OCTOBER 25, 2023

Integrating SPYRO[™] Model into AVEVA's Optimization, Steady-State & Dynamic Simulators

Eric Wagner, Technip Energies



TECHNIP ENERGIES

Streamlining Ethylene Plant Simulations Using Integrated SPYRO[™] Model in AVEVA Software

Challenge

 Technip Energies' proprietary SPYRO[™] program is the industry standard for modeling ethylene furnace operations. Modeling this industrial process becomes arduous as the intricate interplay of thousands of chemical reactions must be painstakingly accounted for. While SPYRO[™] simulates the most important part of the ethylene production process, the furnace model needs to be incorporated into the larger ethylene plant flowsheet.

Solution

 SPYRO[™] was originally a stand-alone design tool that has now been integrated into a variety of convenient platforms, among them AVEVA Process Optimization, AVEVA PRO/II Simulation, and AVEVA Dynamic Simulation.

Results

- SPYRO[™] offers flexibility in designing and supplying various types of ethylene plants.
- A streamlined interface with integrated SPYRO[™] will simplify the overall mass balance and simulation of an ethylene plant, making the process more efficient and effective.





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







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

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

- >50 references for CO₂ removal solutions
- Strategic alliance with Shell CANSOLV[®] on CO₂ capture



Introduction to SPYROTM



SPYRO™ Product Line

SPYRO[™] is the market leader for simulation of steam cracking furnaces

- Used by Technip Energies for cracking furnace design
- Used by ethylene producers to simulate their furnace operations

Our SPYRO™ software versions

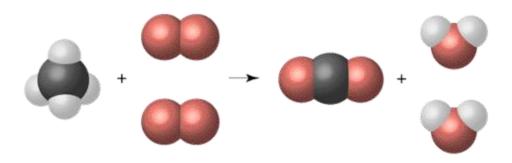


SPYRO™ Kinetic Scheme

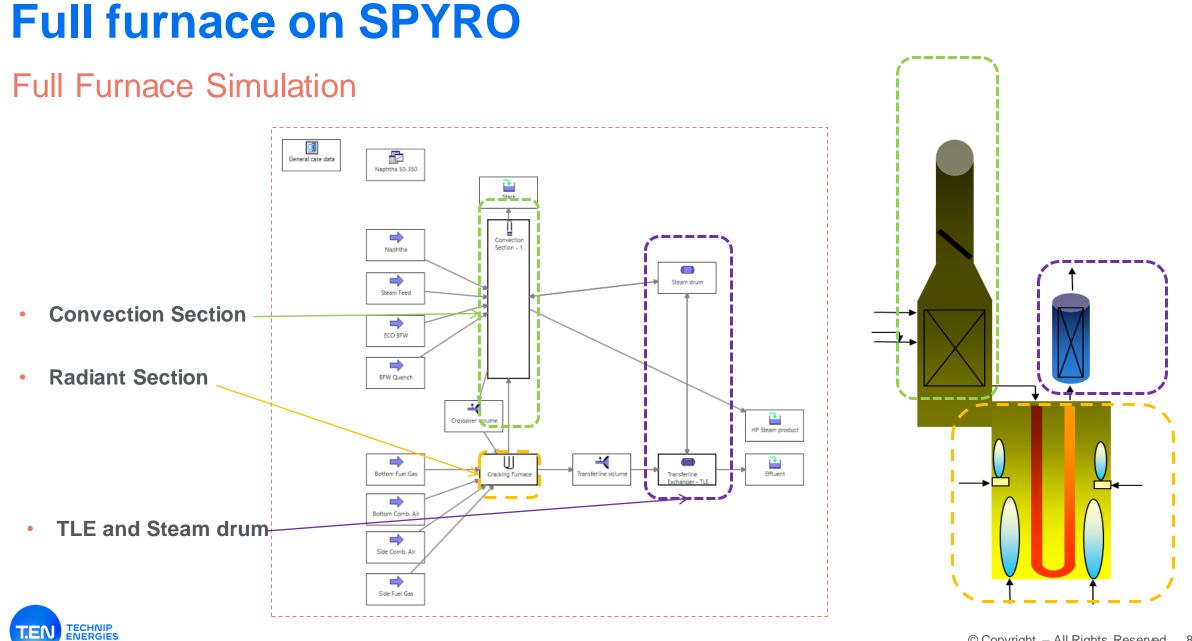
| | KS9002 | KS9306 | KS7 |
|------------|---------------------------------|---------------------------------|---------------------------------|
| Components | 124 | 128 | 218 |
| Radicals | 20 | 20 | 27 |
| Reactions | >3000 | >3000 | >7000 |
| C-range | C ₁ -C ₄₂ | C ₁ -C ₄₂ | C ₁ -C ₃₇ |

