Mitigation of CO_2 Emissions from an Ammonia Synthesis Plant via Green Methanol and DME synthesis

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AVEVA

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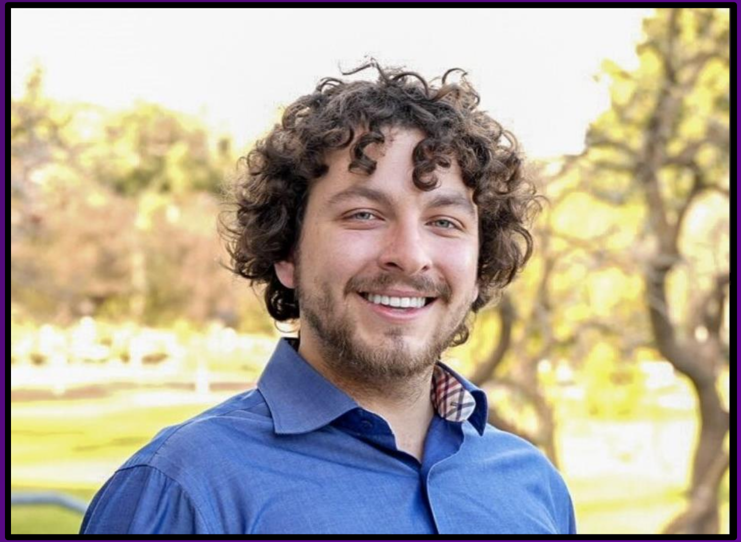


Design Engineer

A class of Cal Poly Pomona seniors investigating reducing GHG emissions of industrial processes to generate synthetic fuels

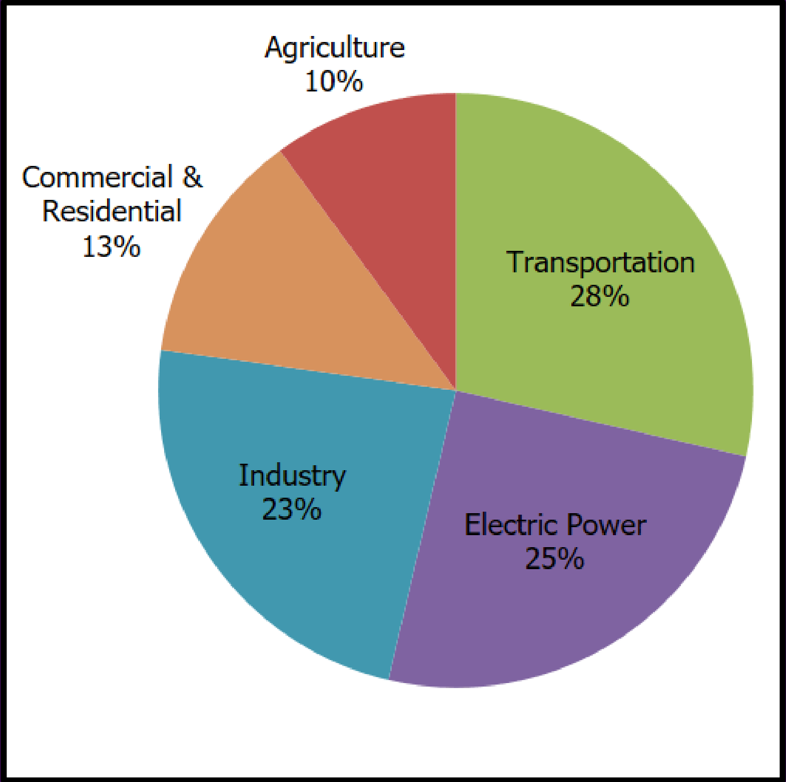


Table 4-21: CO_2 Emissions from Ammonia Production (MMT CO_2 Eq.)

Source	1990	2005	2017	2018	2019	2020	2021
Ammonia Production	14.4	10.2	12.5	12.7	12.4	13.0	12.2

Sources of greenhouse gas emissions | US EPA. (2023, October 5). US EPA. https://www.epa.gov/ghgemissions/sources-greenhouse-gas-emissions#industry
EPA (2023) Inventory of U.S. Greenhouse Gas Emissions and Sinks: 1990-2021. U.S. Environmental Protection Agency, EPA 430-R-23-002. https://www.epa.gov/ghgemissions/inventory-us-greenhouse-gas-emissions-andsinks-1990-2021.

Chemical Industry | United States

Alteragreen wishes to create a feasible synthetic fuel generation plant utilizing green hydrogen

Challenge

- Create a design competitive with other carbon capture and utilization plants
- Analyze novel kinetics for production of both chemicals

Solution

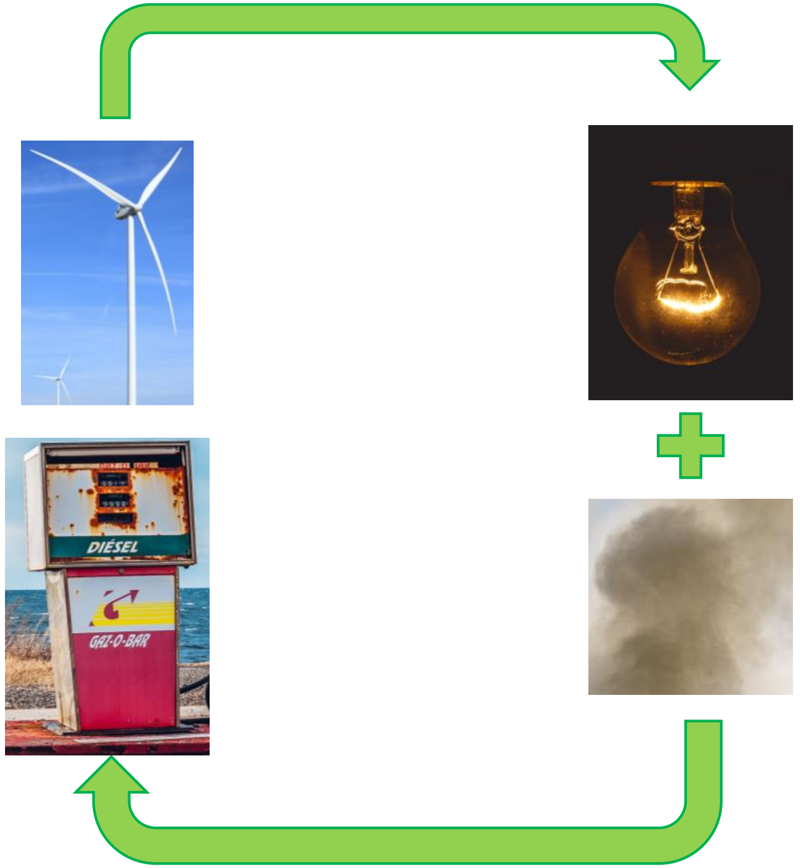
- Design and simulate green methanol and DME production plant required to mitigate CO_2 emissions from ammonia production plant

Results

- **Created a plant design that captures 48 MM SCFD of CO_2**
- **Produced 660,000 tons of methanol and 4,000 tons of DME per year**

Challenge

Reduce carbon footprint in a financially sustainable manor



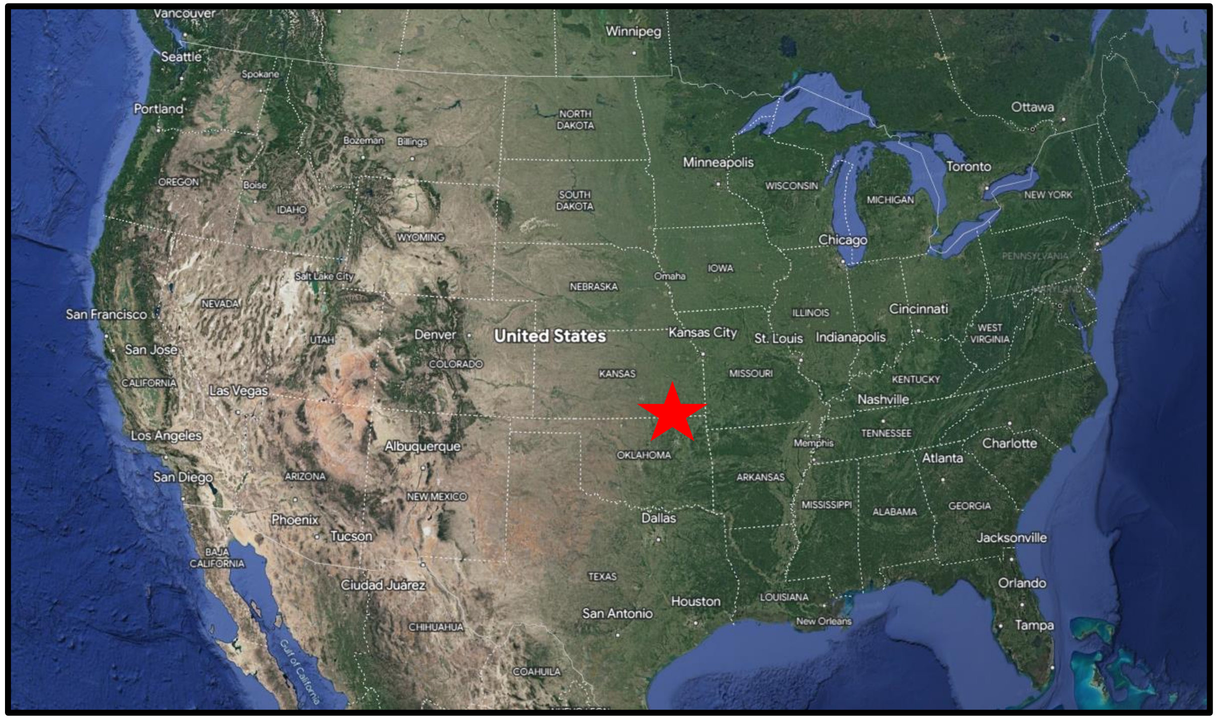
- Increased public action and government incentives in recent years to reduce CO_2 emissions
- Most methanol production is done using steam methane reforming and does not require CO_2 hydrogenation
- Dimethyl Ether production is typically not done using methanol
- Operational challenges with using green generation methods to support industrial stream factors
- Complete technoeconomic analysis to analyze profitability

AVEVA

Solution

Design a green plant using AVEVA software

- Location: CVR Resources in Coffeyville, KS
  - Refinery and fertilizer plant
  - Coke gasification for ammonia hydrogen production
  - Some of the largest wind power availability in the US
  - Data available for stream flowrates and compositions
  - Existing enhanced oil recovery carbon capture system installed
  - Largest existing CCUS system in the fertilizer industry



AVEVA

Solution

Design a green plant using AVEVA software

- AVEVA™ PRO/II™ Simulation for steady state plant design and complete heat integration

- AVEVA™ Dynamic Simulation for dynamic design and HAZOP scenarios

- AVEVA™ E3D Design for isometric plant model and design

- AVEVA™ XR for virtual plant walkthrough to ensure validity of isometric model

AVEVA

Benefits

Utilize AVEVA PRO/II for steady state plant design and complete heat integration

- Aids in making informed decisions that lead to optimized process performance:
  - A blower is required to reduce the high volumetric rates of the feed such that the first compressor is reasonably sized and well designed

