaneous results
- Intuitive user interface

50% reduction in simulation effort across the lifecycle

Collaboration internally and externally

Adaptable for sustainable process development

Improved engineering workflow

Enables true Digital Transformation

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AVEVA Process Simulation Capabilities

SimSci Thermodynamics

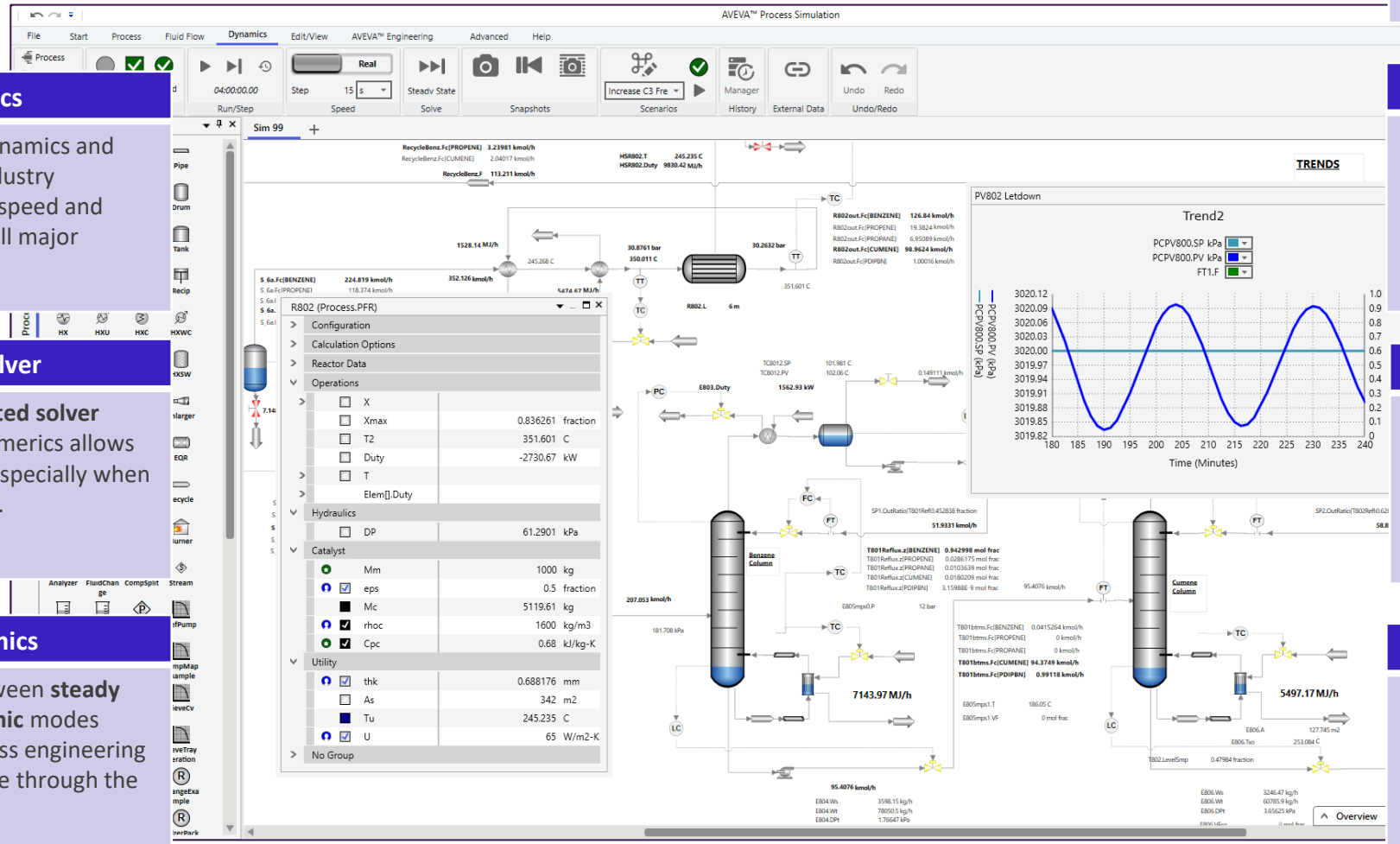
Proven **SimSci** thermodynamics and data import based on industry standards provides high-speed and accurate solutions with all major **thermo methods**.

Equation-Oriented Solver

A robust **equation-oriented solver** using state-of-the-art numerics allows for efficient calculation especially when there are lots of recycles.

Steady-State & Dynamics

Seamless switching between **steady state, rating,** and **dynamic** modes drives collaboration across engineering domains and model reuse through the project lifecycle.



Ease of Use

The **continuously-solved** and **highly-interactive** behavior with **Undo** enables rapid problem exploration and fast adoption by next-generation users.

Library Approach

Model libraries for process utilities (**steam**, **cooling water**, **flares**), as well as **process** simulation allows a common platform for process department simulation.

Open Modeling

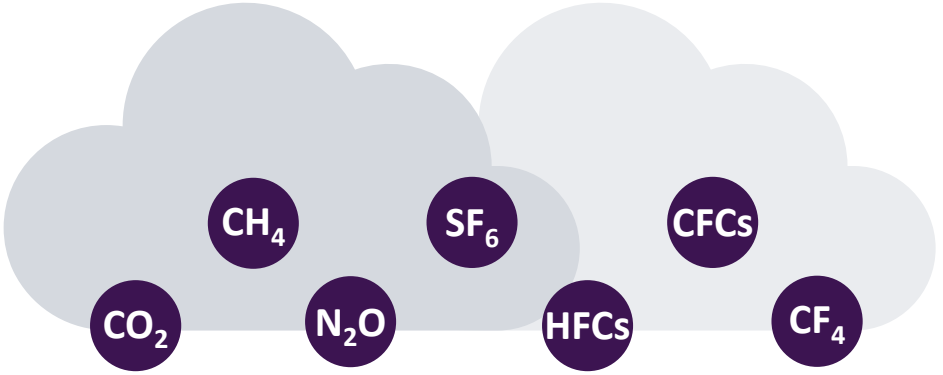
Access to the **mathematical equations** enables process engineers to both customize and add new equipment models without programming.

New Applications

The **open platform extendable** architecture allows the expansion of process simulation into other industries such as batch, power, and more

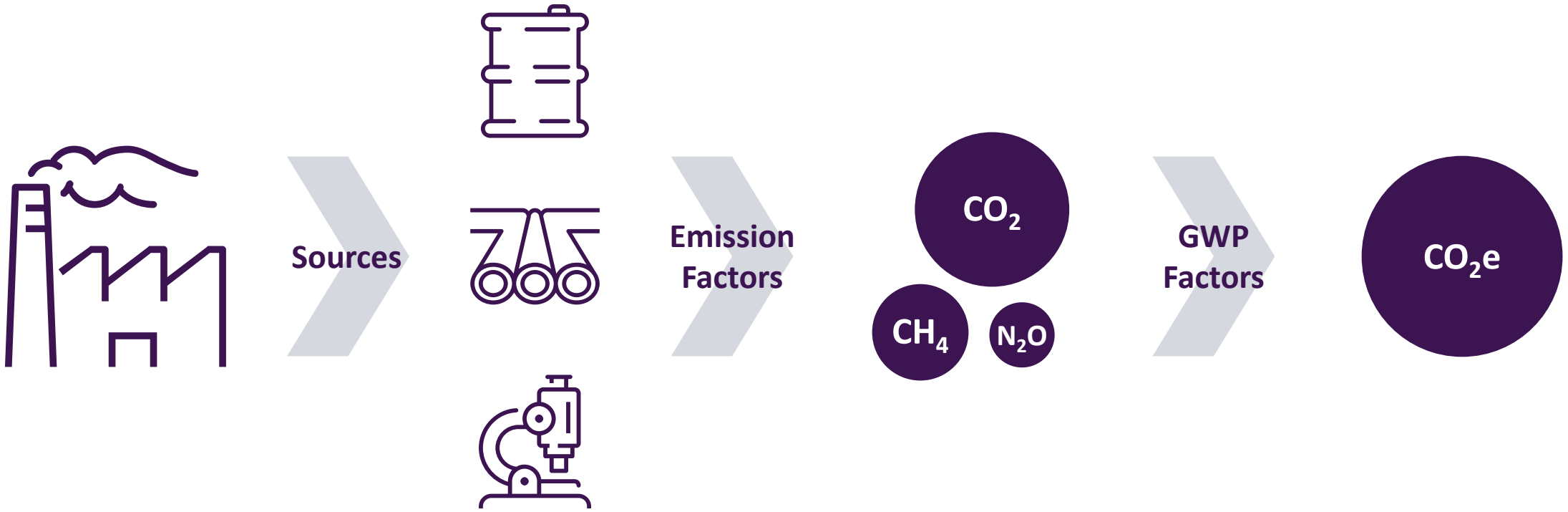
Greenhouse Gas (GHG) Emission Calculations

Greenhouse Gas Emissions

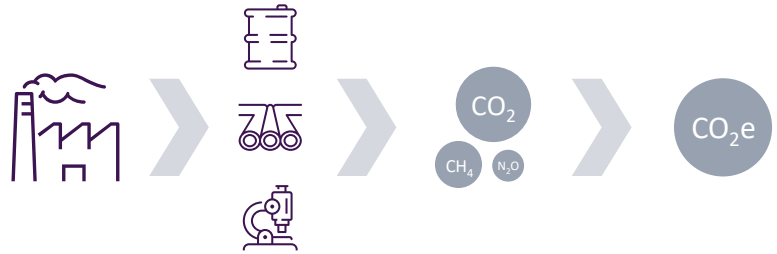


- Nearly all processes release GHGs into the atmosphere through:
  - Stationary combustion
  - Combustion of waste gases
  - Purchased gases
  - Indirect emissions from purchased steam and electricity
- Most countries have begun to limit GHG emissions and have strict targets for reducing them
- AVEVA Process Simulation can calculate greenhouse gas emissions and optimize processes to reduce the overall carbon footprint
- GHG models are included in the **Economics** library of AVEVA Process Simulation

How to Calculate GHG Emissions?



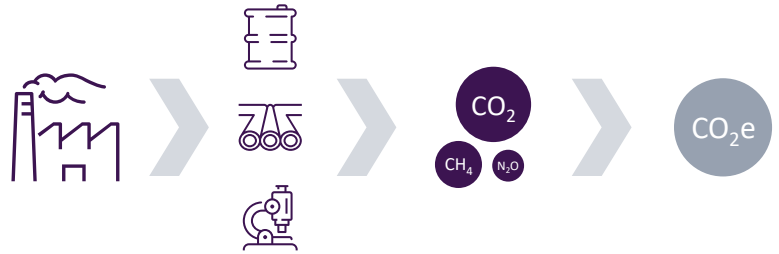
Types of Emission Sources



- The US Environmental Protection Agency (EPA) separates emissions into 3 unique ‘scopes’
- Scope 1 – Direct emissions from your organization
  - Stationary Combustion, Waste Gas, Purchased Gases, Mobile Sources, Refrigeration, Fire Suppression
- Scope 2 – Indirect emissions from energy and steam generation
  - Steam, Electricity
- Scope 3 – Other indirect emissions from your value chain
  - Business Travel, Commuting, Product Transport, Waste

Calculated in AVEVA Process Simulation

Understanding Emission Factors (EFs)



- Emission Factors describe the **quantity of pollutant** released from a material per **unit**
  - For example, stationary combustion of Natural Gas produces about 53.06 [kg CO_2 / MMBtu] = 0.0544 [kg CO_2 / scf]
- Common units are mass of pollutant per weight, volume, energy, or time
- EFs can be calculated for every material at various stages of the product lifecycle
  - What quantity of emissions are produced per kg of material produced?
  - What quantity are produced per kg of material burned?

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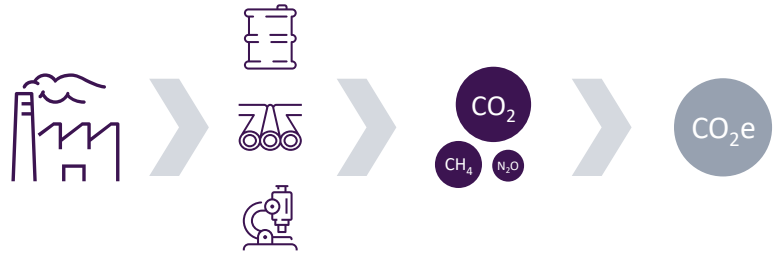
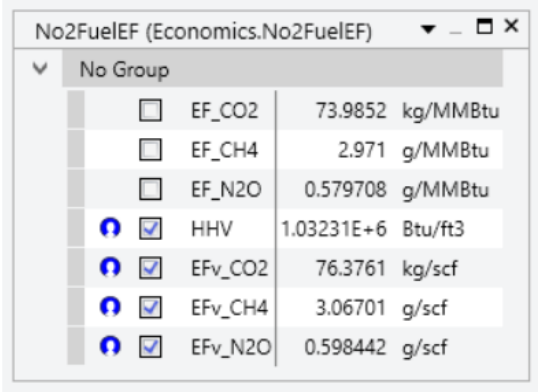
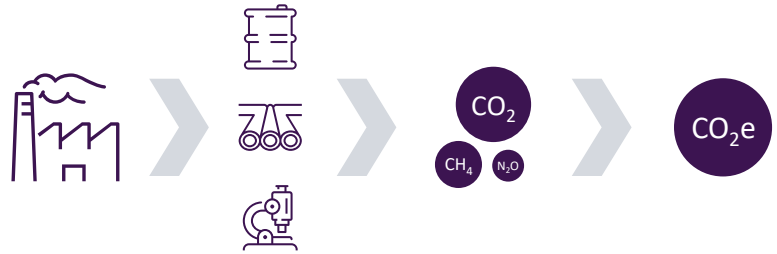
EFs in AVEVA Process Simulation



- AVEVA Process Simulation provides default emission factor submodels for common fuels:
  - Natural Gas (**NatGasEF**)
  - No. 2 Fuel Oil (**No2FuelEF**)
  - No. 6 Fuel Oil (**No6FuelEF**)
- You can use the **DefEF** submodel as a template for defining emission factors for other materials
- AVEVA Process Simulation requires a mass per energy basis for EFs. Conversion from other units can be done within the custom submodel.