 KS9002 → KS9306: Little more detail in small olefins (C5, C6 and C7)

 KS9306 → KS7: Extended detail in heavier components (>C12)



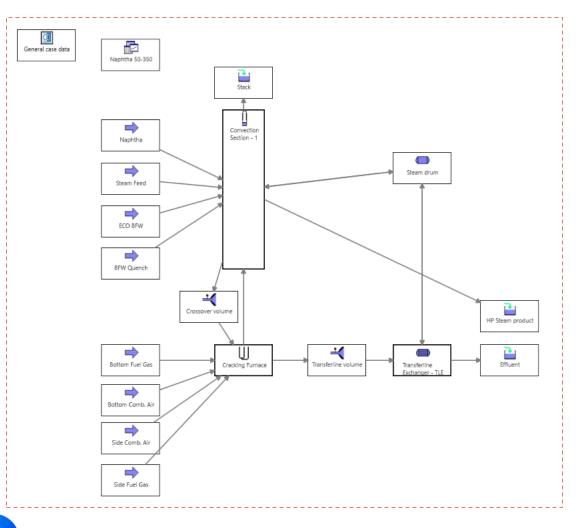




SPYRO™ Steam Cracking Furnace

Offline simulation of furnace operations

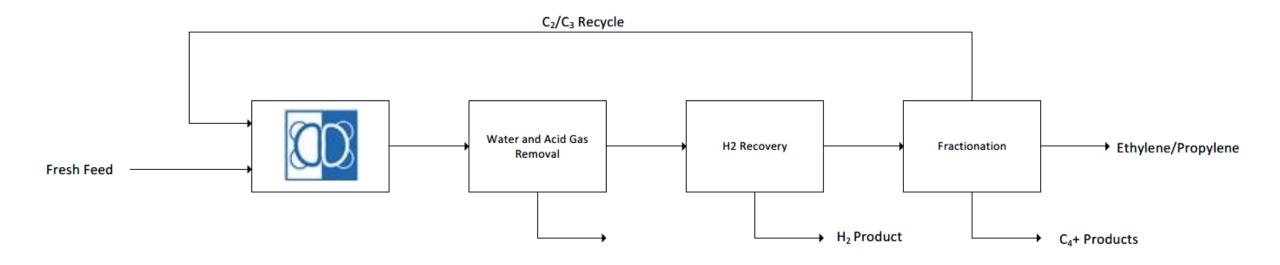
TECHNIP ENERGIES



- Product yieldsCoke formation
- Fuel gas, HP steam, etc.

- Feedstock evaluation
- Optimization of operating conditions
- Prediction of furnace run lengths
- Generation of input data for production planning

Overview of an Ethylene Plant





Running Integrated SPYRO[™] in AVEVA Process Optimization

INPUTS from Simulation (Feed Composition, Feed Rate, Temperature, etc.)



OUTPUTS to Simulation (Effluent Yields, Outlet Temperature, Outlet Pressure, etc.)



Integrated SPYRO[™]

What inputs does Integrated SPYRO[™] need?