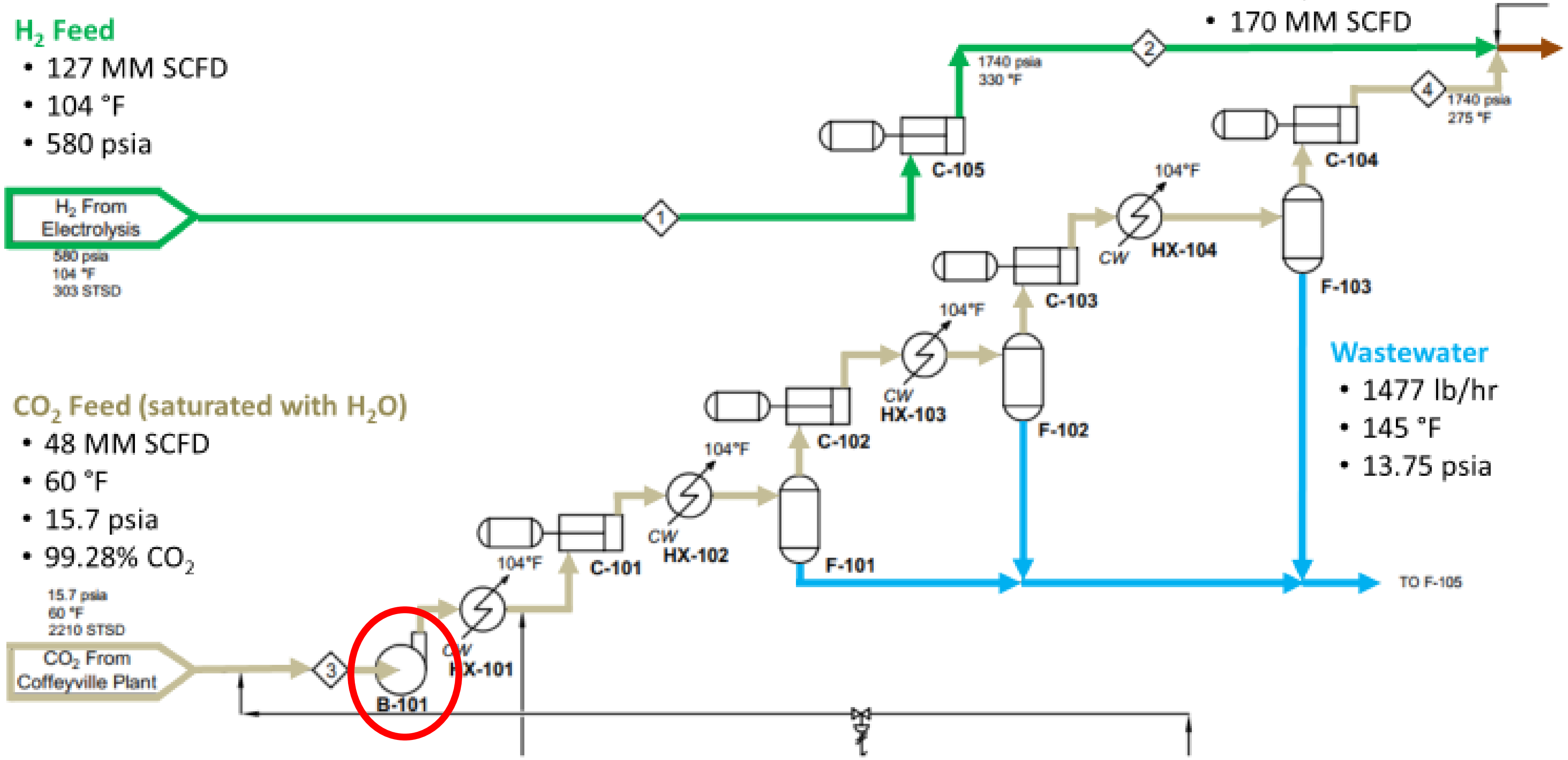
Compression

Compressed Feed
- 1740 psia
- 170 MM SCFD

H_2 Feed
- 127 MM SCFD
- 104 °F
- 580 psia

Wastewater
- 1477 lb/hr
- 145 °F
- 13.75 psia

CO_2 Feed (saturated with H_2O)
- 48 MM SCFD
- 60 °F
- 15.7 psia
- 99.28% CO_2



Benefits

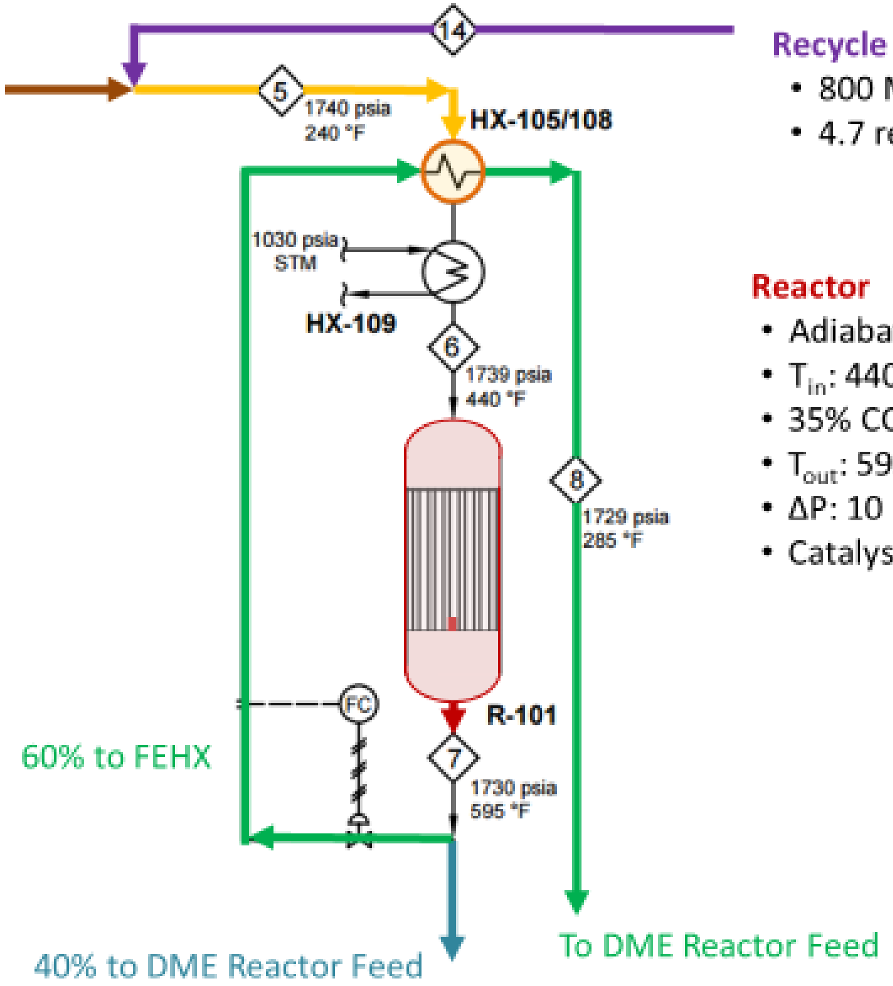
AVEVA PRO/II for steady state plant design and complete heat integration

- Aids in making informed decisions that lead to optimized process performance:
  - A blower is required to reduce the high volumetric rates of the feed such that the first compressor is reasonably sized and well designed
  - An adiabatic reactor was made in conjunction with the kinetics of CO_2 to methanol synthesis and to limit steam production. This would improve equipment process longevity, reduce electrical and hydrogen requirement for operating the plant

Methanol Synthesis

Compressed Feed
- 1740 psia
- 170 MM SCFD

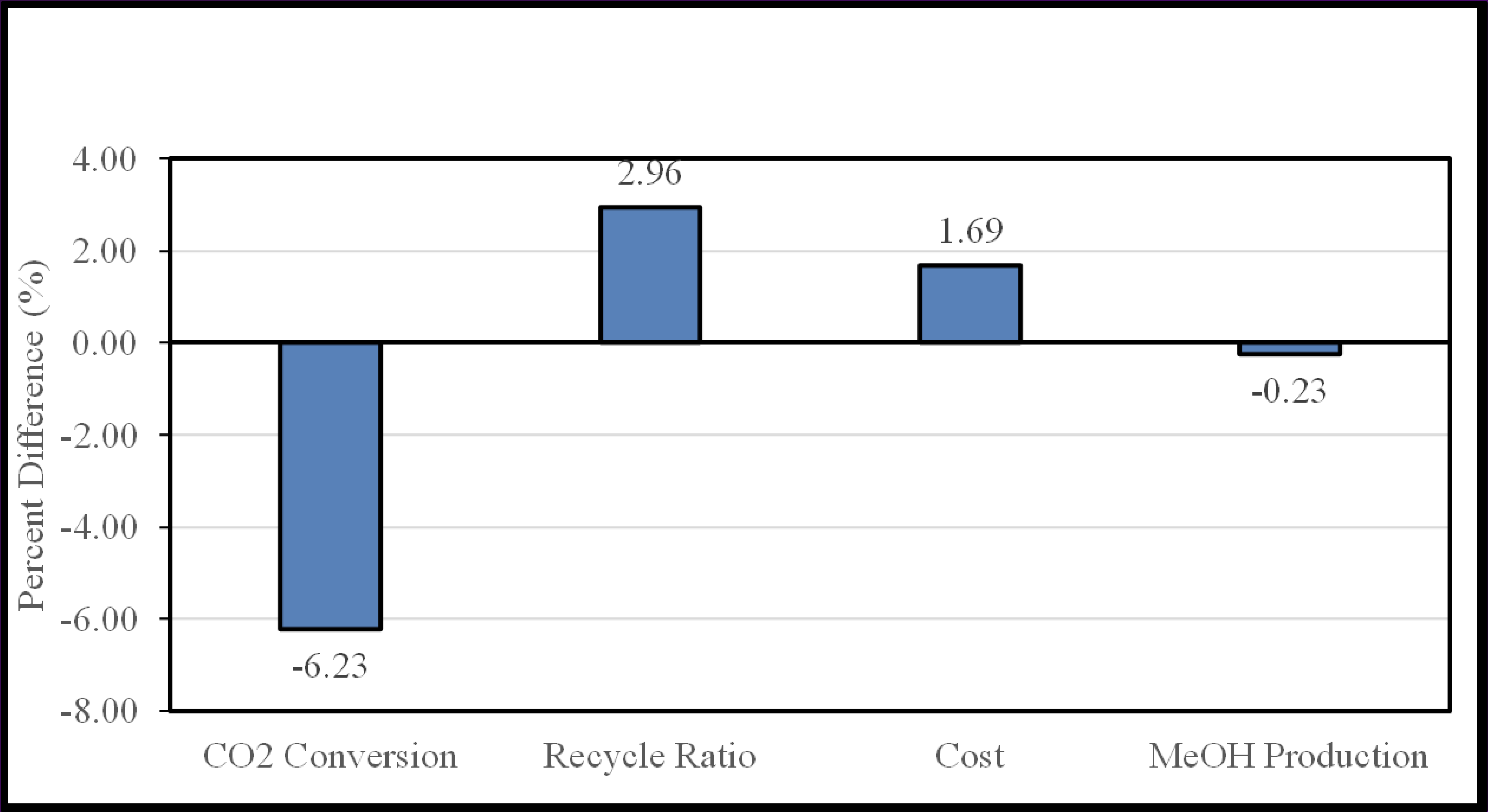
Combined Feed
- 970 MM SCFD
- 240 °F
- 1740 psia



Recycle
- 800 MM SCFD
- 4.7 recycle: process feed ratio

Reactor
- Adiabatic
- T_{in}: 440 °F
- 35% CO_2 Conversion
- T_{out}: 595 °F
- ΔP: 10 psi
- Catalyst: Cu/ZnO-Cr2O3-SiO2

Adiabatic vs Isothermal Reactor



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  - High vapor:liquid ratio was identified for the MeOH plant and pressure energy was recovered for electricity using an Isogen hydraulic turboexpander.