What is Global Warming Potential (GWP)?



- Not all GHG emissions have the same warming potential
- Global Warming Potential (GWP) factors are used to align emissions to a common scale
- GWP = energy absorbed by 1 ton of Gas A / energy absorbed by 1 ton of CO_2 (typically over 100 years)
- Measured experimentally while accounting for:
  - Radiative Efficiency – how much energy does the GHG absorb?
  - Lifetime – how long will the GHG remain in the atmosphere before being broken down?

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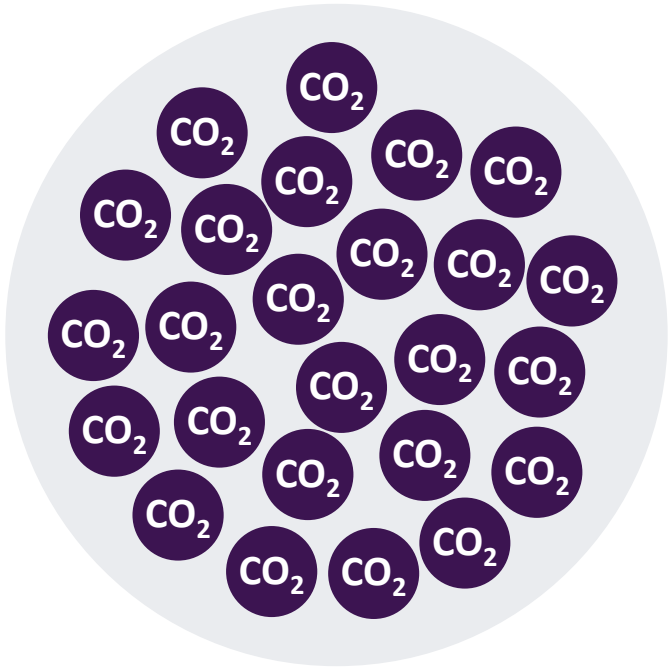
Visualizing Global Warming Potential

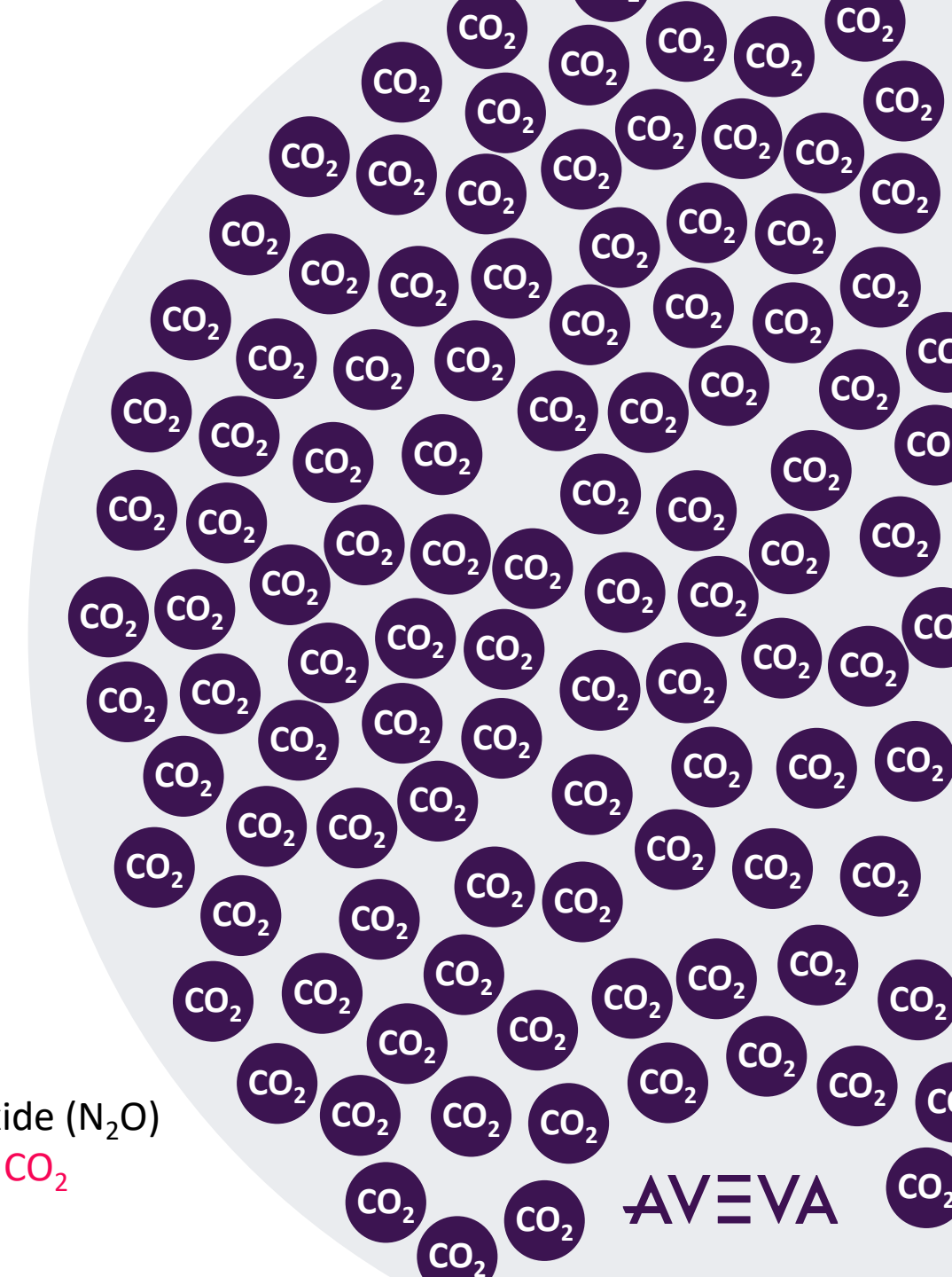
Carbon Dioxide (CO_2)

1x CO_2



Methane (CH_4)

25x CO_2



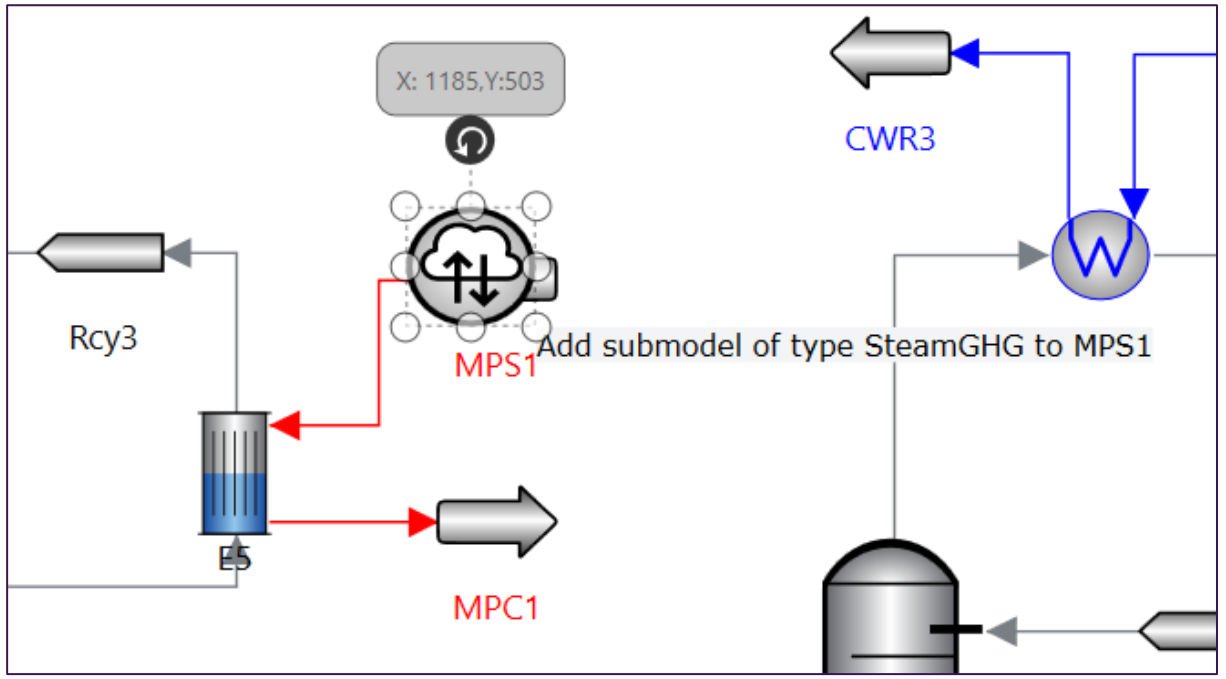
Nitrous Oxide (N_2O)

298x CO_2

Calculating GHG Emissions in AVEVA Process Simulation

Introduction

- AVEVA Process Simulation calculates the CO2-equivalent emissions (CO2e) across the entire simulation
- Drag + Drop GHG submodels on top of existing models in the simulation
- Access the full features of AVEVA Process Simulation
  - Optimization
  - Dynamic studies
  - Steady-state design



Calculating GHG Emissions in AVEVA Process Simulation

SummaryGHG Model

- Provides a single location to view total CO2e emissions
- Automatically sums emissions from all GHG submodels in the simulation

View and Edit GWP Factors

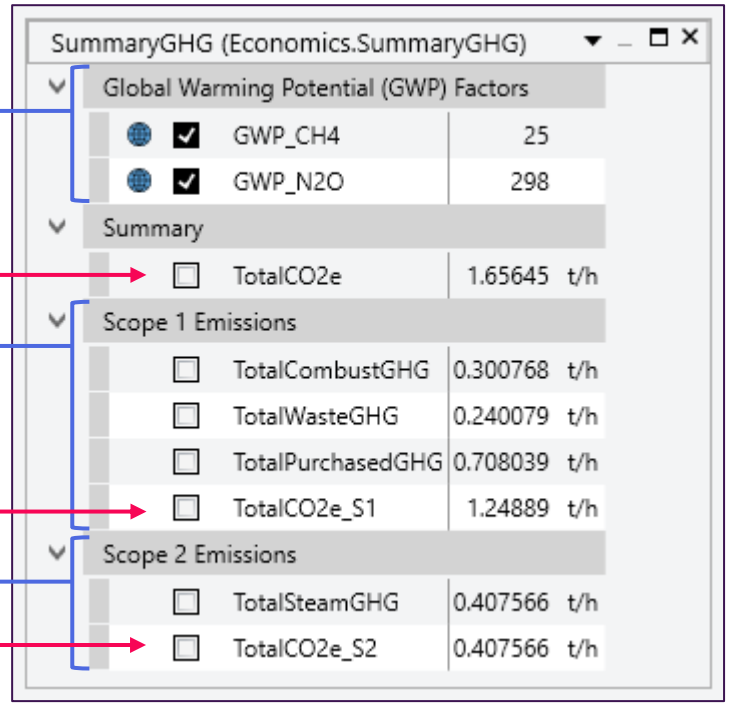
Total CO2e emissions for all emission sources

CO2e emissions for each source in Scope 1

Total Scope 1 CO2e emissions

CO2e emissions for each source in Scope 2

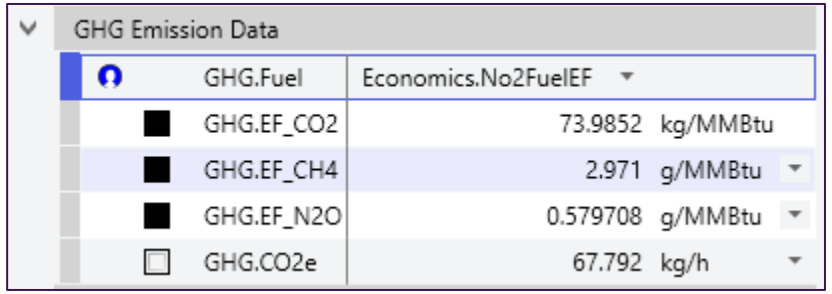
Total Scope 2 CO2e emissions



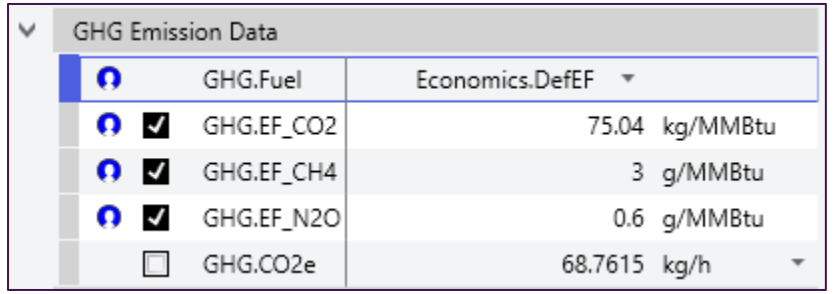
Calculating GHG Emissions in AVEVA Process Simulation