- Convergence Option
 - COT / Severity / Conversion of Ethane or Propane / Radiant Wall Temperature
- Pressure
- At the coil inlet, coil outlet, or effluent
 - Feed Composition and Dilution Steam Ratio
- Feed Flowrate
- Coil Inlet Temperature
- Coke Thickness

| | Position | Name | Description |
|---|----------|---------|--|
| ľ | 1-4 | - | Reserved |
| | 5 | NKEY | Key component number if CONOP1 specifies convergence |
| | | | on conversion. |
| | 6 | CONOP1 | Type of convergence for severity / conversion / temper- |
| | | | ature, see below. |
| | 7 | CONVAL1 | Severity / conversion / temperature, required if $CONOP1 \neq 0$. |
| | 8 | CONOP2 | Type of pressure convergence (0=coil inlet, 1=coil out- let, 2=effluent). |
| | 9 | CONVAL2 | Coil outlet /effluent pressure [kgf/cm ² abs.], required if |
| | 9 | CUNVALZ | CONOP2 $\neq 0$. |
| | 10 | TOLF | Convergence tolerance [-], see below. |
| | 11 - 138 | | Feed Composition on dry weight basis [dry wt%]. See |
| | | | Appendix A for component indices. |
| | 139 | - | Binary option flag $(0 - 3)$ |
| | 140 | - | Type of output in DSPYOUT $(0/1)$ |
| | 141 | FLOWR | HC flow rate [kg/hr] |
| | 142 | DS | Dilution steam ratio |
| | 143 | CIP | Coil inlet pressure [kgf/cm ²] |
| | 144 | Trw | Radiating wall temperature [°C] |
| | 145 | CIT | Coil inlet temperature [°C] |
| | 146 | DpAdia | Pressure drop in transfer line [kgf/cm ²] |
| | 147-166 | COKET | Coke thickness for tube 1–20 [m] |
| | 167 | FLUXP | Adjustment parameter for flux profile |
| | 168 | HCOE | Adjustment multiplier for heat transfer coefficient |
| | 169 | FRIC | Adjustment multiplier for friction factor |
| | 170 | FOULC | Adjustment multiplier for fouling coefficient |
| | 171 | PARCO | Adjustment multiplier for coke thermal conductivity |
| | 172 | COKAD | Adjustment multiplier for coking |



Integrated SPYRO[™]

What does the user get out of Integrated SPYRO™?

- Effluent Yields
- Radiant Wall and Coil Outlet Temperatures
- Absorbed Duty
- Process Pressure and Temperature Profiles
- Maximum Tube Metal Temperature
- Heat Flux and Tube Skin Temperature Profiles
- Coking Rates
- Information Passed Back to APO Model

| Position | Description |
|-----------|---|
| 1 - 128 | Effluent Composition [dry wt%]. See Appendix A for |
| | details. |
| 129 - 136 | Reserved |
| 137 | Coil inlet pressure [kgf/cm ²] |
| 138 | Pressure drop across coil [kgf/cm ²] |
| 139 | Radiant wall temperature [°C] |
| 140 | Coil outlet temperature [°C] |
| 141 | Absorbed duty [kcal/h/coil] |
| 142 | Number of tubes per coil |
| 143 - 163 | Process temperature profile (Tube 1 through NTUBE plus |
| | the transfer line immediately following the last tube) [°C] |
| 164–184 | Process pressure profile (Tube 1 through NTUBE plus the transfer line immediately following the last tube) [kgf/cm ²] |
| 185-204 | Maximum tube metal temperature (Tube 1 through NTUBE) [°C] ¹ |
| 205-224 | Heat flux profile based on inside surface area (Tube 1 through NTUBE) [kcal/hr/m ²] |
| 225 - 244 | Coking rate (Tube 1 through NTUBE) [mm/30 days] |
| 245 - 644 | Tube skin temperature profile per collocation point [°C |



02 SPYRO™ in PRO/II



SPYRO[™] in PRO/II (Available Q1 2024)

AVEVA is currently developing a SPYRO[™] Unit Operation in PRO/II

- Scheduled to be released along with the next release of PRO/II
- Integrated SPYRO[™] license will be required
- No additional licenses will be needed for PRO/II