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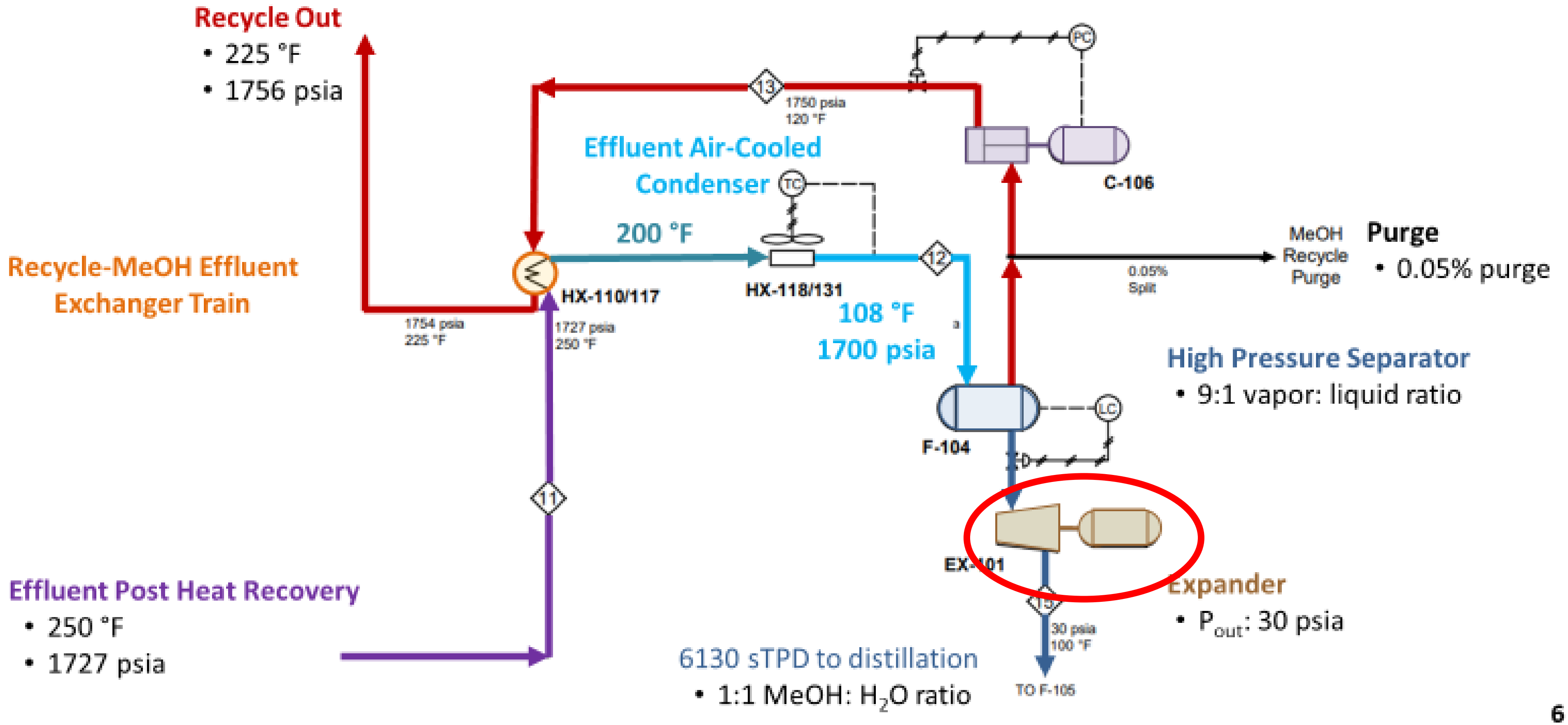
High Pressure Separation and Cooling



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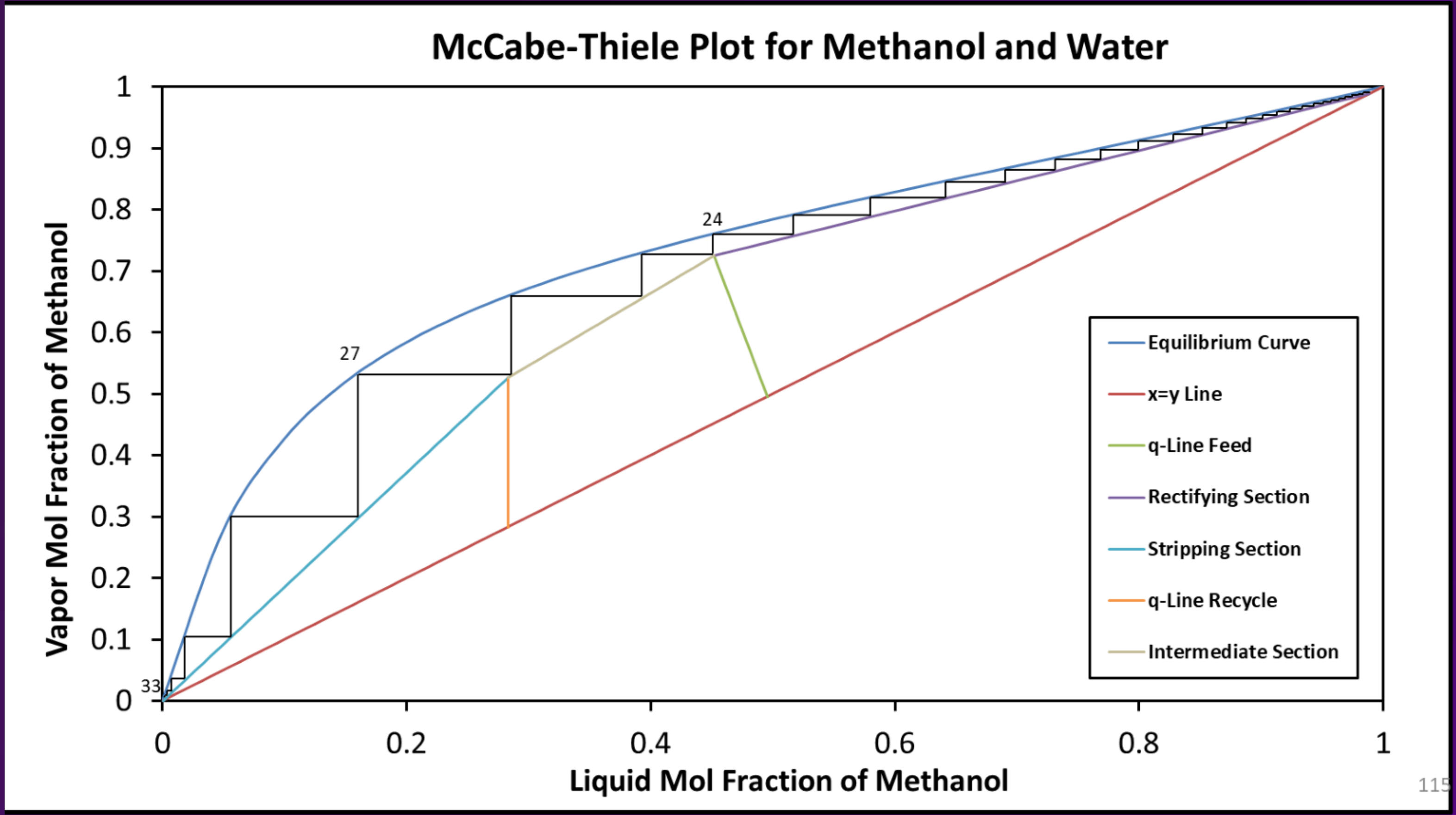
  - Optimizing the tower in PRO II reduced the reboiler duty and lightened the load on the heat exchanger network.



Methanol Tower	
Top Tray Pressure	14.5 PSIA
Reflux Ratio	0.984
Theoretical Trays	33
Distillate Composition	99.53 mol %

Benefits

AVEVA PRO/II for steady state plant design and complete heat integration

- Aids in making informed decisions that lead to optimized process performance:
  - ➢ A blower is required to reduce the high volumetric rates of the feed such that the first compressor is reasonably sized and well designed.
  - ➢ An adiabatic reactor was made in conjunction with the kinetics of CO_2 to methanol synthesis and to limit steam production. This would improve equipment process longevity, reduce electrical and hydrogen requirement for operating the plant.
  - ➢ High vapor:liquid ratio was identified for the MeOH plant and pressure energy was recovered for electricity using an Isogen hydraulic turboexpander.
  - ➢ Optimizing the Methanol tower in PRO II reduced the reboiler duty and lightened the load on the heat exchanger network.
  - ➢ Without complete heat integration, the hydrogen requirement would nearly double, drastically increasing the capital investment of the facility, potentially by more than $1 billion.
  - ➢ Heat integration data was corroborated using 3 different simulation software and HTRI and AVEVA PRO/II showed the most corroboration for a two-phase system and is desirably preferred .

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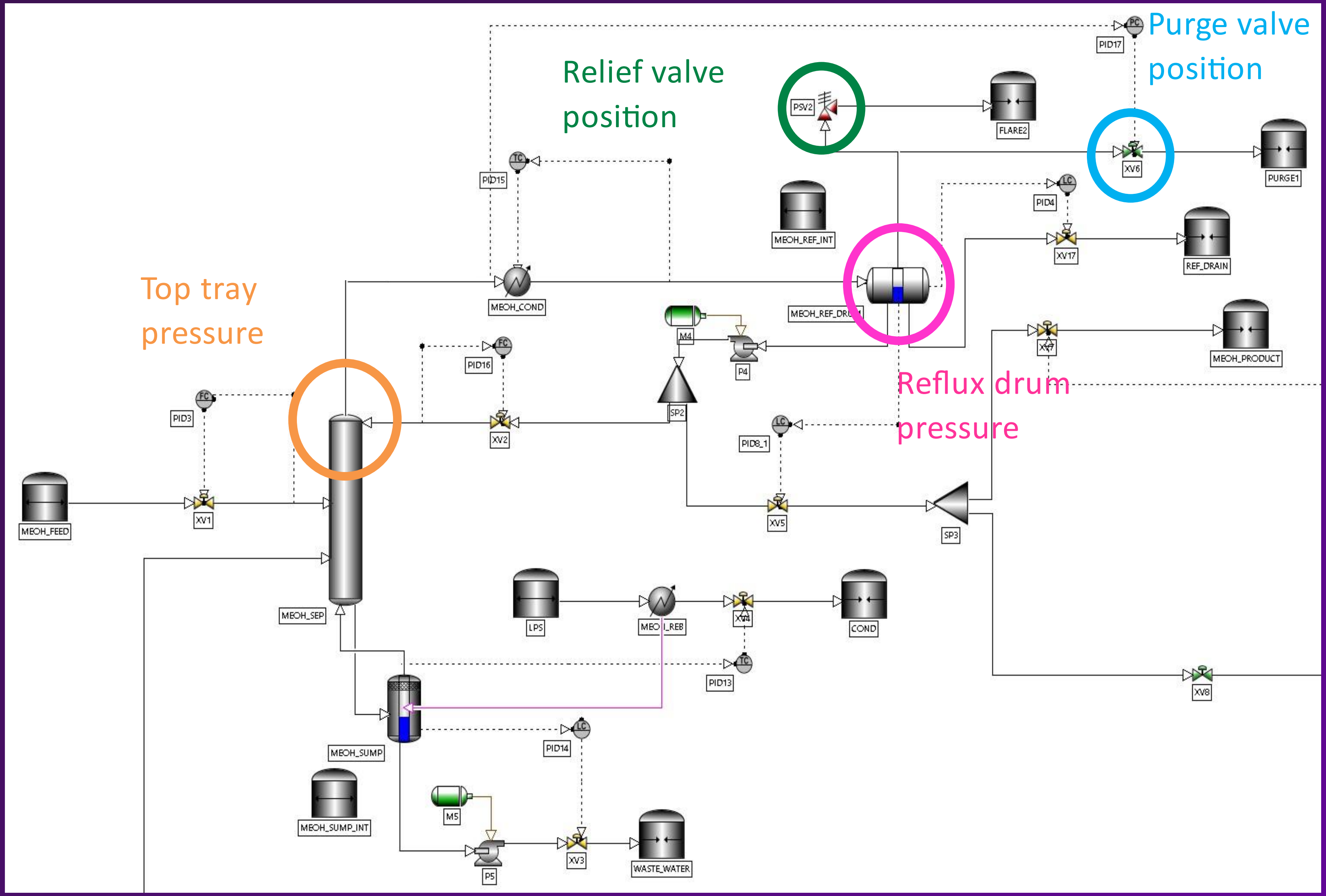
Benefits