CombustGHG Submodel

- Calculate emissions for stationary combustion (for example: burners, boilers, and furnaces)
- Emission Factors must be defined for the fuel:
  - Select a submodel (**Fuel**) that provides the correct emission factors *or*
  - Use the DefEF submodel and manually specify **EF_CO2**, **EF_CH4**, and **EF_N2O**
- **CO2e** is calculated from individual CO_2, CH_4, and N_2O emissions with GWP factors defined in SummaryGHG model



Emission Factors for No. 2 Fuel Oil

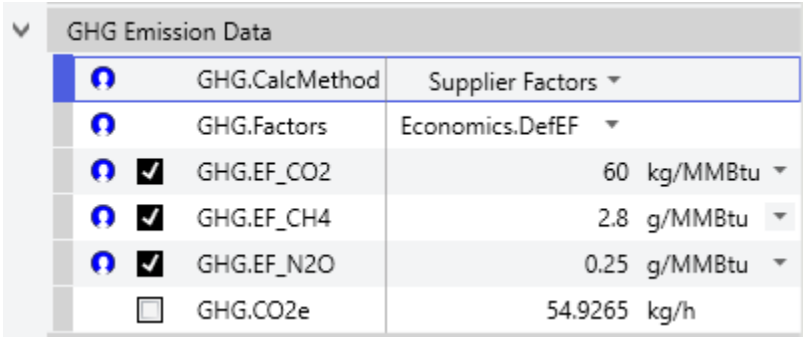


Emission Factors Specified with DefEF

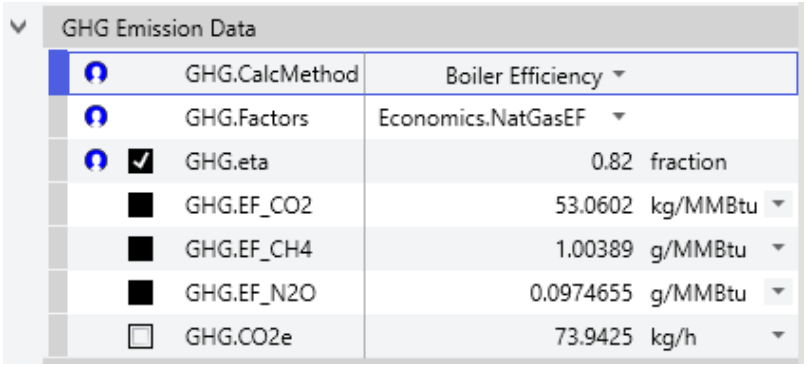
Calculating GHG Emissions in AVEVA Process Simulation

SteamGHG Submodel

- Calculate emissions for purchased steam
- Supports both calculation methods set by the US EPA
  - Set **CalcMethod = Supplier Factors** to manually specify emission factors from the steam supplier (*preferred*)
  - Set **CalcMethod = Boiler Efficiency** if supplier factors are unknown. Then, select a fuel and specify a boiler efficiency (**eta**).
- **CO2e** is calculated from individual CO_2, CH_4, and N_2O emissions with GWP factors defined in SummaryGHG model



Supplier Factor Method

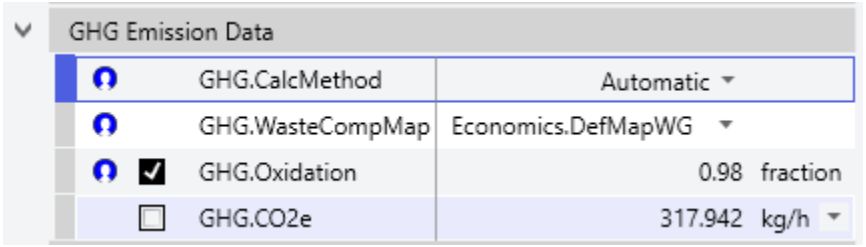


Boiler Efficiency Method

Calculating GHG Emissions in AVEVA Process Simulation

WasteGHG Submodel

- Calculate emissions for waste gas combustion (for example: flaring, thermal oxidizers)
- To automatically calculate carbon content of waste stream, set **CalcMethod = Automatic**
- To manually map your fluid components to a standard waste composition, set **CalcMethod = Map Components**
  - Recommended for fluids where exact chemical formulas are not known for every component
  - You must provide a mapping submodel (see **DefMapWG**)
- CO2e emissions are calculated from flow rate, carbon content, and **Oxidation** fraction

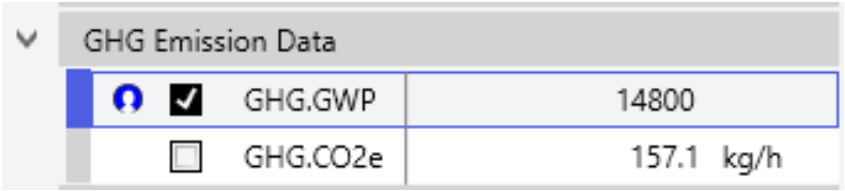


Automatically Calculate Carbon Content

Calculating GHG Emissions in AVEVA Process Simulation

PurchasedGHG Submodel

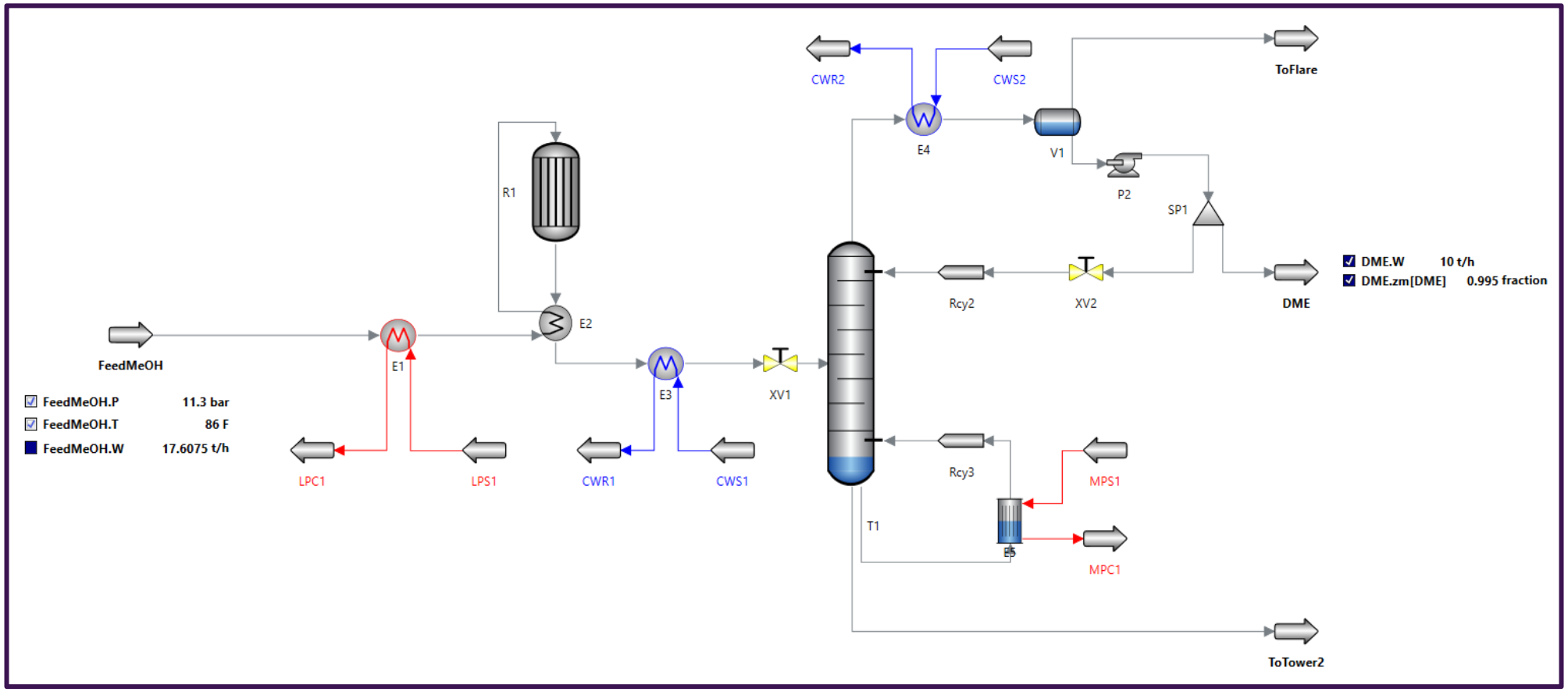
- Calculate emissions for purchased industrial gases (for example: refrigerants, laboratory gases)
- Specify the GWP factor for the purchased gas
  - Not sure? Visit the US EPA Center for Corporate Climate Leadership's GHG Emission Factors Hub



CO2e emissions for HFC-23

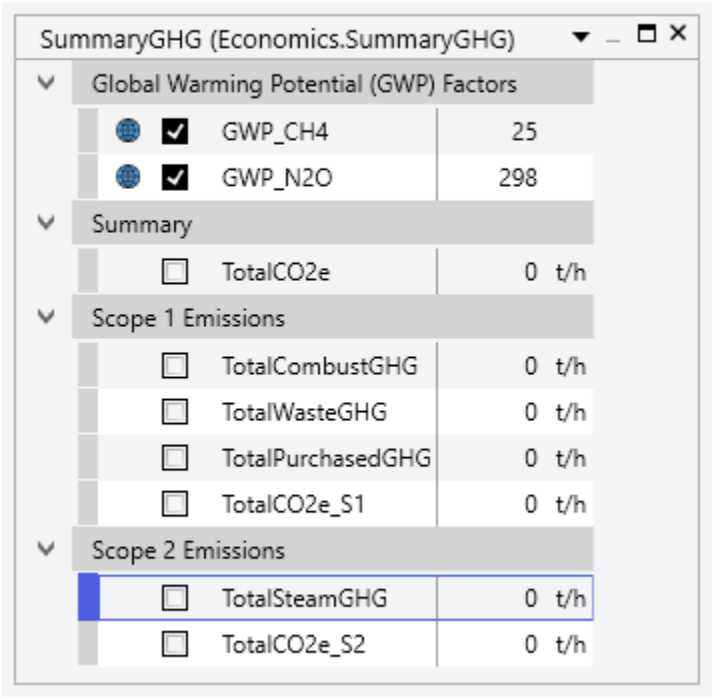
Calculating GHG Emissions in AVEVA Process Simulation