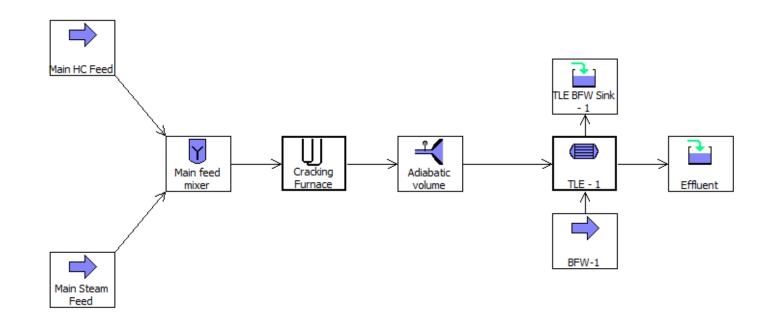
Features to Be Included

- Compatibility with KS9306 and KS7 SPYRO[™] Kinetic Schemes
- Ability to converge on all available convergence options available in Integrated SPYRO™
- Ability to input coke thicknesses in the radiant section of the SPYRO[™] files
- SPYRO[™] output data will be able to be exported to an Output Report
- TLEs can be included in SPYRO[™] geometry files
- Multiple SPYRO[™] unit operations can be used in the same simulation



SPYRO™ Geometry File

SPYRO[™] Geometry File is used by Integrated SPYRO[™] when called from PRO/II





Component Mapping

A default mapping will be provided depending on the SPYRO[™] kinetic scheme

- KS9306 contains 128 components
- KS7 contains 213 components

Mapping is not one-to-one

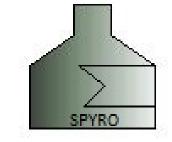
User can change mapping, but not the components

| M Range | Help | | | | |
|---------|----------|-------|-------------------------------|---------------------------|---|
| | | | | | |
| | SimSci | SPYRO | Input to SimSci Components | SPYRO Component Output | |
| | NC15 | NC15 | 0.333 | 1 | ^ |
| | NC15 | NAF15 | 0.334 | 1 | |
| | NC15 | ISO15 | 0.333 | 1 | |
| | 1EICOSE | NAF20 | 0.333 | 1 |] |
| | 1EICOSE | EIC1 | 0.334 | 1 | |
| | 1EICOSE | OLC20 | 0.333 | 1 | |
| | 2MNP | OLN11 | 1 | 1 | |
| | C10CYH | OLN16 | 0.334 | 1 | |
| | C10CYH | OLC16 | 0.333 | 1 | |
| | C10CYH | EXA1 | 0.333 | 1 | |
| | C9BZ | C15AR | 1 | 1 | |
| | C14BENZ | C20AR | 0.5 | 1 | |
| | C14BENZ | DNA20 | 0.5 | 1 | |
| | NC20 | NC20 | 0.5 | 1 | |
| | NC20 | ISO20 | 0.5 | 1 | |
| | 1PNAP | C15CO | 1 | 1 | |
| | C10NAPH | C20CO | 1 | 1 | |
| | 1HEPTYNE | DIA7 | 1 | 1 | |
| | TED1 | DIA14 | 1 | 1 | |
| | 4IPDPH | DNA15 | 1 | 1 | |
| | NC32 | CH32 | 0.25 | 1 | ¥ |



SPYRO™ – PRO/II Interface Summary

- AVEVA is developing a new unit operation in PRO/II that will allow Integrated SPYRO[™] to be run from the PRO/II flowsheet
 - This new unit operation is scheduled to be released along with the next release of PRO/II
- SPYRO[™] geometry file provides the coil geometry to be simulated
- KS9306 and KS7 will be compatible with this new unit operation
- SPYRO[™] output data will be accessible via the PRO/II output reports
- Multiple instances of SPYRO[™] can be called in the same flowsheet





103 SPYRO[™] for Dynamic Real-time Environment (SPYDRE)



Integrating SPYRO[™] into AVEVA Dynamic Simulation

What?