AVEVA Dynamic Simulation for dynamic design and HAZOP scenarios

- Aided our understanding of transient responses:
  - Relief Valve Sizing

Understanding the Transient Responses using a Pressure Relief Valve



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- Enables users to simulate various scenarios and assess its impact:
  - Spiked water in MEOH feed into MEOH separation tower demo

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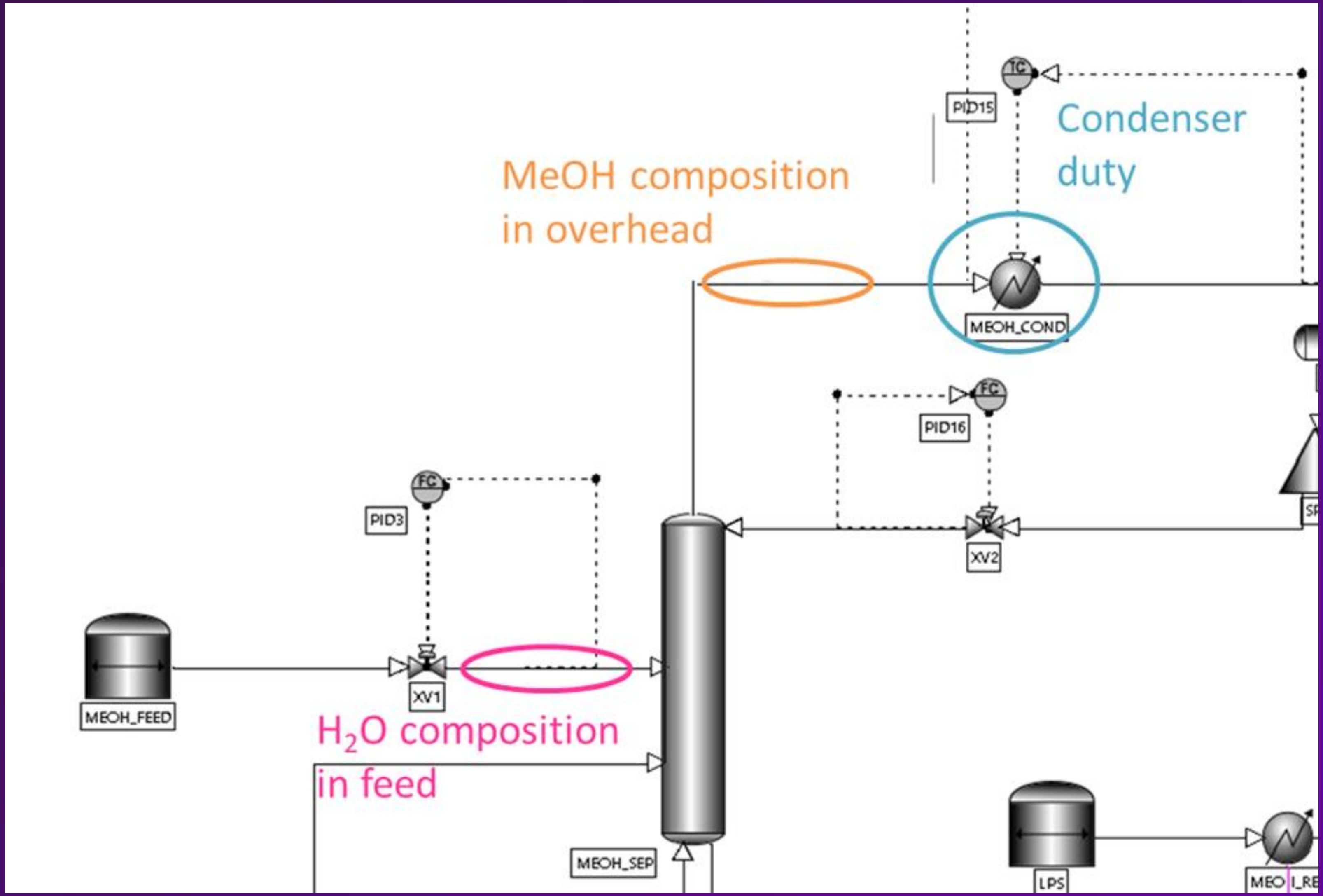
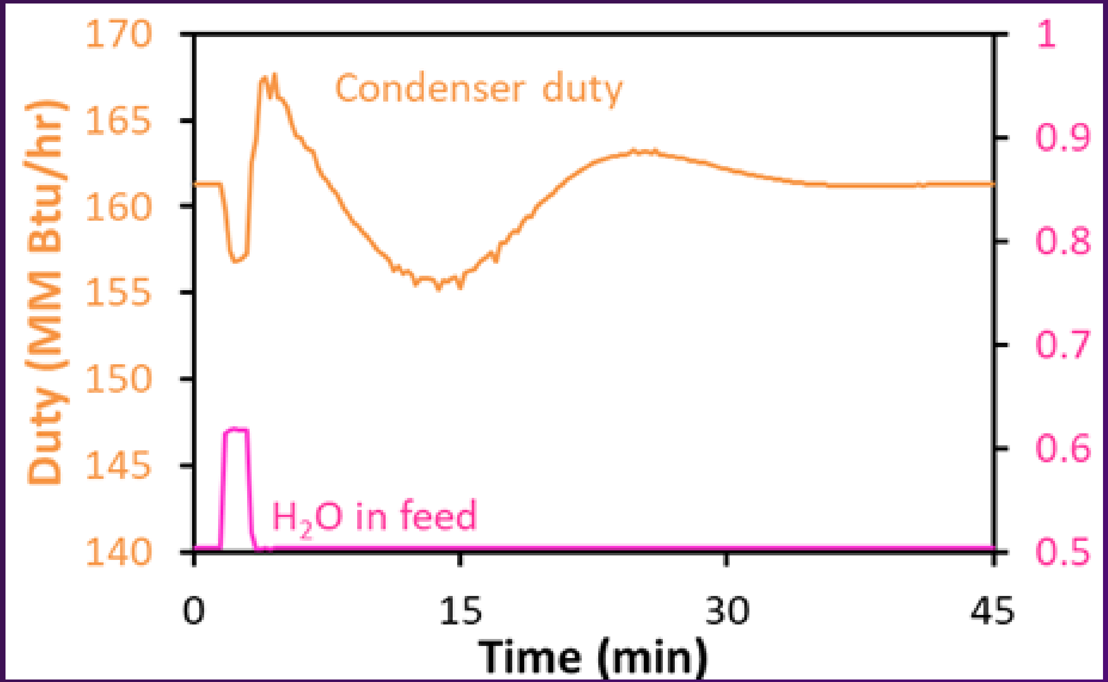
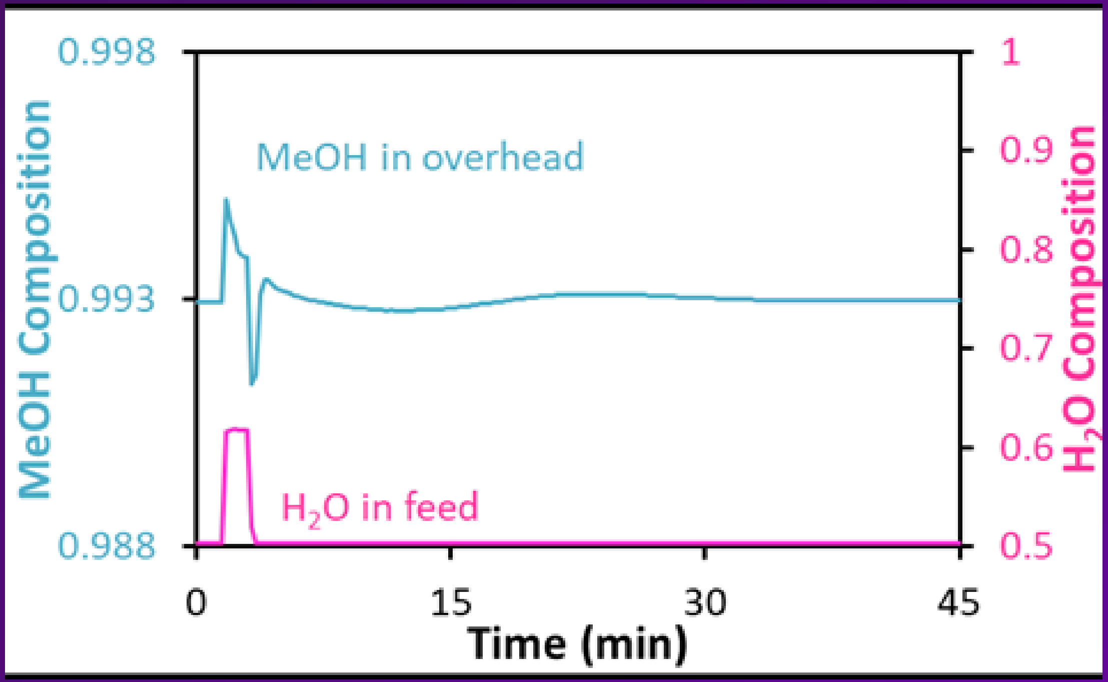
Spiked Water in MeOH Feed into MeOH Separation Tower



Results from Spiked Water in MeOH Feed into MeOH Separation Tower





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- Allows for the study of abnormal situations, startups, shutdowns, emergencies, & operator training:
  - Startup demo