Full Example with Optimization



Calculating GHG Emissions in AVEVA Process Simulation

Step 1: Add SummaryGHG Model to Simulation and Confirm GWP Factors



SummaryGHG

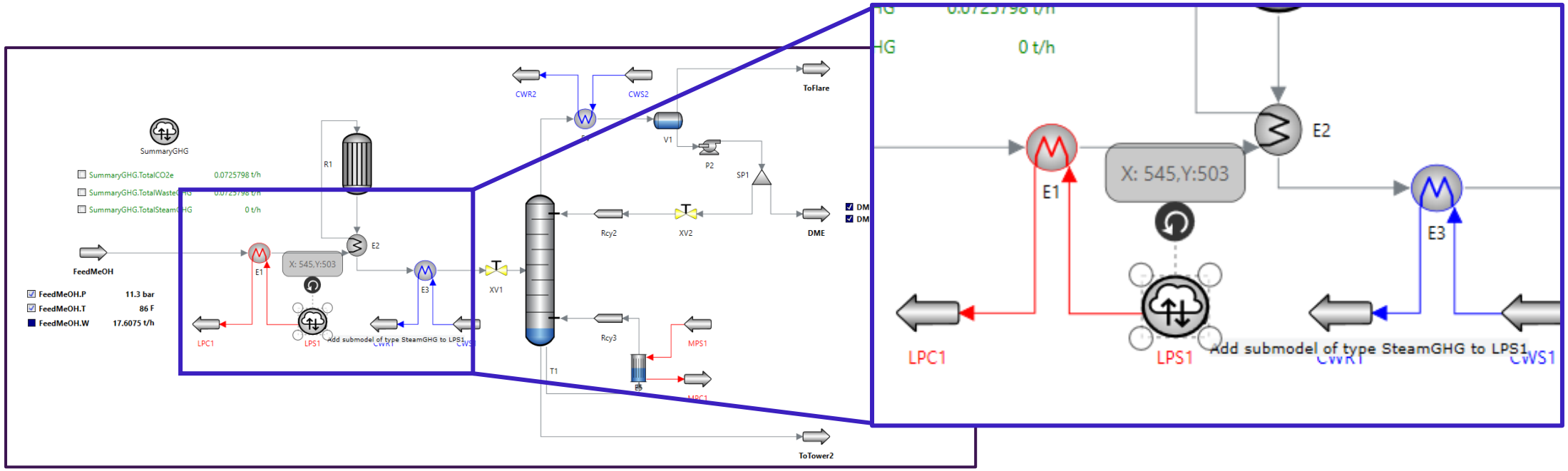
SummaryGHG.TotalCO2e 0 t/h

SummaryGHG.TotalWasteGHG 0 t/h

SummaryGHG.TotalSteamGHG 0 t/h

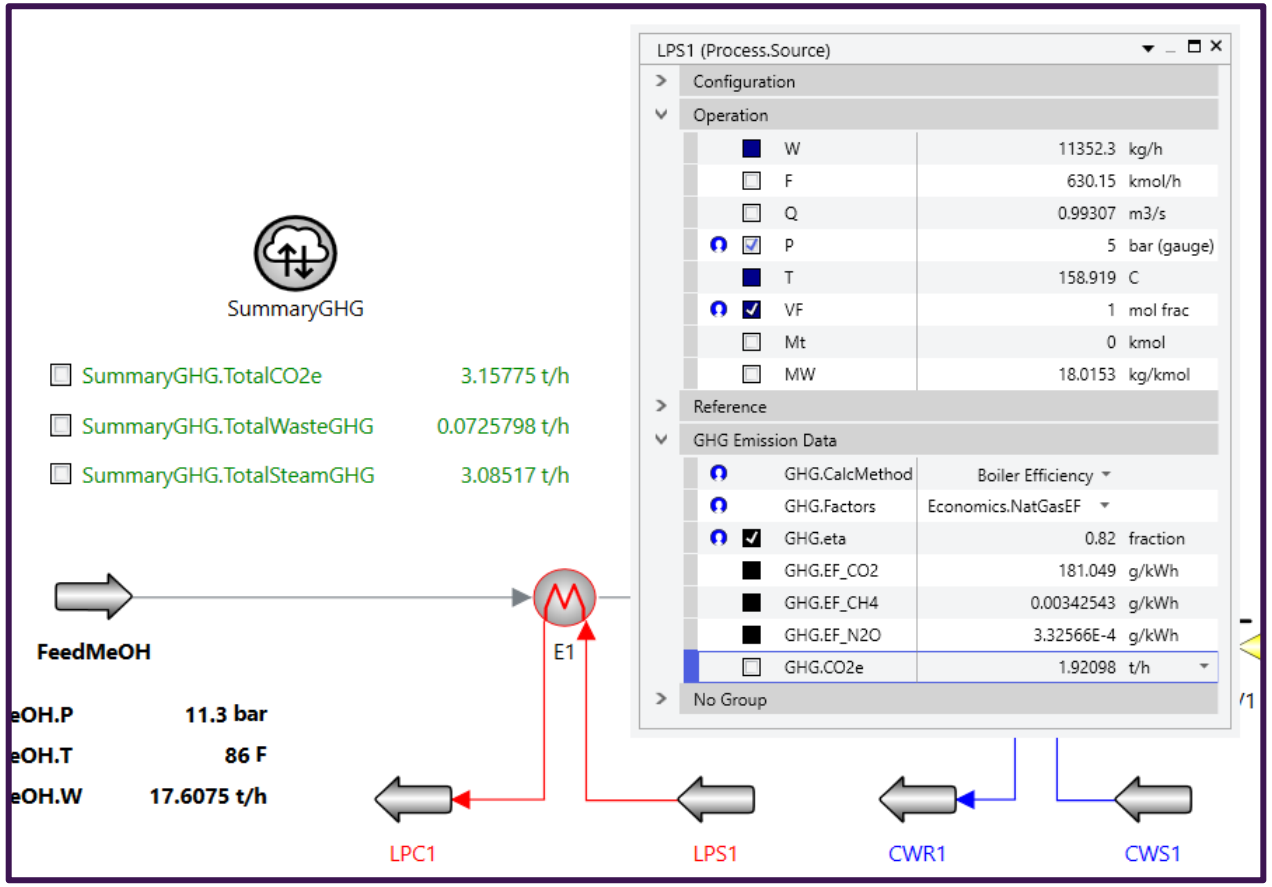
Calculating GHG Emissions in AVEVA Process Simulation

Step 2: Drag-and-Drop GHG Submodels into Steam Sources and Waste Gas Sinks



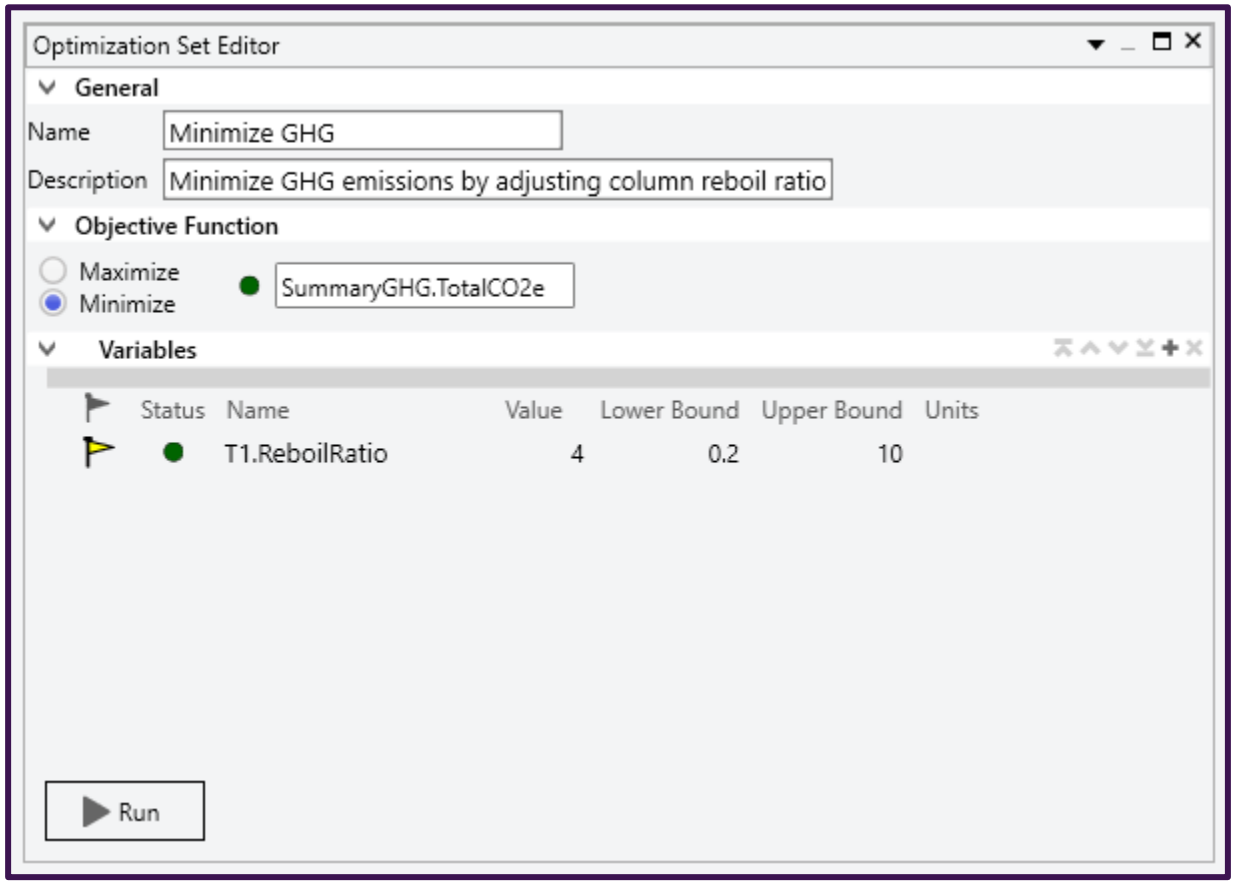
Calculating GHG Emissions in AVEVA Process Simulation

Step 3: Select Fuel Type and Set Efficiency in SteamGHG Submodels



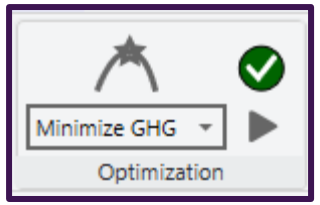
Calculating GHG Emissions in AVEVA Process Simulation

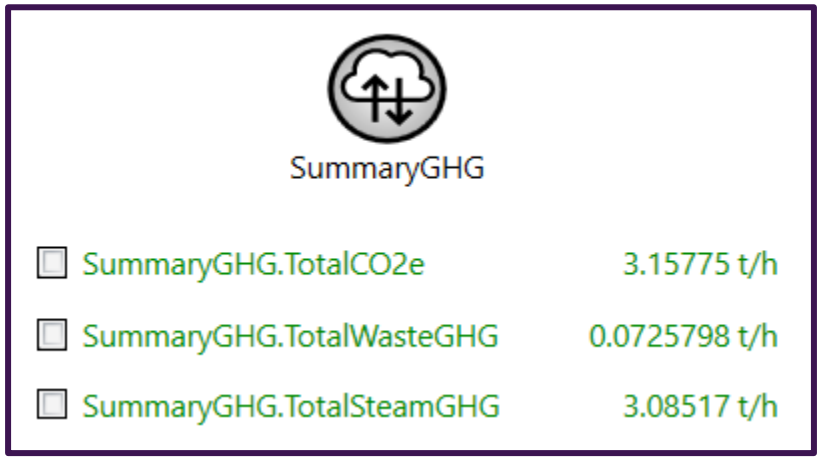
Step 4: Create an Optimization Set



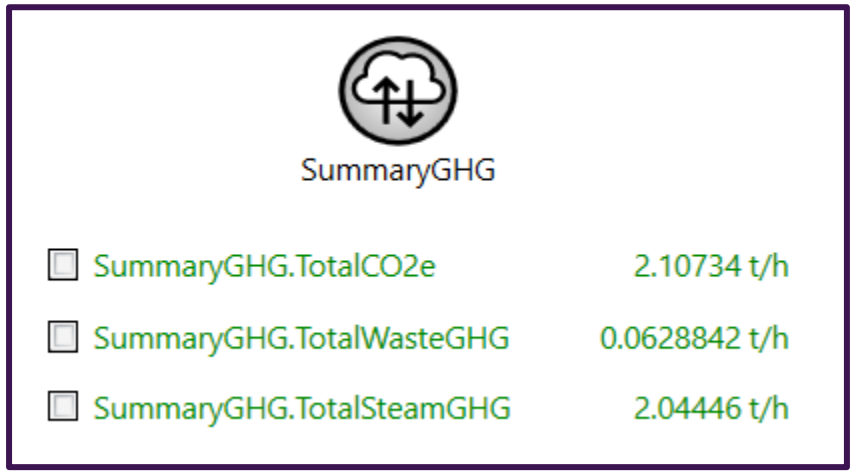
Calculating GHG Emissions in AVEVA Process Simulation

Step 5: Run Optimization and Review Results





Before Optimization



After Optimization

Hydrogen Production

Hydrogen Production – Grey, Blue, or Green?

- Steam Methane Reforming (SMR) with Water Gas Shift (WGS) reactions
- CO_2 is a byproduct of both SMR and WGS reactions
- High reaction temperatures require large industrial furnaces
- **No carbon capture or storage**

- Steam Methane Reforming (SMR) with Water Gas Shift (WGS) reactions
- Carbon is **captured and stored** underground (CCS)
- However, not all carbon can be captured with current technologies

- Renewable energy sources to power water electrolysis
- Water is split into H_2 and O_2 with **no carbon** byproducts
- Only accounts for a small portion of all current hydrogen production

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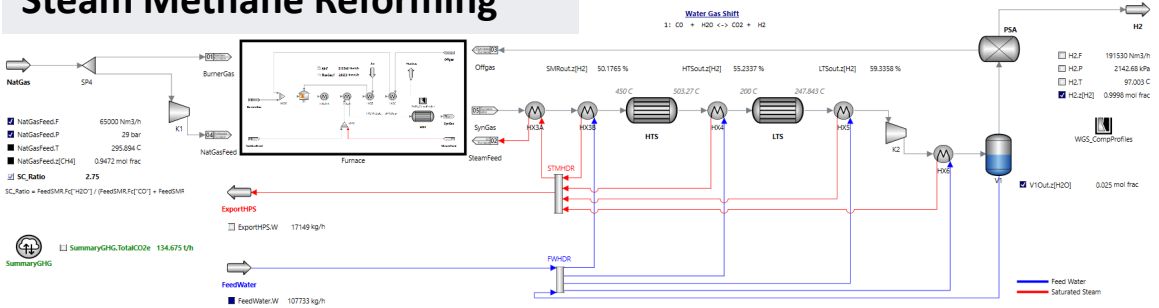
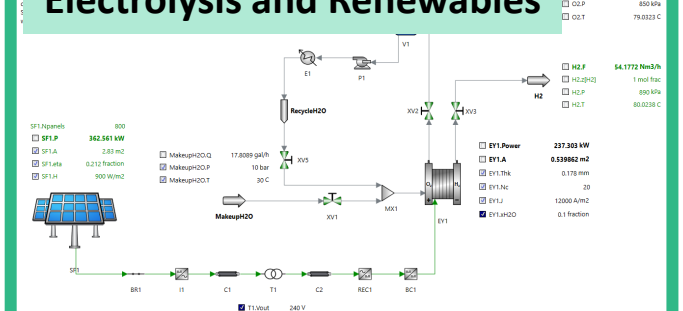
Hydrogen Processing in AVEVA Process Simulation