• SPYRO[™] is Technip Energies' proprietary software for an ethylene cracker yield model for furnace design and performance prediction

How?

• The hydrocarbon cracking reaction kinetic model set and radiant coil heat transfer embedded in SPYRO[™] is integrated into the ADS OTS via DLL I/O

Why?

- Take advantage of the rigorous radiant coil cracking solution provided by SPYRO[™] in ADS OTS to predict overall system dynamic behavior
 - Overcome limitations of regression-based OTS models



First Principle High Fidelity Dynamic Model of an Ethylene Furnace

Rigorous Comprehensive Simulation of Key Equipment in an Ethylene Unit/Furnace

- Radiant Coils
- Radiant Furnace
- Convection Section
- Transfer Line Exchangers
- Recovery Section

Simulate Ethylene Unit/Furnace Operating Transitions

- Start-up/Shutdown
- HSSB to Cracking and vice-versa
- HSSB to Decoking and vice-versa
- Trip condition to HSSB

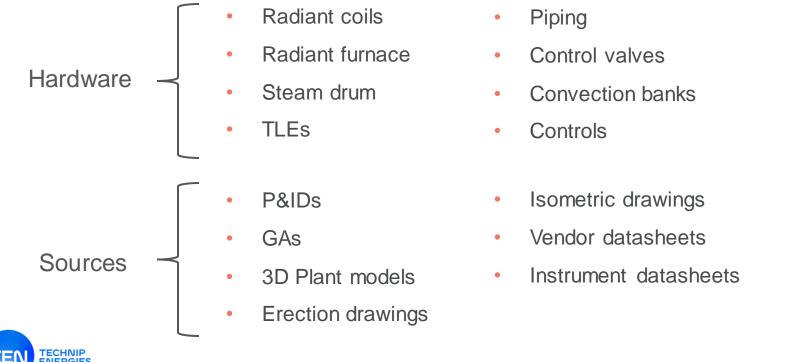


Customized Furnace Model

Case-by-case Configuration of Ethylene Unit/Furnace

The dynamic simulation model is built and tuned specifically for each individual application

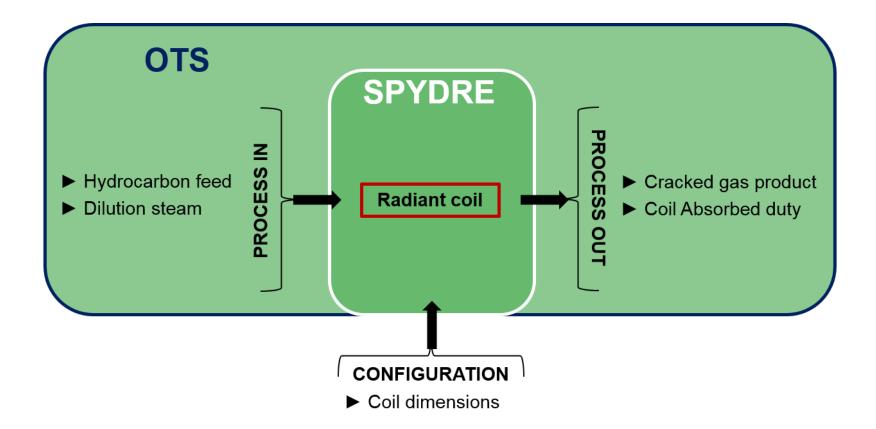
Detailed information obtained from Client's engineering design and vendor documentation is used to develop sections in the model when supplied