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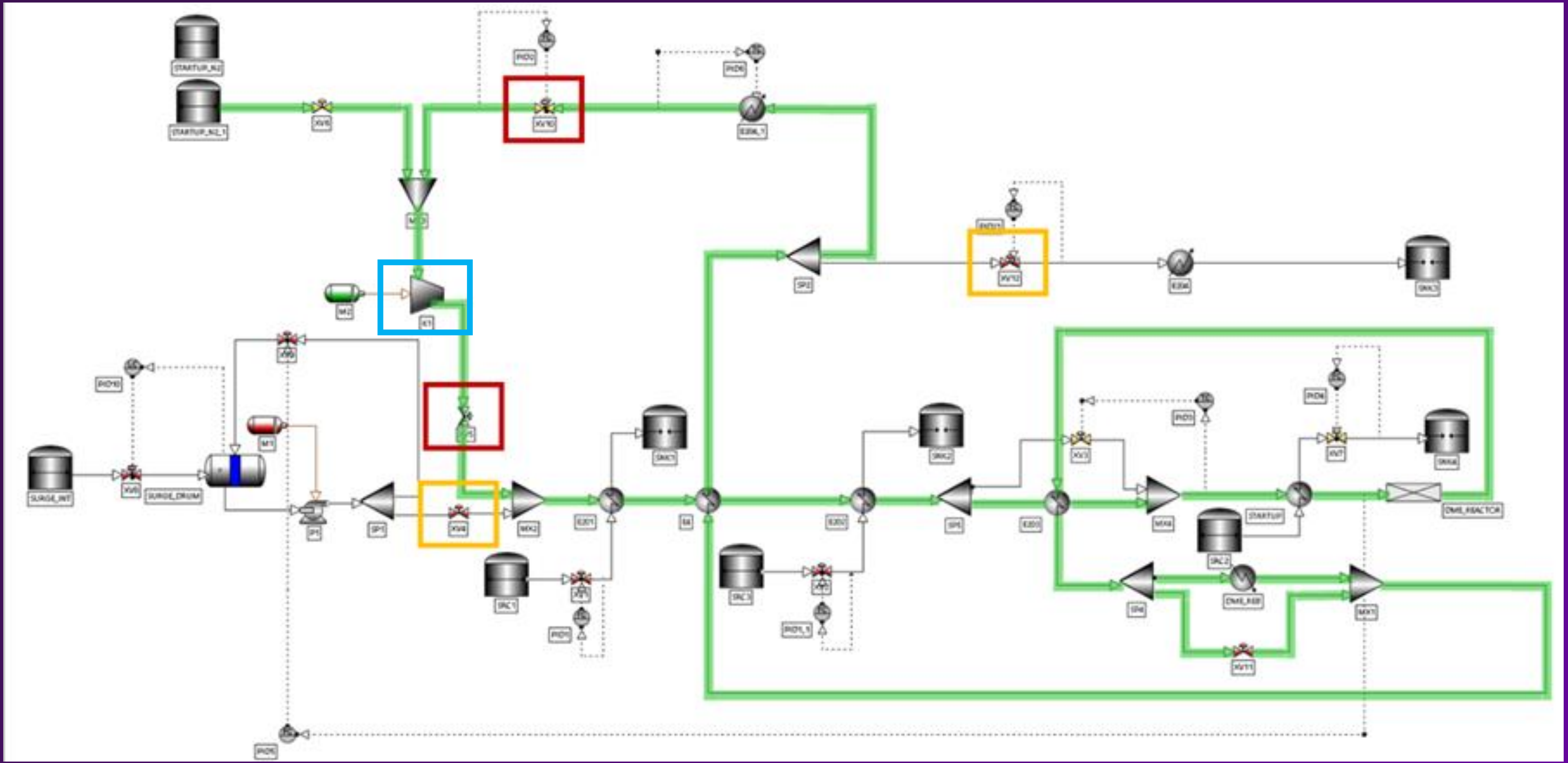
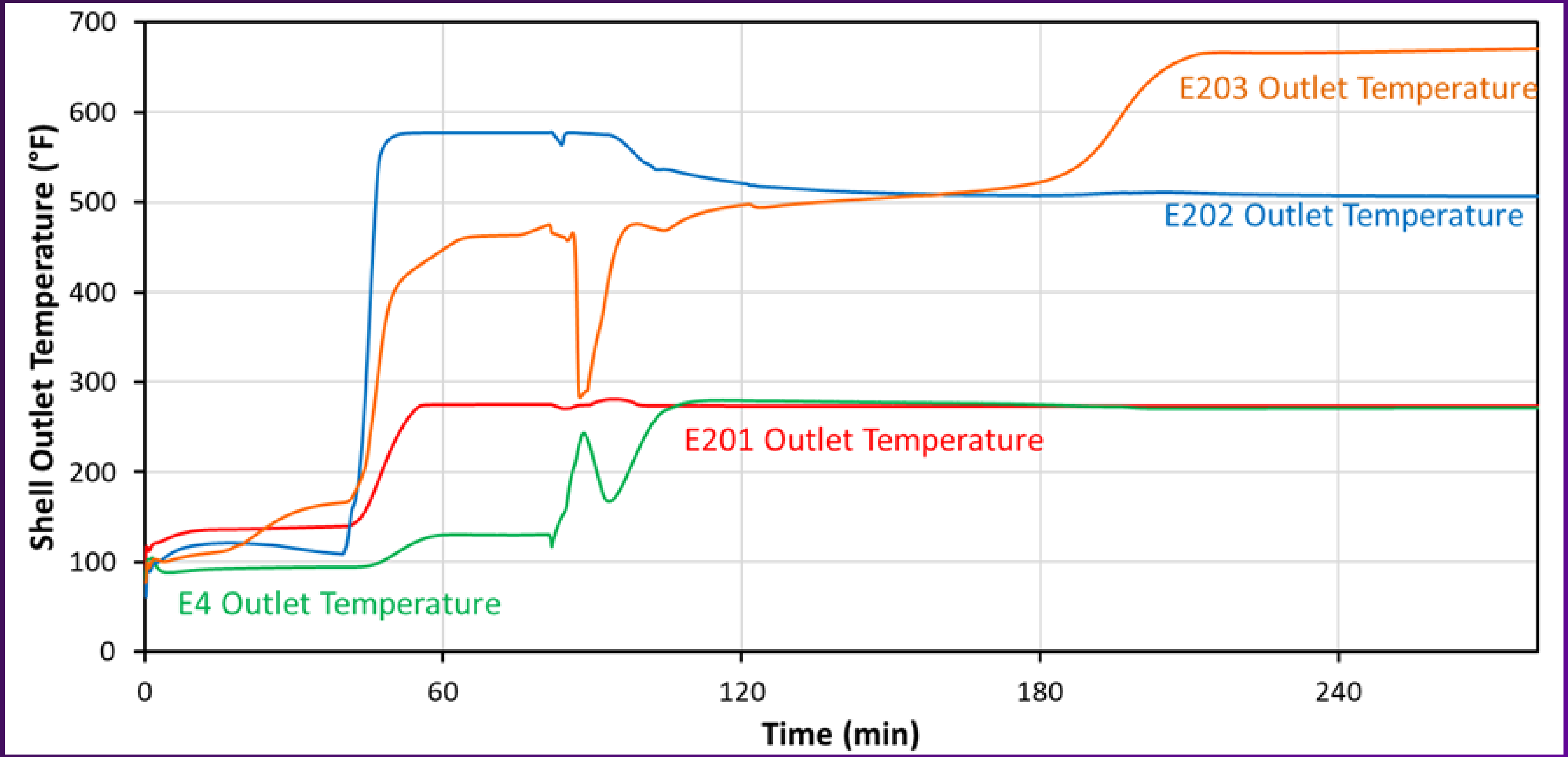
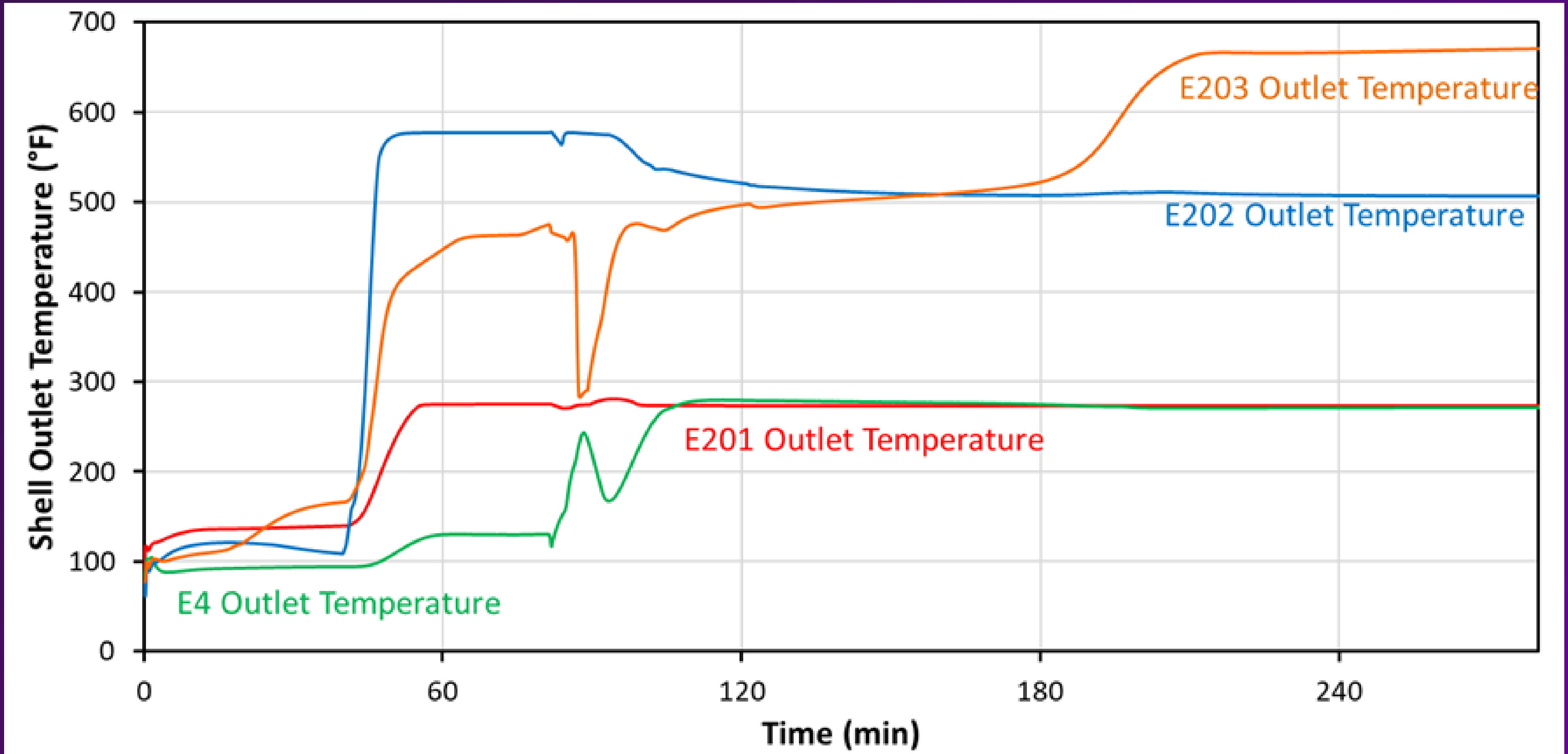
Startup - Flow Pathway Closed Nitrogen Loop (Green)