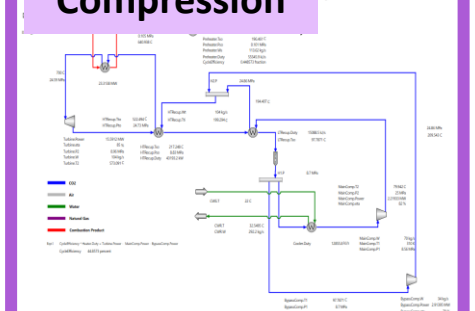
Steam Methane Reforming



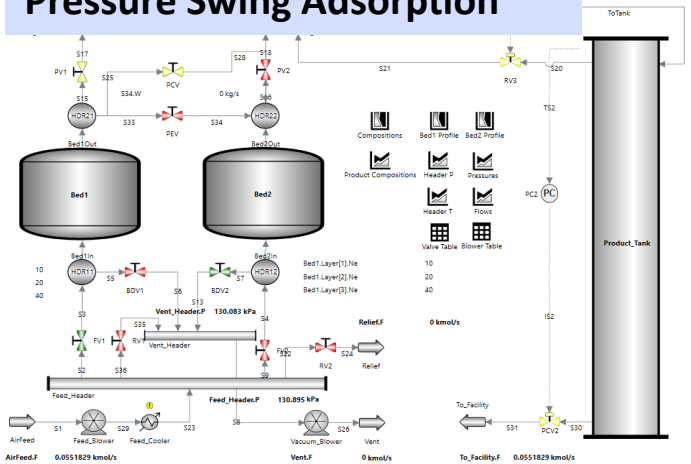
Electrolysis and Renewables



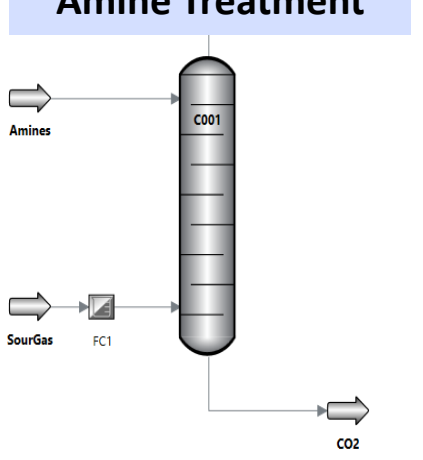
Compression



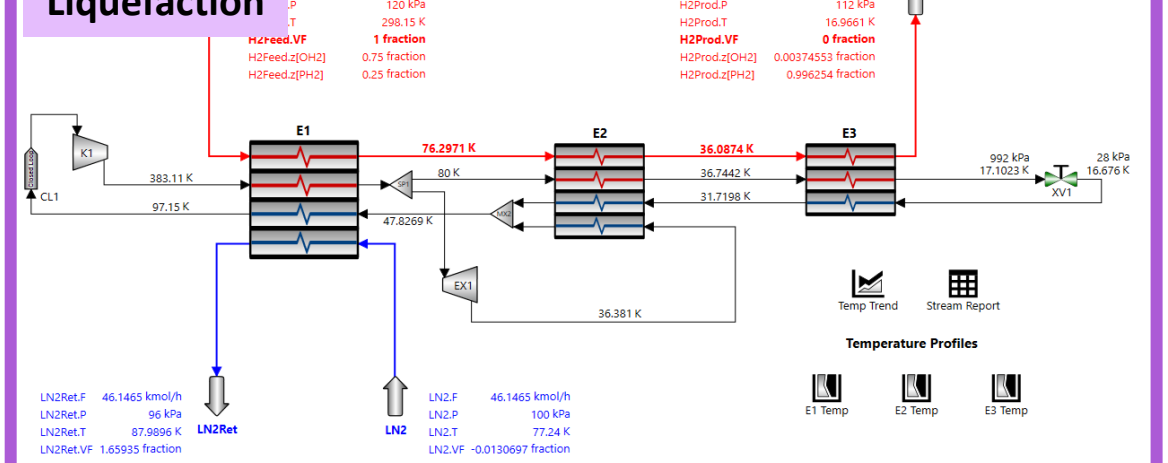
Pressure Swing Adsorption



Amine Treatment

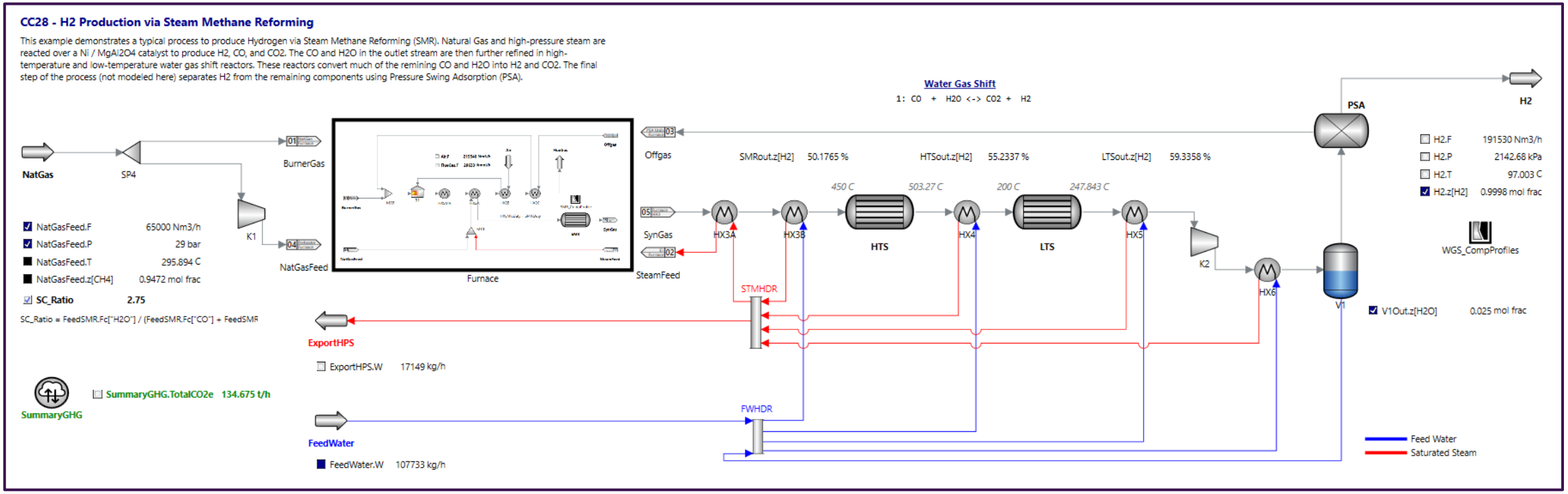


Liquefaction

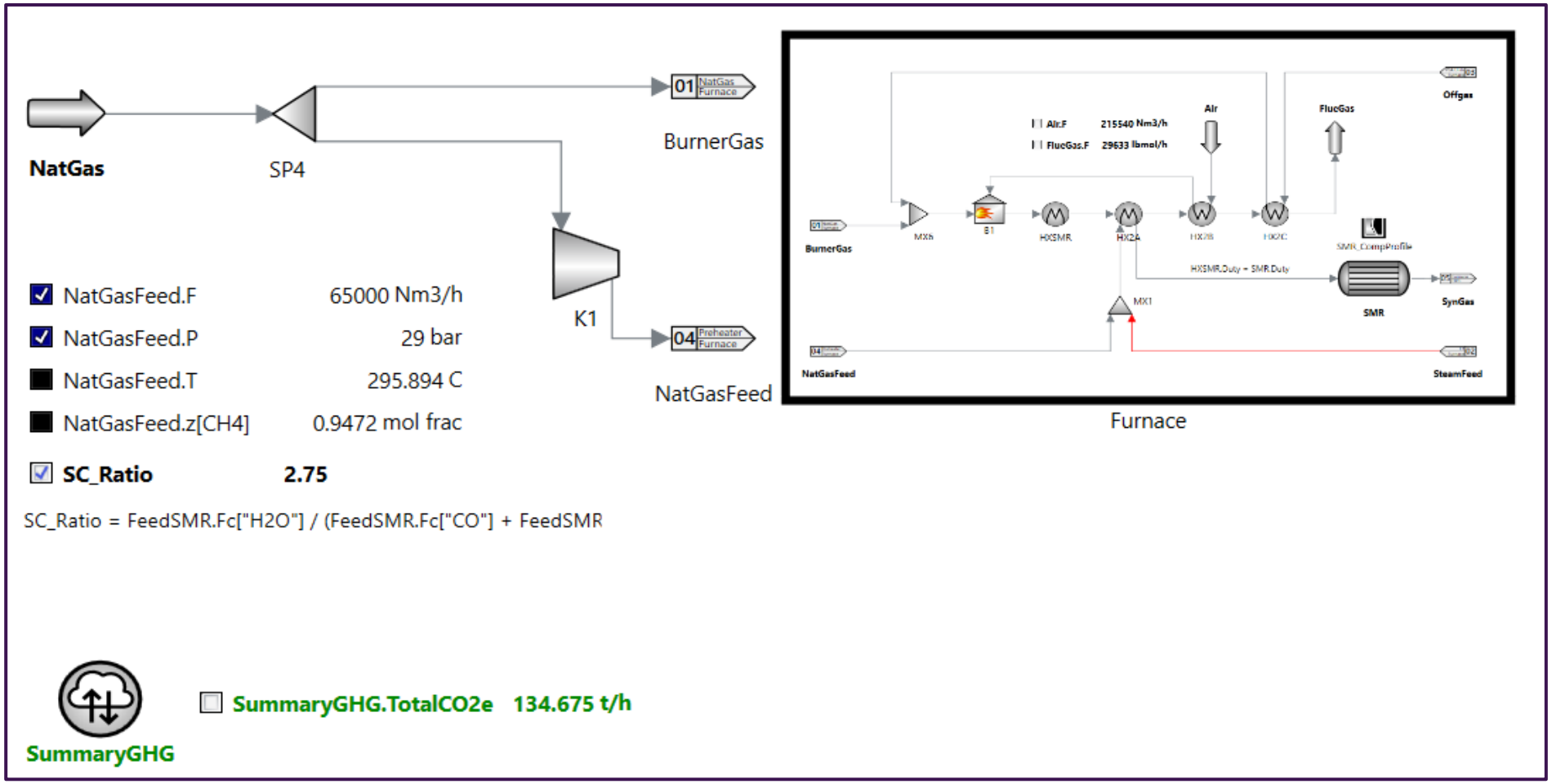


Grey Hydrogen – SMR in AVEVA Process Simulation

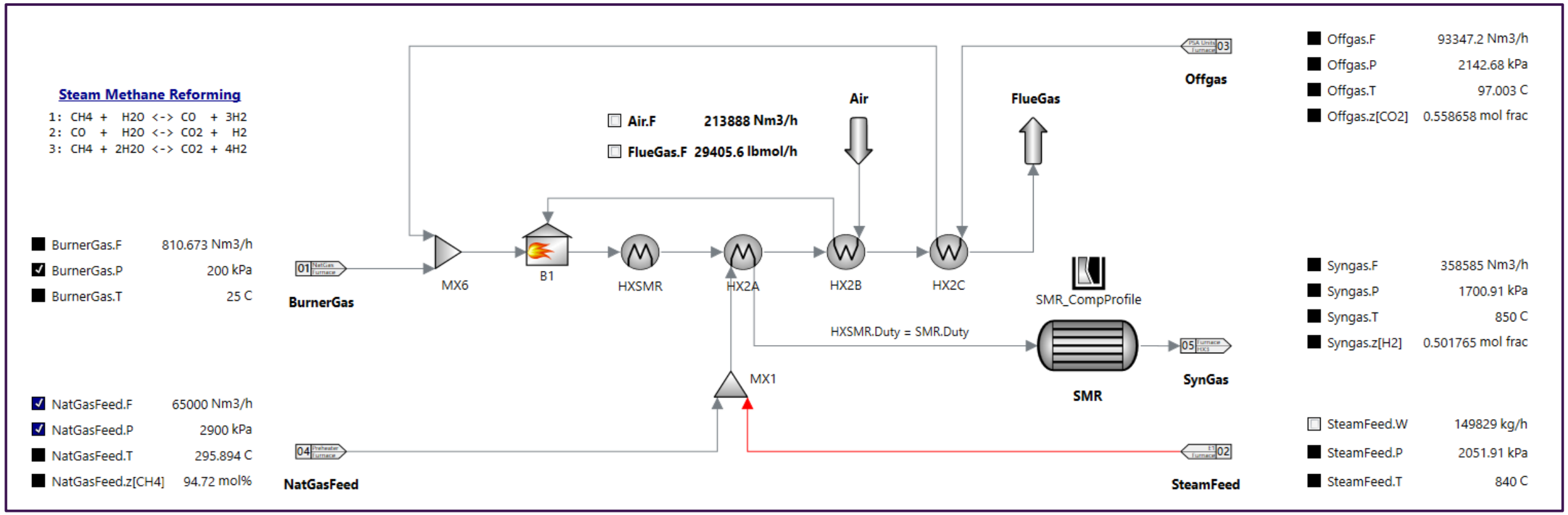
- See Documented Example CC28 – H2 Production via Steam Methane Reforming