- Transmitters
- ID Fan

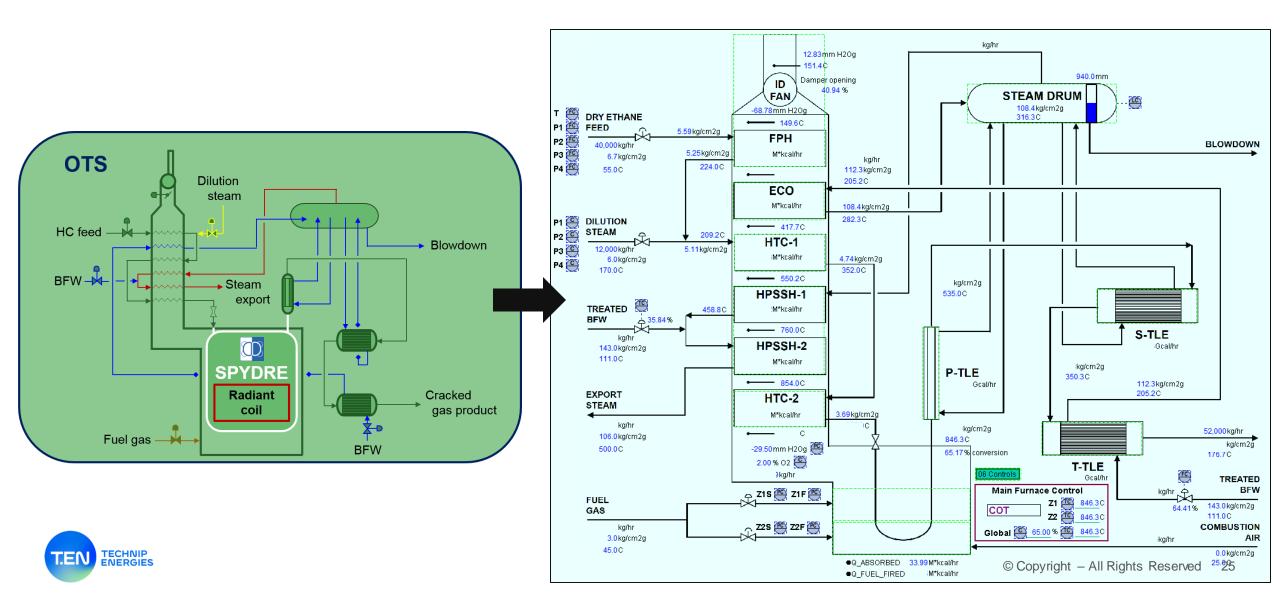
- Mechanical Assembly and Shop drawings
- Cause and Effect matrix