Startup – Feed Effluent Exchanger Outlet Temperatures



0-30 minutes: Nitrogen flow due to pressure differential from compressor



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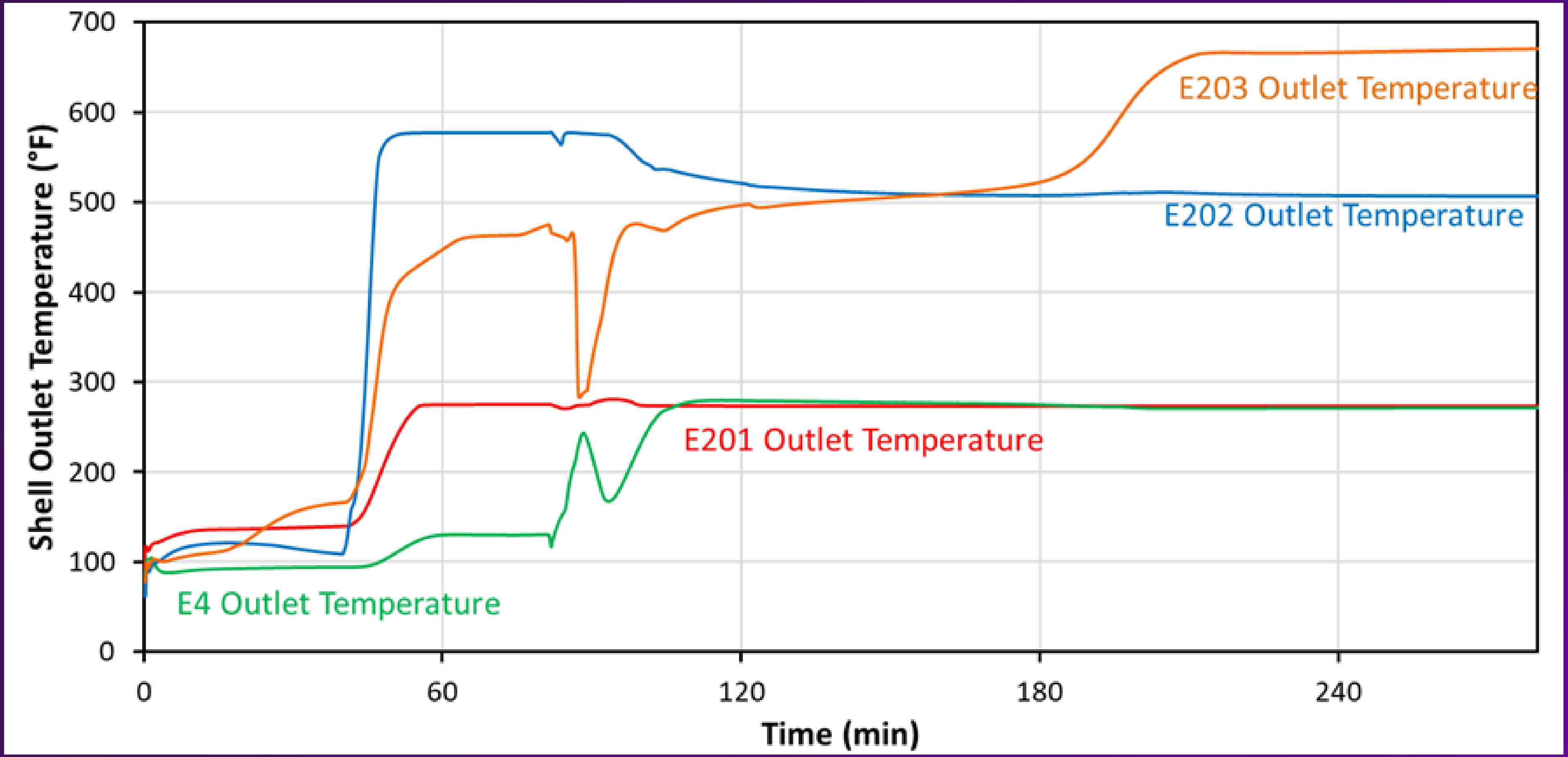
30-60 minutes: Bringing heat exchangers up to temperature by heating nitrogen



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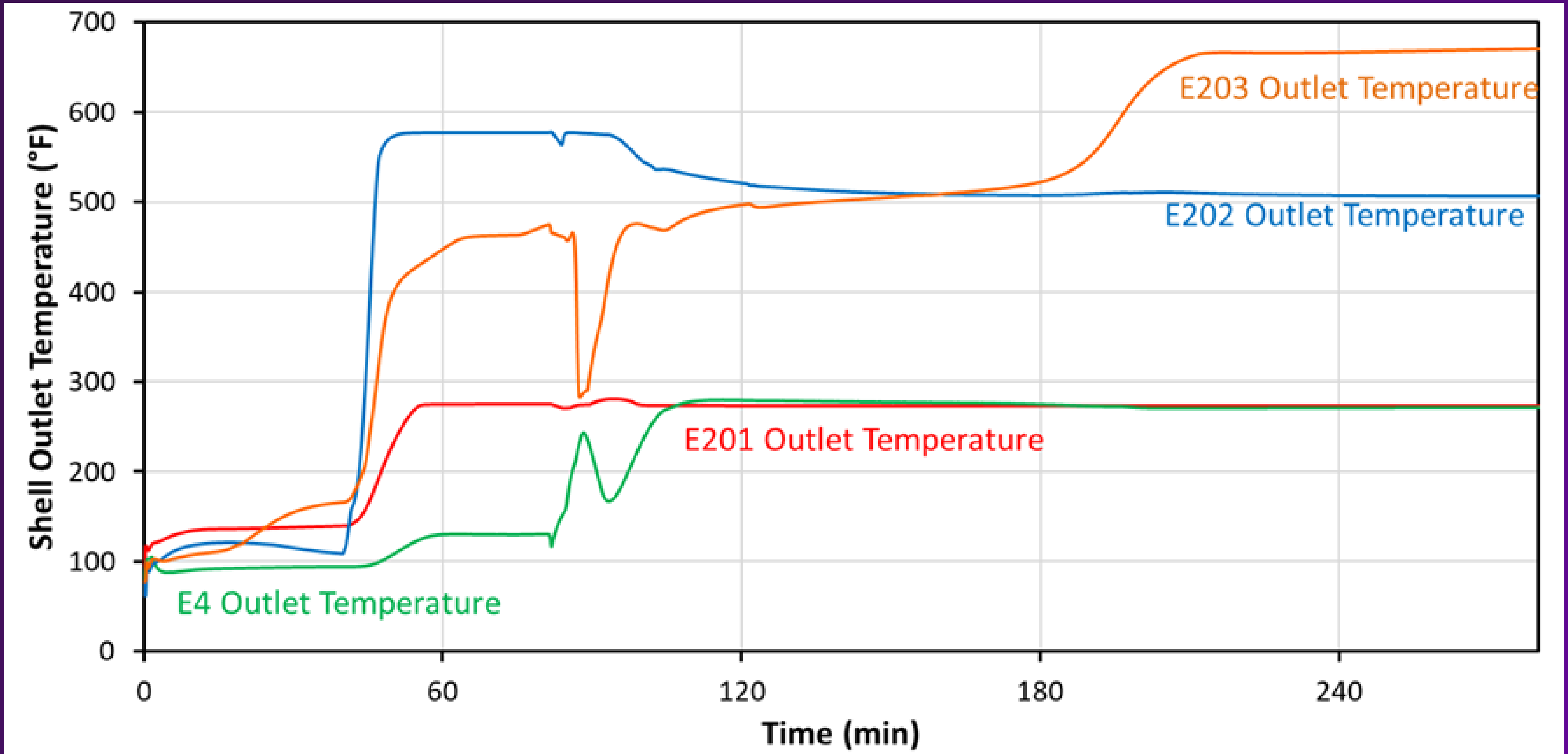
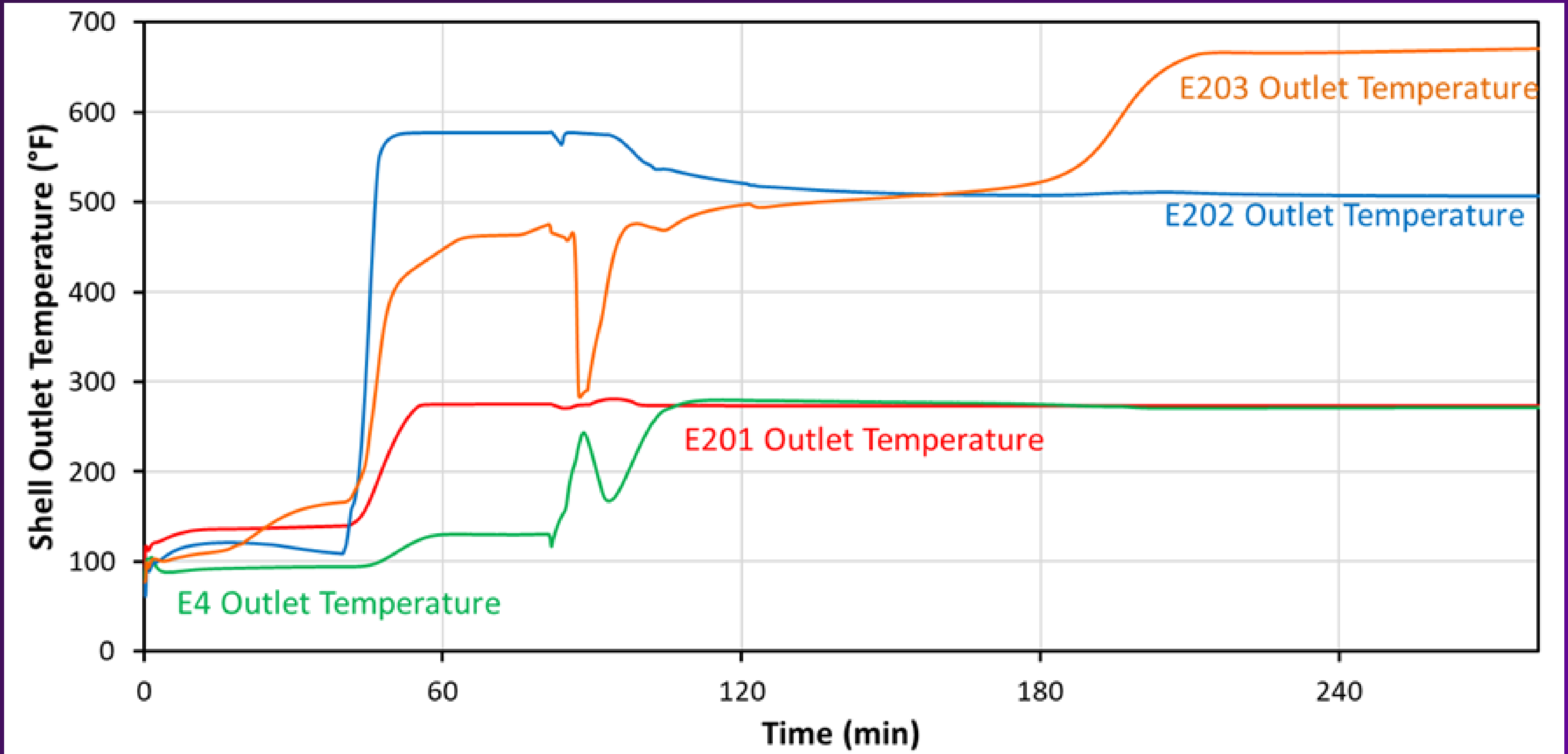
90th minute: Cold methanol is introduced