SMR – Design Specifications



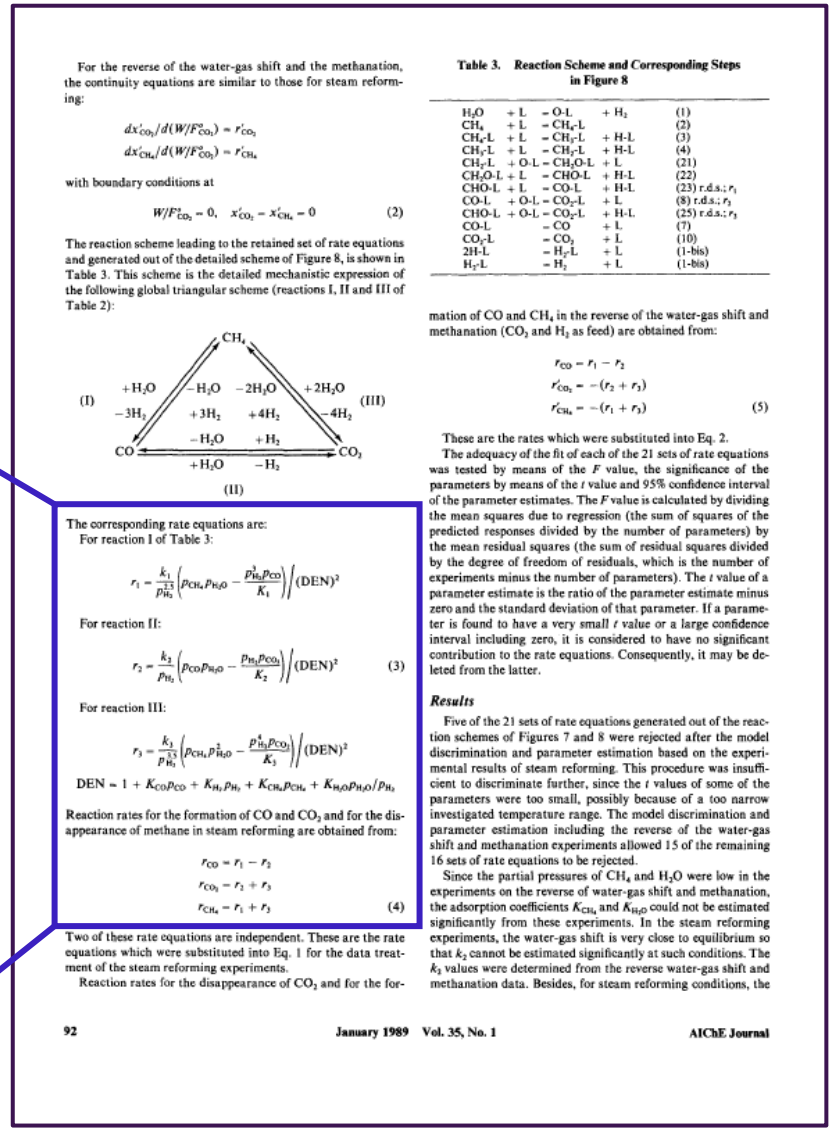
SMR – Reformer Furnace



SMR – Reaction Kinetics

Equations

Condition	Name	Status	Formula
	Eqn3	●	Rate["H2O"] = -RateRxn[1] - RateRxn[2] - 2 * RateRxn[3]
	Eqn4	●	Rate["H2"] = 3 * RateRxn[1] + RateRxn[2] + 4 * RateRxn[3]
	Eqn5	●	Rate["CO"] = RateRxn[1] - RateRxn[2]
	Eqn25	●	Rate[not{"CO2", "CH4", "H2O", "H2", "CO"}] = 0
	Eqn6	●	Py = P / 100 * tear(z)
	Eqn7	●	k[1] = 4.225E15 * exp(-240100 / (R * T))
	Eqn8	●	k[2] = 1.955E6 * exp(-67130 / (R * T))
	Eqn9	●	k[3] = 1.020E15 * exp(-243900 / (R * T))
	Eqn10	●	Keq[1] = exp(-26830 / T + 30.114)
	Eqn11	●	Keq[2] = exp(4400 / T - 4.036)
	Eqn12	●	Keq[3] = Keq[1] * Keq[2]
	Eqn13	●	Ka["CO"] = 8.23E-5 * exp(70650 / (R * T))
	Eqn14	●	Ka["H2"] = 6.12E-9 * exp(82900 / (R * T))
	Eqn15	●	Ka["CH4"] = 6.65E-4 * exp(38280 / (R * T))
	Eqn16	●	Ka["H2O"] = 1.77E5 * exp(-88680 / (R * T))
	Eqn17	●	Ka[not{"CO", "CH4", "H2O", "H2"}] = 0
	Eqn18	●	den = 1 + Ka["CO"] * Py["CO"] + Ka["H2"] * Py["H2"] + Ka["CH4"] * Py["CH4"] + Ka["H2O"] * Py["H2O"] / Py["H2"]
	Eqn19	●	RateRxn[1] * den^2 * 3600 = k[1] * Py["H2"]^(-2.5) * (Py["CH4"] * Py["H2O"] - (Py["H2"]^3 * Py["CO"]) / Keq[1])
	Eqn20	●	RateRxn[2] * den^2 * 3600 = k[2] * Py["H2"]^(-1) * (Py["CO"] * Py["H2O"] - (Py["H2"] * Py["CO2"]) / Keq[2])
	Eqn21	●	RateRxn[3] * den^2 * 3600 = k[3] * Py["H2"]^(-3.5) * (Py["CH4"] * Py["H2O"]^2 - (Py["H2"]^4 * Py["CO2"]) / Keq[3])



For the reverse of the water-gas shift and the methanation, the continuity equations are similar to those for steam reforming:

$$dx'_{CO_2}/d(W/F^\circ_{CO_2}) = r'_{CO_2}$$
$$dx'_{CH_4}/d(W/F^\circ_{CO_2}) = r'_{CH_4}$$

with boundary conditions at

$$W/F^\circ_{CO_2} = 0, \quad x'_{CO_2} = x'_{CH_4} = 0 \qquad (2)$$

The reaction scheme leading to the retained set of rate equations and generated out of the detailed scheme of Figure 8, is shown in Table 3. This scheme is the detailed mechanistic expression of the following global triangular scheme (reactions I, II and III of Table 2):

The corresponding rate equations are:
For reaction I of Table 3:

$$r_1 = \frac{k_1}{p_{H_2}^{2.5}}\left(p_{CH_4}p_{H_2O} - \frac{p_{H_2}^3 p_{CO}}{K_1}\right)\Big/(\mathrm{DEN})^2$$

For reaction II:

$$r_2 = \frac{k_2}{p_{H_2}}\left(p_{CO}p_{H_2O} - \frac{p_{H_2}p_{CO_2}}{K_2}\right)\Big/(\mathrm{DEN})^2 \qquad (3)$$

For reaction III:

$$r_3 = \frac{k_3}{p_{H_2}^{3.5}}\left(p_{CH_4}p_{H_2O}^2 - \frac{p_{H_2}^4 p_{CO_2}}{K_3}\right)\Big/(\mathrm{DEN})^2$$

$$\mathrm{DEN} = 1 + K_{CO}p_{CO} + K_{H_2}p_{H_2} + K_{CH_4}p_{CH_4} + K_{H_2O}p_{H_2O}/p_{H_2}$$

Reaction rates for the formation of CO and CO_2 and for the disappearance of methane in steam reforming are obtained from:

$$r_{CO} = r_1 - r_2$$
$$r_{CO_2} = r_2 + r_3$$
$$r_{CH_4} = r_1 + r_3 \qquad (4)$$

Two of these rate equations are independent. These are the rate equations which were substituted into Eq. 1 for the data treatment of the steam reforming experiments.

Reaction rates for the disappearance of CO_2 and for the formation of CO and CH_4 in the reverse of the water-gas shift and methanation (CO_2 and H_2 as feed) are obtained from:

$$r_{CO} = r_1 - r_2$$
$$r'_{CO_2} = -(r_2 + r_3)$$
$$r'_{CH_4} = -(r_1 + r_3) \qquad (5)$$

These are the rates which were substituted into Eq. 2.

The adequacy of the fit of each of the 21 sets of rate equations was tested by means of the F value, the significance of the parameters by means of the t value and 95% confidence interval of the parameter estimates. The F value is calculated by dividing the mean squares due to regression (the sum of squares of the predicted responses divided by the number of parameters) by the mean residual squares (the sum of residual squares divided by the degree of freedom of residuals, which is the number of experiments minus the number of parameters). The t value of a parameter estimate is the ratio of the parameter estimate minus zero and the standard deviation of that parameter. If a parameter is found to have a very small t value or a large confidence interval including zero, it is considered to have no significant contribution to the rate equations. Consequently, it may be deleted from the latter.

Results

Five of the 21 sets of rate equations generated out of the reaction schemes of Figures 7 and 8 were rejected after the model discrimination and parameter estimation based on the experimental results of steam reforming. This procedure was insufficient to discriminate further, since the t values of some of the parameters were too small, possibly because of a too narrow investigated temperature range. The model discrimination and parameter estimation including the reverse of the water-gas shift and methanation experiments allowed 15 of the remaining 16 sets of rate equations to be rejected.

Since the partial pressures of CH_4 and H_2O were low in the experiments on the reverse of water-gas shift and methanation, the adsorption coefficients K_{CH_4} and K_{H_2O} could not be estimated significantly from these experiments. In the steam reforming experiments, the water-gas shift is very close to equilibrium so that k_2 cannot be estimated significantly at such conditions. The k_2 values were determined from the reverse water-gas shift and methanation data. Besides, for steam reforming conditions, the

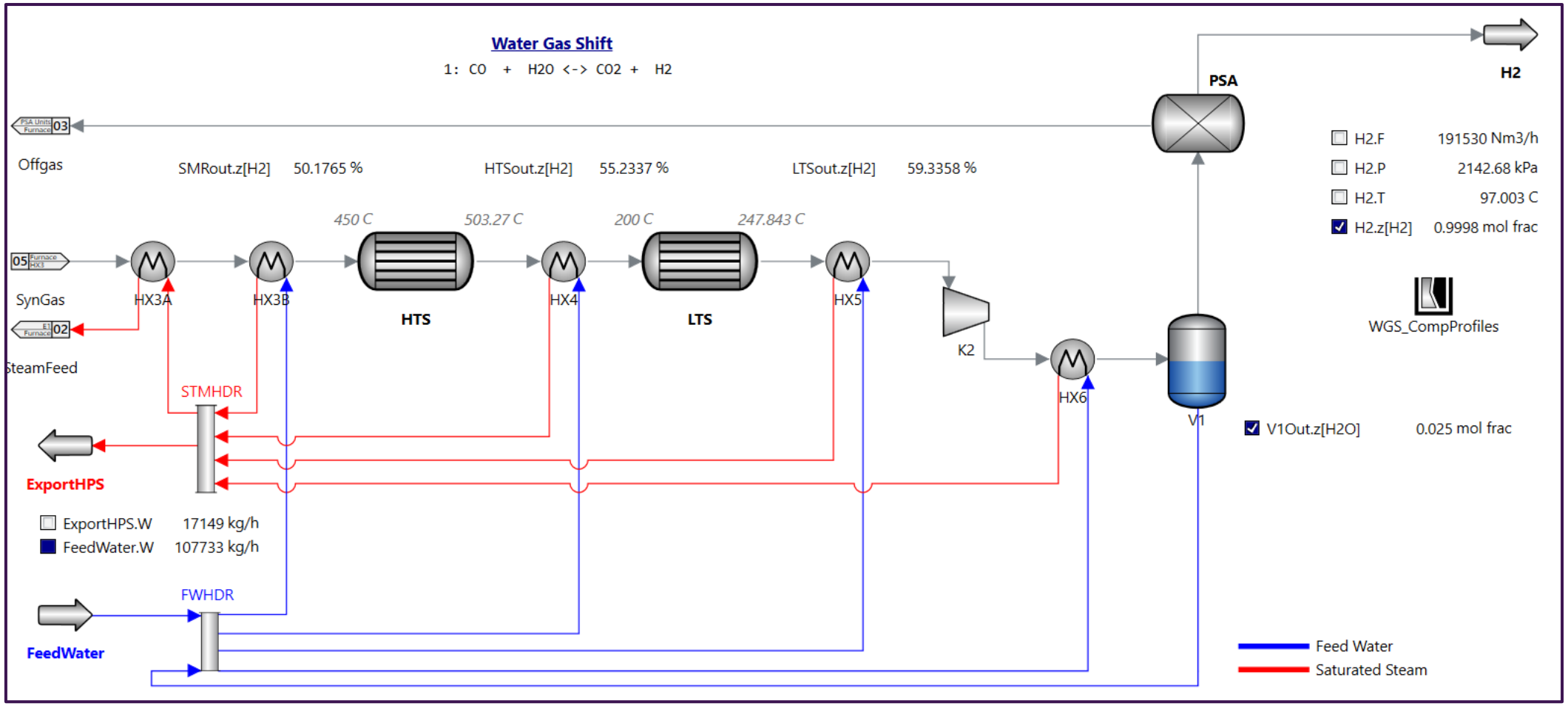
Table 3. Reaction Scheme and Corresponding Steps in Figure 8

H_2O	+ L	= O-L	+ H_2	(1)
CH_4	+ L	= CH_4-L		(2)
CH_4-L	+ L	= CH_3-L	+ H-L	(3)
CH_3-L	+ L	= CH_2-L	+ H-L	(4)
CH_3-L	+ O-L	= CH_3O-L	+ L	(21)
CH_2O-L	+ L	= CHO-L	+ H-L	(22)
CHO-L	+ L	= CO-L	+ H-L	(23) r.d.s.; r_1
CO-L	+ O-L	= CO_2-L	+ L	(8) r.d.s.; r_2
CHO-L	+ O-L	= CO_2-L	+ H-L	(25) r.d.s.; r_3
CO-L		= CO	+ L	(7)
CO_2-L		= CO_2	+ L	(10)
2H-L		= H_2-L	+ L	(1-bis)
H_2-L		= H_2	+ L	(1-bis)

J. Xu, G.F. Froment, Methane Steam Reforming, Methanation and Water-Gas Shift: I. Intrinsic Kinetics, AIChE J. 35 (1989) 88–96.