OTS Interface with SPYDRE





Ethylene Furnace Overview in ADS OTS

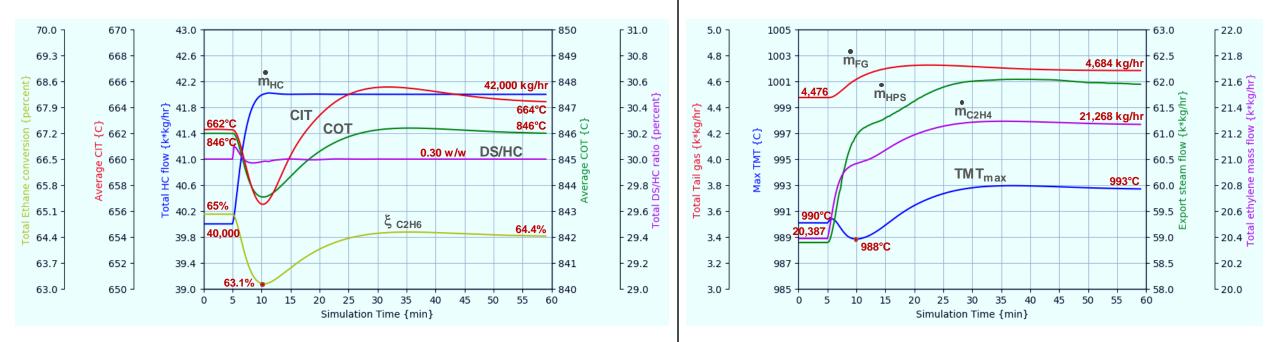


Transient Scenario #1

Increase Total HC Feed to Furnace by 5% with COT control

- Initial condition:
 - All 4 passes at 10,000 kg/hr HC each
 - COT = 846°C

- 97 wt% C2H6 dry basis in HC feed
- C2H6 Conversion = 65%



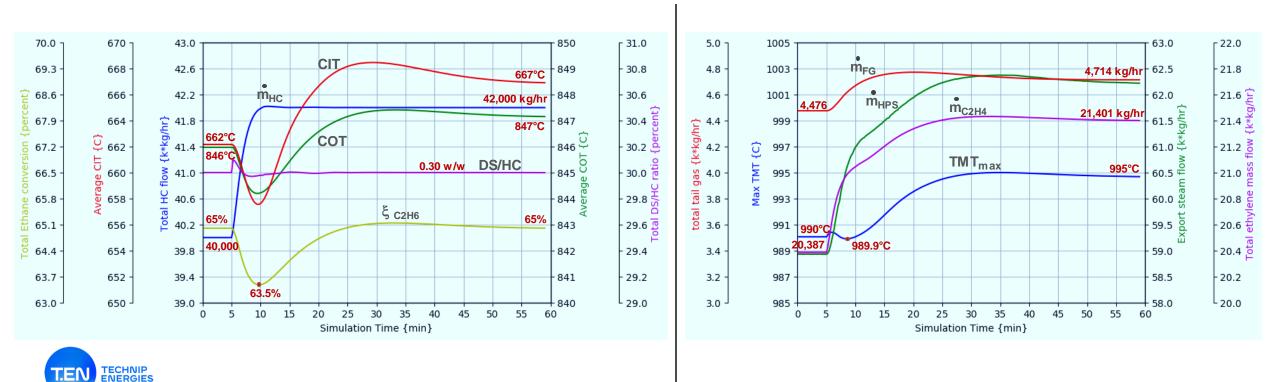


Transient Scenario #2

Increase Total HC Feed to Furnace by 5% with Conversion control

- Initial condition:
 - All 4 passes at 10,000 kg/hr HC each
 - COT = 846°C

- 97 wt% C2H6 dry basis in HC feed
- C2H6 Conversion = 65%

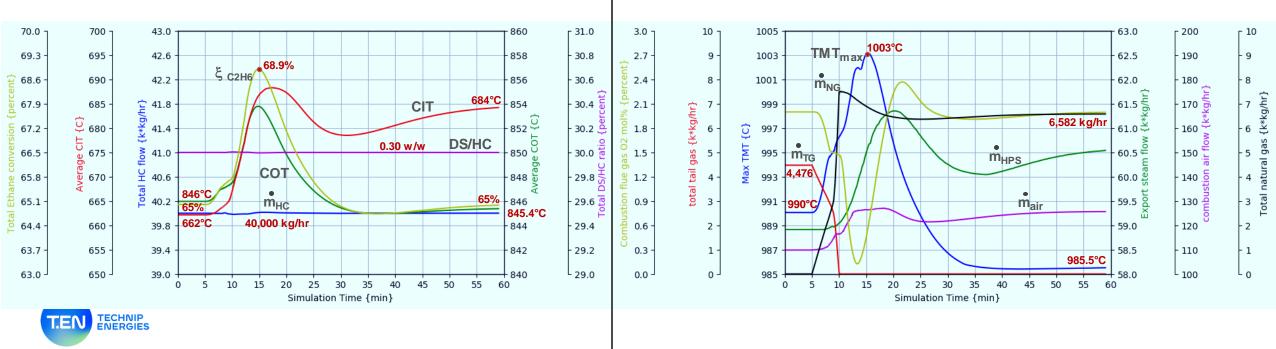


Transient Scenario #3

Transition Combustion Fuel from H2 Rich Tail Gas to NG

- Initial condition:
 - Fuel gas:
 - 79 mol% H2 + 20 mol% CH4
 - COT = 846°C

- Final condition:
 - Fuel gas:
 - 100 mol% CH4
 - COT = 846°C



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!