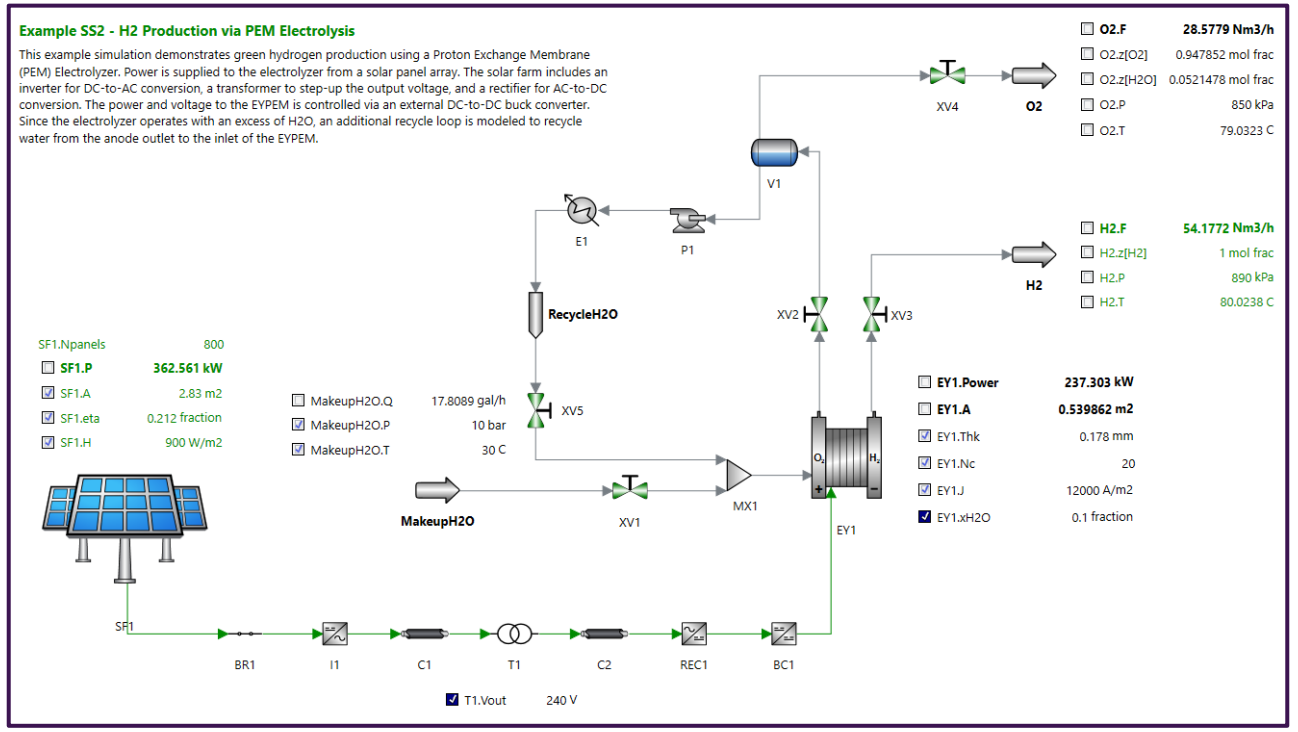
AVEVA

SMR – Shift Reactors and Heat Integration



Green Hydrogen – Electrolysis in AVEVA Process Simulation

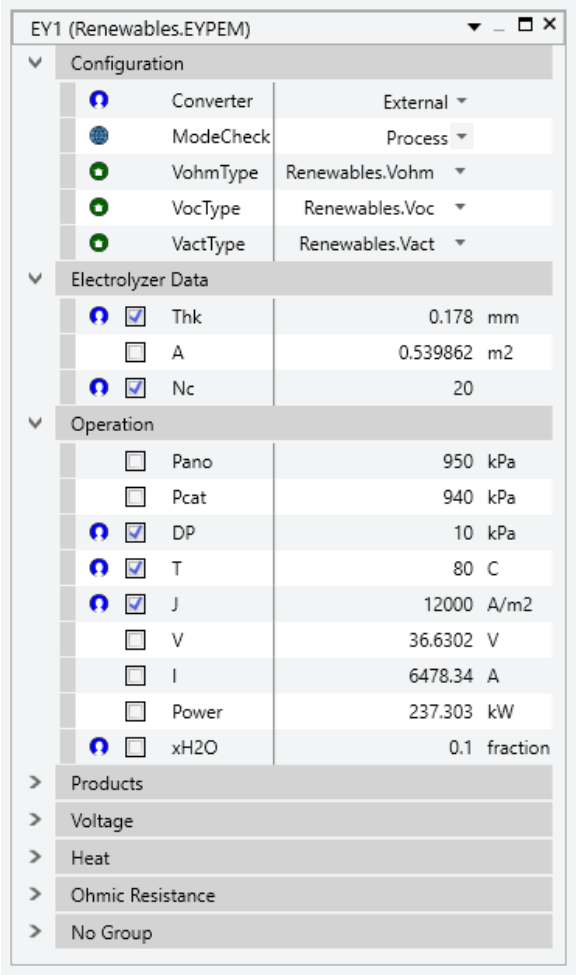
- See Undocumented Example SS2 – H2 Production via PEM Electrolysis



Electrolysis Modeling

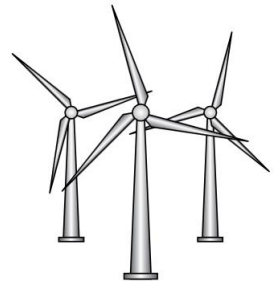
Electrolyzer Characteristics

- AVEVA Process Simulation allows you to edit key characteristics of the PEM Electrolyzer model and see the impact on overall hydrogen production:
  - Number of cells in series, **Nc**
  - Current density on electrolyzer stack, **J** (typically ~12 kA/m^2)
- The EYPEM model includes an optional electrical connection
  - Electrolyzers require DC inputs so AC voltage must be first converted with a **Rectifier**
  - DC voltage is then stepped down with a Buck **Converter.** Choose between an Internal or External converter.



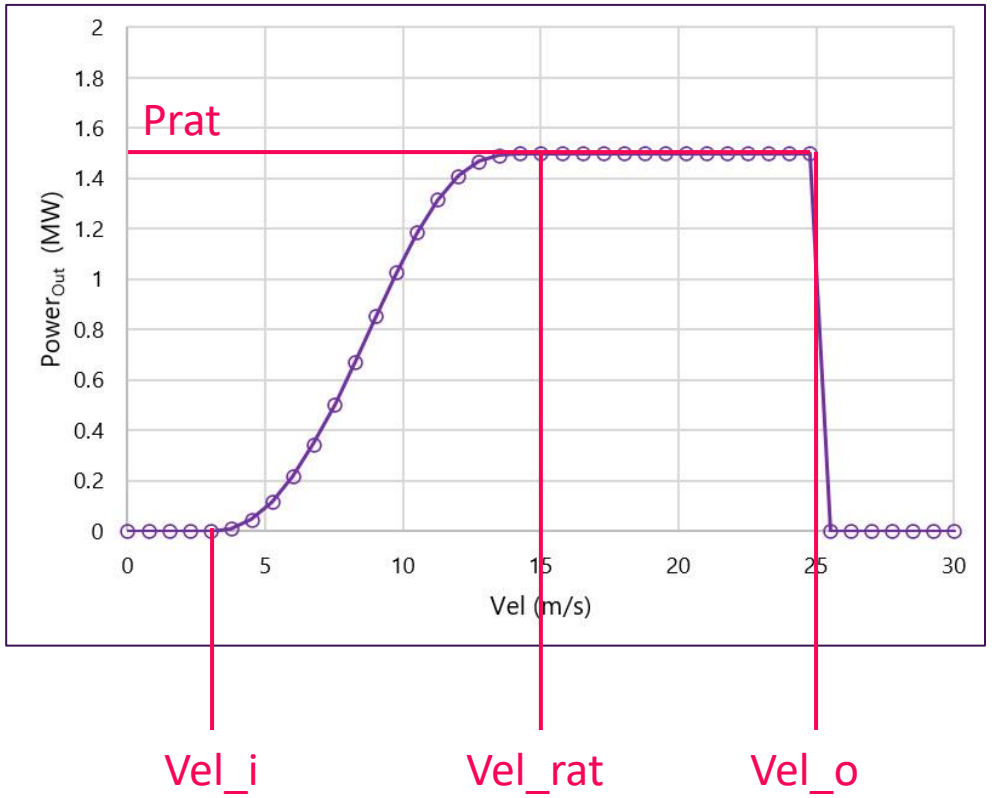
Renewable Energy Models in AVEVA Process Simulation

Wind Farm Modeling

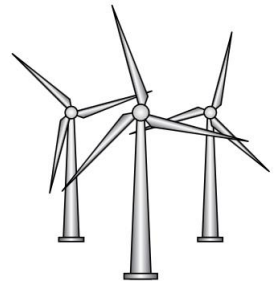


Power Curves

- AVEVA Process Simulation uses turbine power curves for calculating output power and the power coefficient
- **DefWFPower** is the default scaled power curve and represents a typical turbine. You should specify:
  - Prat – Rated power output of the turbine
  - Vel_i – Cut-in velocity (typically 3-4 m/s)
  - Vel_rat – Wind velocity at rated power (typically 11-17 m/s)
  - Vel_o – Cut-out velocity (typically ~25 m/s)
- You can also select a custom power curve for your turbines

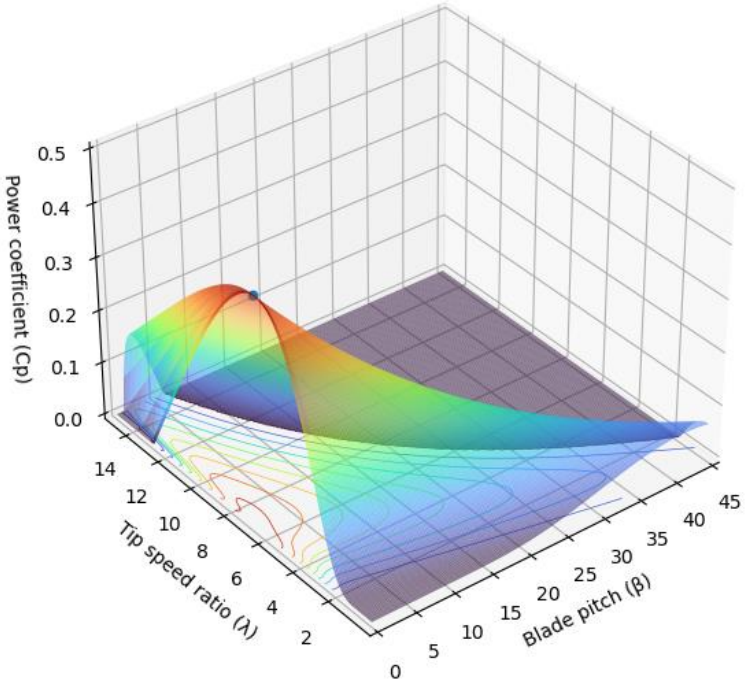


Wind Farm Modeling

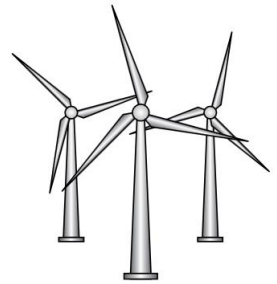


What is the Power Coefficient (Cp)?

- Indicates how much of the total wind energy is captured by the turbine after aerodynamic, mechanical, and electrical losses
- It has an upper limit of 59.3% for an ideal turbine (Betz's Law)
- Broadly, Cp is a function of:
  - Blade tip speed ratio (λ) – wind speed vs. rotational speed of turbine
  - Blade pitch angle (β)
- Turbine controllers attempt to maintain Cp_{max} by adjusting λ and β
- AVEVA Process Simulation calculates Cp directly from the power output

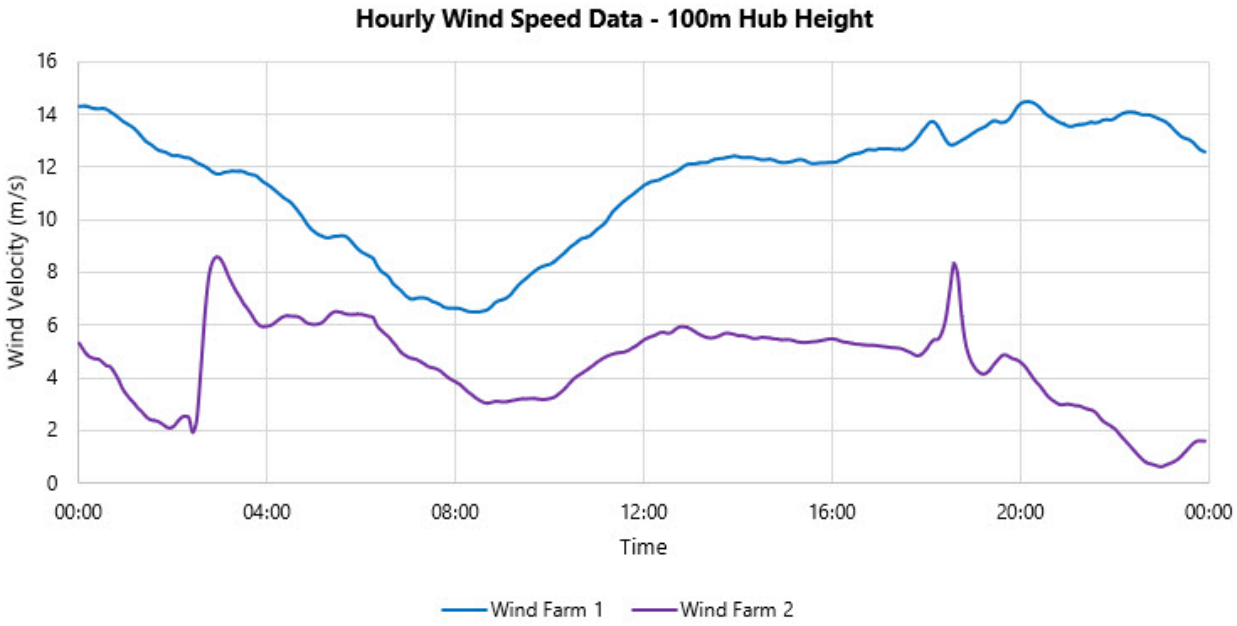


Wind Farm Modeling

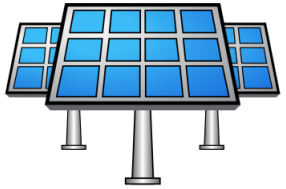


Specifying Wind Velocity

- In Process mode, specify the average velocity, **Vel**, to calculate output power
- In Dynamics mode, provide a time vs. velocity trend and use the curve tracing features to see how power output changes throughout the day
- Where to find wind resource data?
  - National Renewable Energy Laboratory (NREL) Wind Integration National Dataset (WIND)

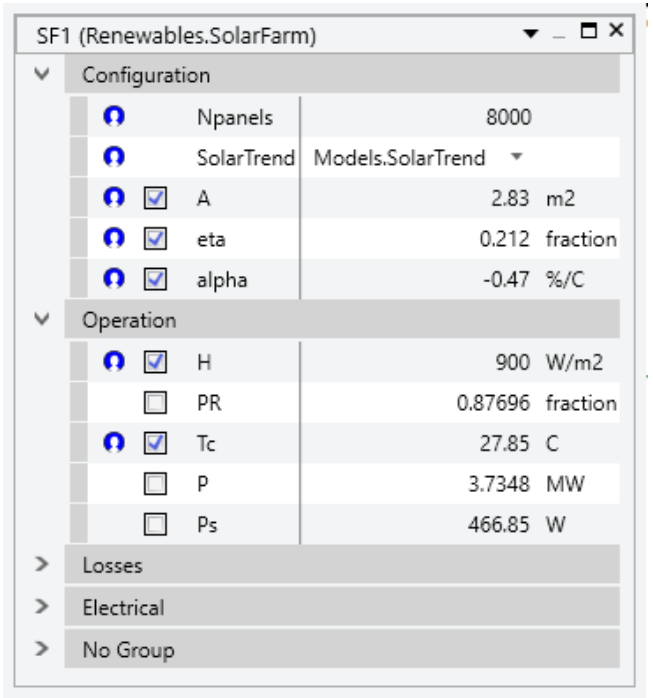


Solar Farm Modeling

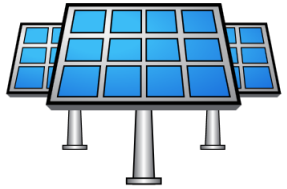


Panel Characteristics

- Solar panel output power is a function of:
  - Solar irradiance (**H**)
  - Panel area (**A**)
  - Module efficiency (**eta**) – fraction of total energy captured by the panel at standard test conditions (H = 1000W/m^2, T = 25°C). This is provided by the manufacturer and typically ranges from 10 – 25%.
  - Cell temperature (**Tc**) and temperature coefficient of power (**alpha**)
  - Performance Ratio (**PR**) – accounts for total losses beyond those reported by manufacturer

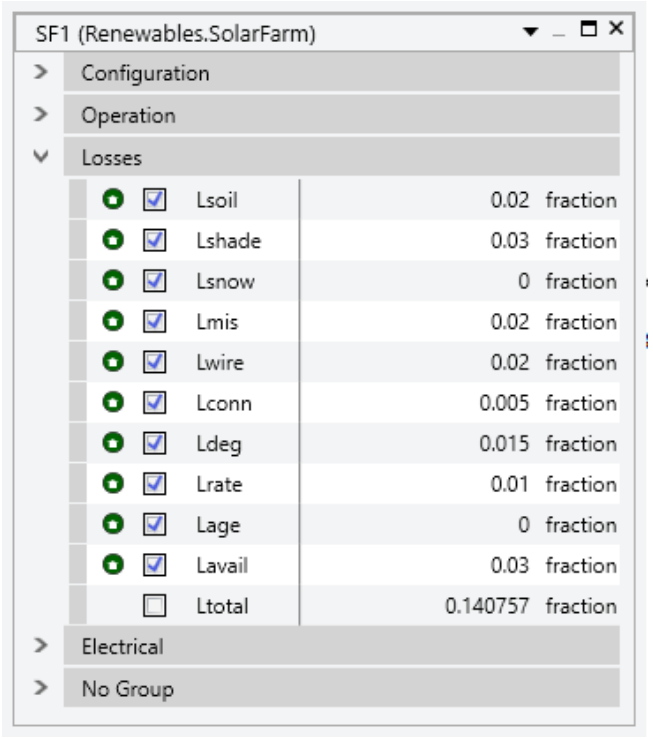


Solar Farm Modeling

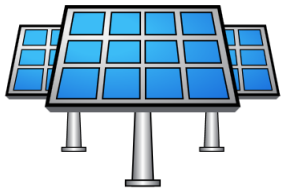


Performance Ratio

- Performance Ratio (PR) accounts for losses not measured by manufacturer:
  - Soiling – dust and dirt on panels
  - Shade
  - Snow
  - Mismatched voltage and current characteristics between panels
  - Panel age
  - Light-induced degradation
- AVEVA Process Simulation uses default values recommended by the National Renewable Energy Laboratory (NREL)

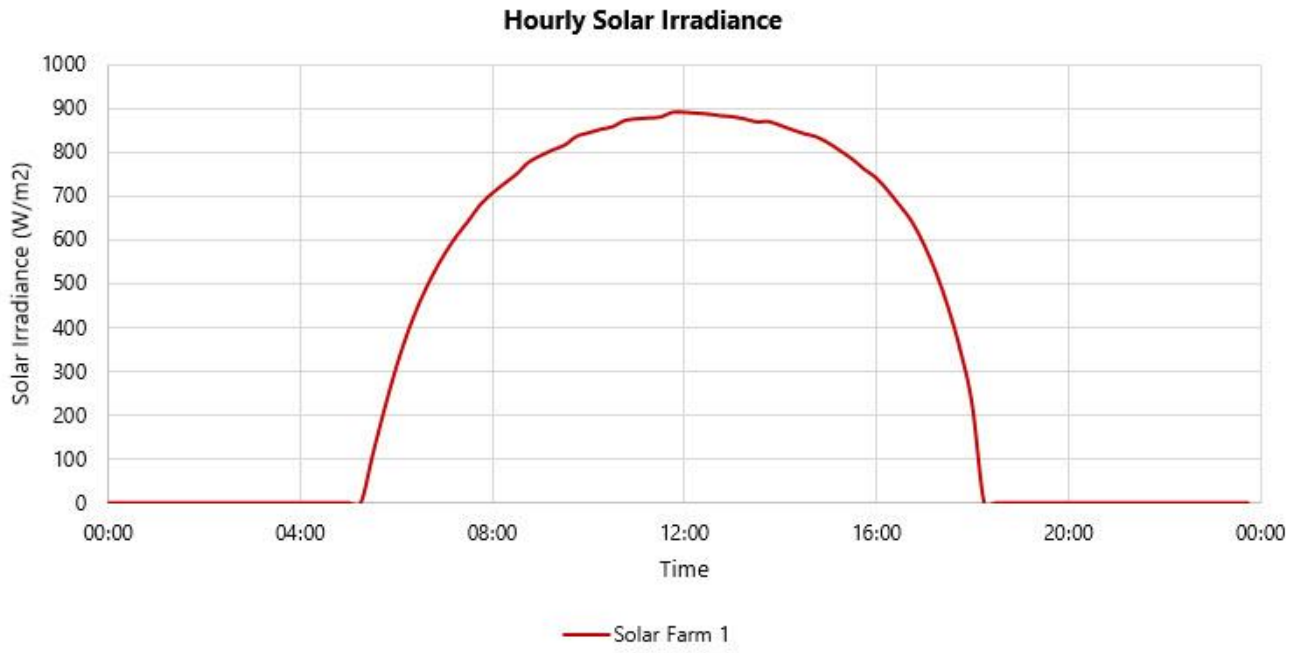


Solar Farm Modeling



Specifying Solar Irradiance

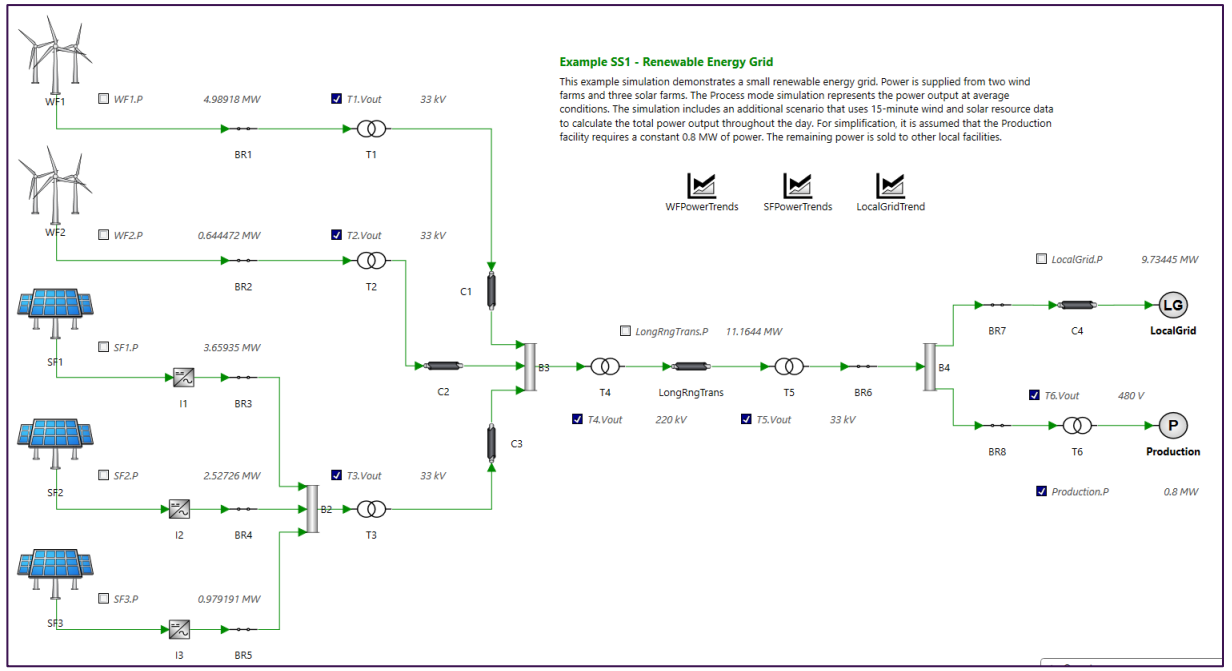
- In Process mode, specify the average solar irradiance, **H**, to calculate output power
- In Dynamics mode, provide a time vs. solar resource trend and use the curve tracing features to see how power output changes throughout the day
- Where to find solar resource data?
  - National Renewable Energy Laboratory (NREL) National Solar Radiation Database (NSRDB) – data available for the United States, South Asia, and Mexico/Central America



Renewable Grid Modeling

Connecting Renewable Energy Sources to Plant Equipment

- AVEVA Process Simulation includes a variety of simplified models to simulate a full renewable energy grid:
  - Transformer (AC → AC)
  - Converter (DC → DC)
  - Inverter (DC → AC)
  - Rectifier (AC → DC)
  - Transmission Cable
  - Busbar
  - Breaker
  - Generator



See Example SS1 – Renewable Energy Grid

Takeaways – Why AVEVA Process Simulation?

Optimize Existing Plants and Processes

Greenhouse Gas Emissions

- Use AVEVA Process Simulation to add greenhouse gas emission calculations to your simulations
- Almost every process has emissions that can be reduced
- GHG models are drag-and-drop and require almost no additional engineering effort
- Access the full range of features in AVEVA Process Simulation for optimization and dynamic studies

AVEVA

Quicky Adapt to Emerging Technologies

Hydrogen Production and Renewable Energy

- AVEVA Process Simulation can be used to model the entire hydrogen value chain
- There are opportunities for improving Grey Hydrogen processes with advanced reaction kinetics and GHG models
- Pivot to new technologies with the Renewables library (renewable energy and water electrolysis)
- The open model writing framework allows you to quickly adapt to changing technologies as they become available commercially

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