90+ minute: Bringing the reactor up to temperature & reaction light-off



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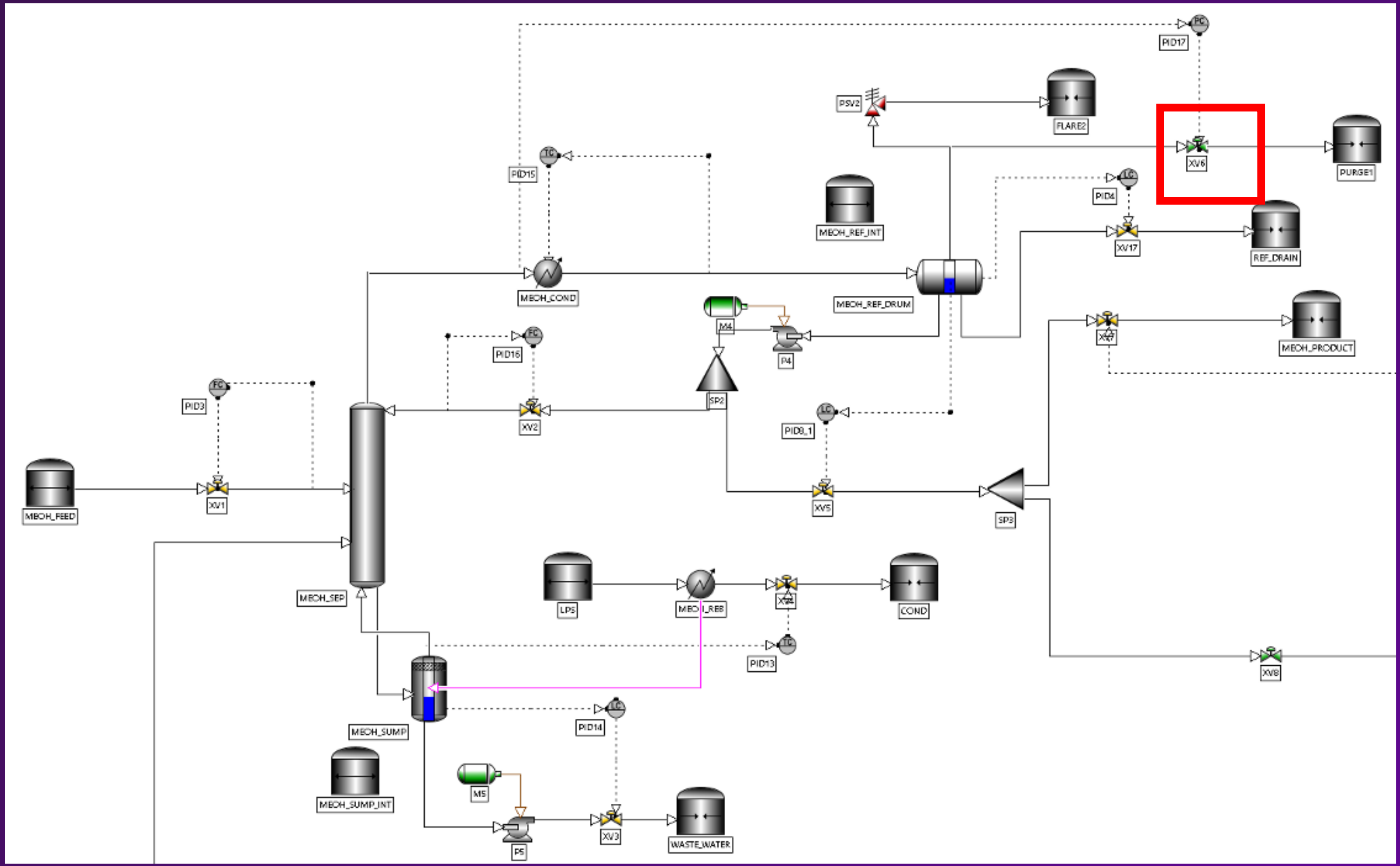
- Enables users to simulate various scenarios and assess its impact:
  - Spiked water in MEOH feed into MEOH separation tower demo
- Allows for the study of abnormal situations, startups, shutdowns, emergencies, & operator training:
  - Startup demo
  - HAZOP study
  - XR studios

HAZOP study – Indication of vapor purge valve location



HAZOP study – Results

Parameter	Guideword	Deviation	Cause	Consequences	Safeguard
Flow	More	More Flow	• Mechanical Failure • Controller Failure	• Pressure in reflux drum decreases • Pressure in tower decreases	• Install pressure gauge at top tray
	Less	Less Flow	• Mechanical Failure • Controller Failure • Blockage	• Pressure in reflux drum increases • Pressure in tower increases	• Install pressure gauge at top tray • Install pressure relief valve
	No	No Flow	• Mechanical Failure • Controller Failure • Blockage	• Pressure in reflux drum increases • Pressure in tower increases	• Install pressure gauge at top tray • Install pressure relief valve

Benefits

AVEVA E3D Design for isometric plant model and design

Challenges:

- Construction of plot plan
- Weather conditions

Goal: A complete 3D model

Plot Plan references

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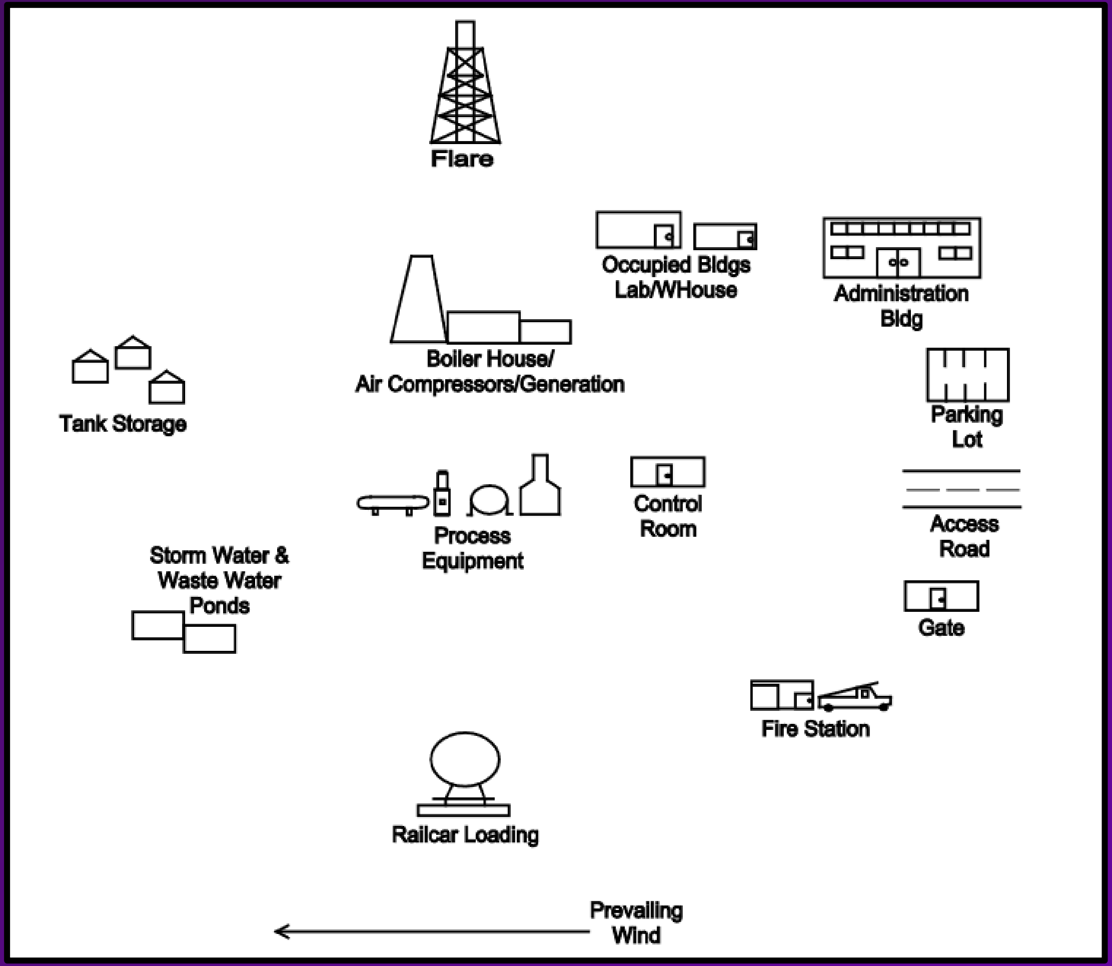
Solution:

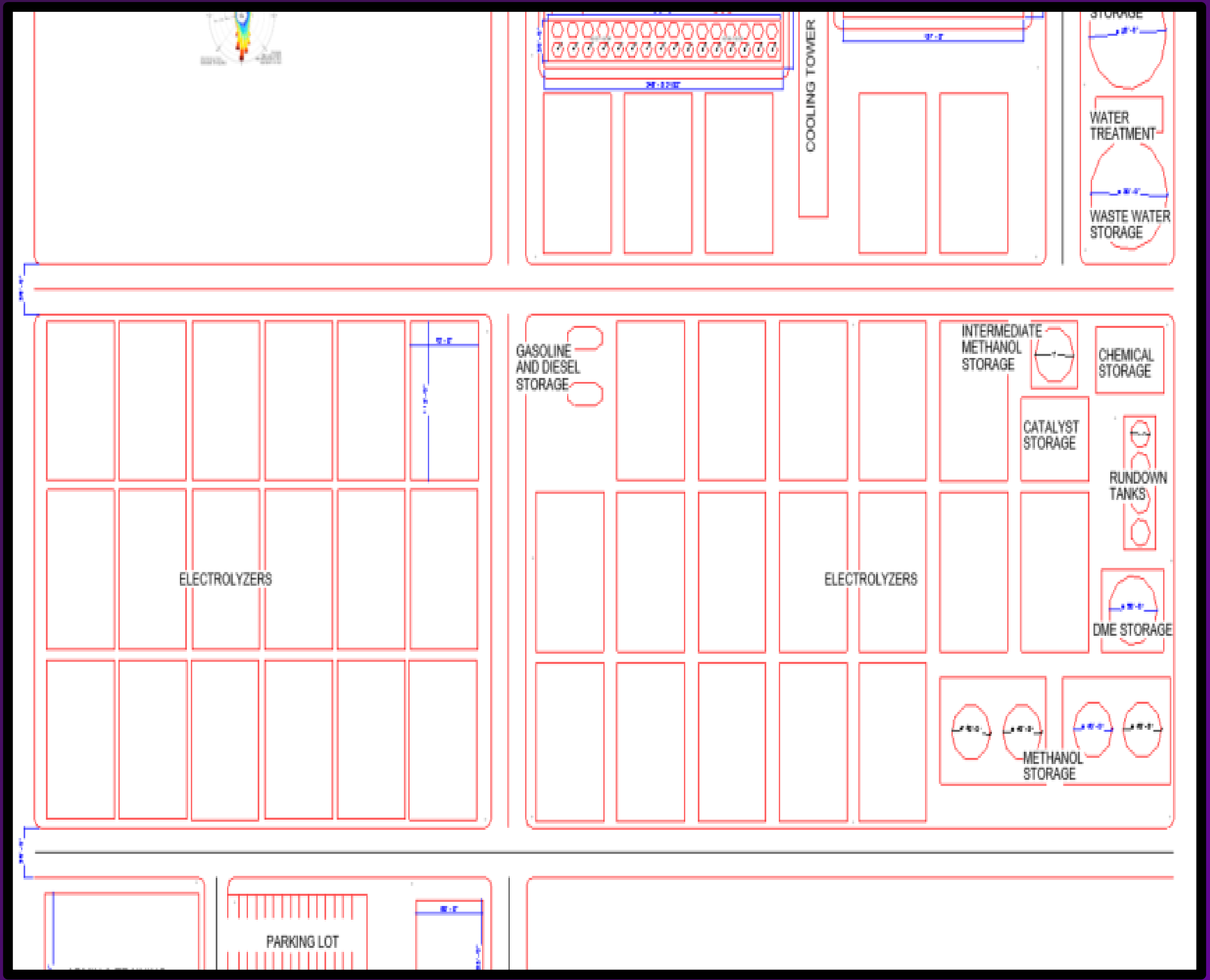
- Dr. Richard Turton’s *Analysis, Synthesis, and Design of Chemical Processes* and AXA XL Risk Consulting *Oil and Chemical Plant Layout and Spacing*
- Generalized pipe sizing was used

Dr. Richard Turton's Heuristics:

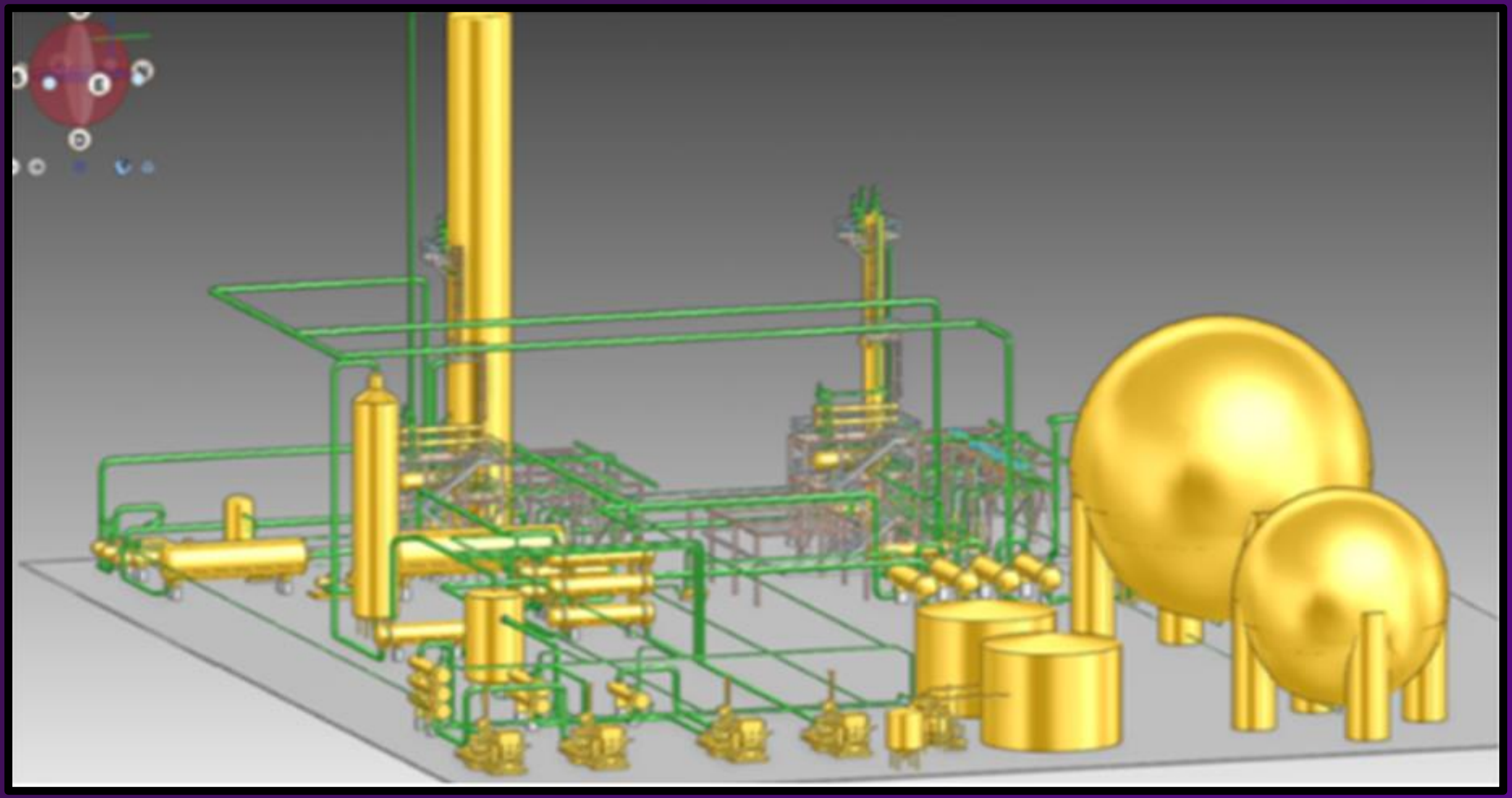
	Service B	Motor Control C Electrical Substati	Utilities Areas	Cooling Towers	Control Rooms	Compressor Buildings	Large Pump Houses	Process Units Moderate Hazard	Process Units Intermediate Hazard	Process Units High Hazard	Atmospheric Storage Tanks	Pressure Storage Tanks
Motor Control C Electrical Substati	/											
Utilities Areas	/	/										
Cooling Towers	50	50	/									
Control Rooms	50	50	100	50 (1)								
Compressor Buildings	/	/	100	100	/							
Large Pump Houses	100	100	100	100	100	30						
Process Units Moderate Hazard	100	100	100	100	100	30	30					
Process Units Intermediate Hazard	100	100	100	100	100	30	30	50				
Process Units High Hazard	200	100	100	100	200	50	50	100	100			
Atmospheric Storage Tanks	400	200	200	200	300	100	100	200	200	200		
Pressure Storage Tanks	250	250	250	250	250	250	250	250	300	350	*	
Refrigerated Storage Tanks Dome Roof	350	350	350	350	350	350	350	350	350	350	*	*

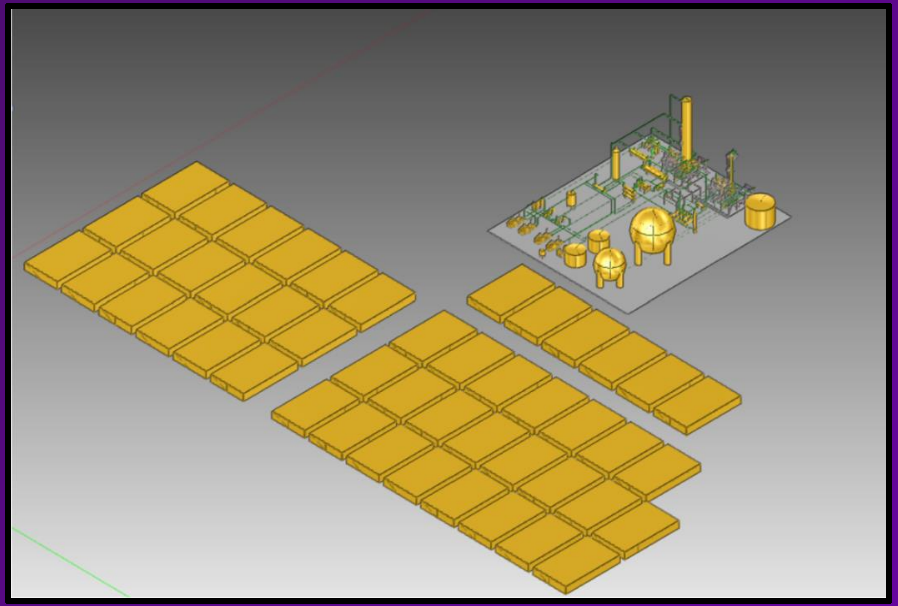


Plot Plan



COOLING TOWER
WATER TREATMENT
WASTE WATER STORAGE
GASOLINE AND DIESEL STORAGE
INTERMEDIATE METHANOL STORAGE
CHEMICAL STORAGE
CATALYST STORAGE
RUNDOWN TANKS
ELECTROLYZERS
ELECTROLYZERS
DME STORAGE
METHANOL STORAGE
PARKING LOT





Benefits

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- Weather conditions

Goal: Develop isometric model

Solution:

- Dr. Richard Turton's *Analysis, Synthesis, and Design of Chemical Processes* and AXA XL Risk Consulting *Oil and Chemical Plant Layout and Spacing* referenced
- Generalized pipe sizing used

Results/Future Work:

- E3D played a significant role early in the design phase
- Validated equipment was operating safely and efficiently by identifying potential safety issues
- Add pipe racks and air coolers

Benefits

AVEVA XR for virtual plant walkthrough to ensure validity of isometric model

Goals:

- Show the benefits of using virtual reality in plant design
- Import a fully designed plant and make the plant interactive

Challenges:

- Time
- No former experience

Results & Future Work:

- The plant was successfully imported from E3D Design
- Make the virtual plant fully interactive with applications of DynSim

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Alteragreen's Virtual Plant

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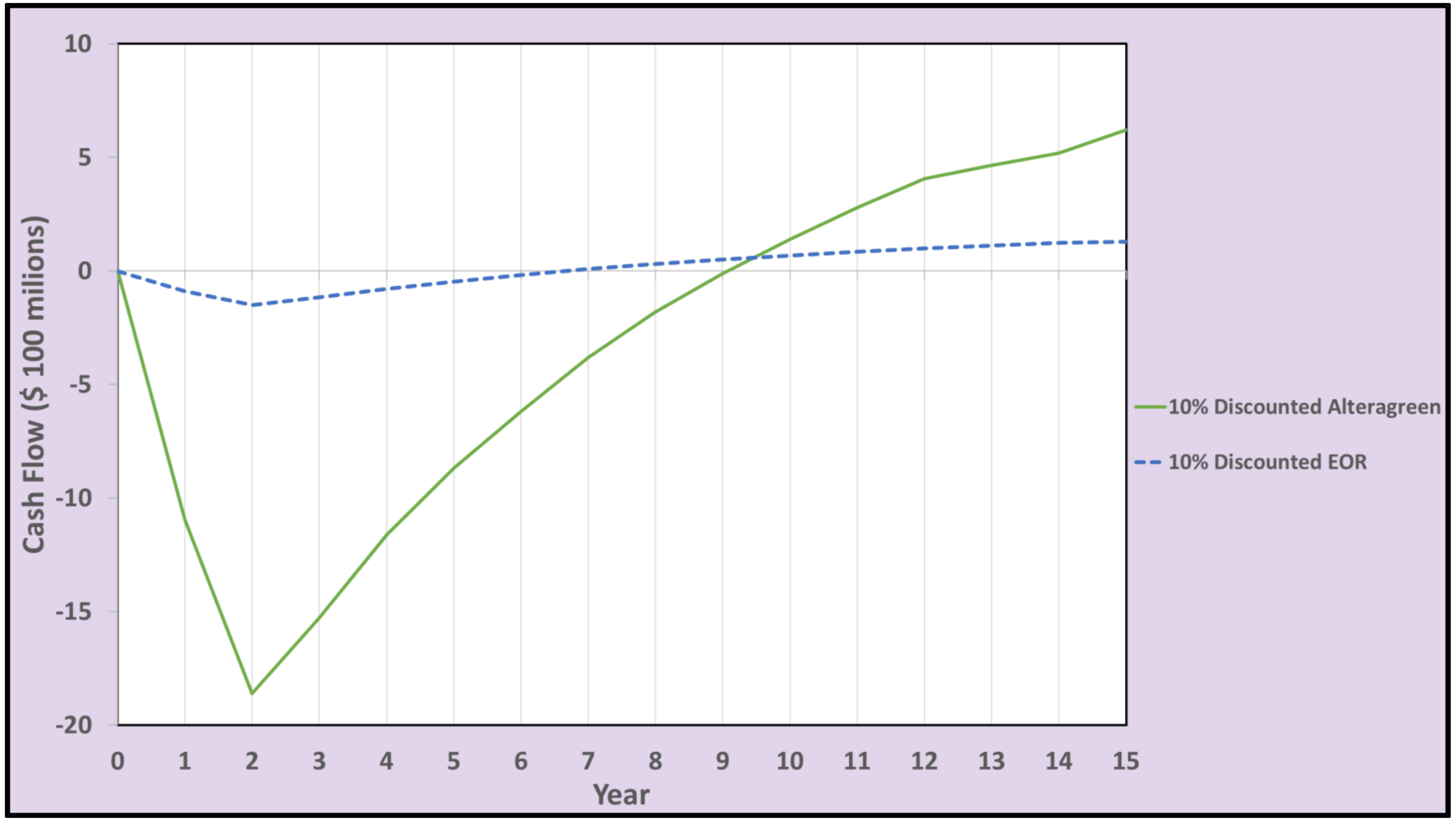
Conclusions

Designing a green plant using AVEVA software proved to be extremely effective for the task

- The plant was constructed in a steady state and dynamic mode, modelled isometrically, and costed
- Net present value was ~5x greater than the existing enhanced oil recovery system, resulting in a $500 million differential
- Proved the viability of synthetic fuel generation plants
- Profitability will grow in coming years with new subsidies



Alteragreen

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References

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Green Hydrogen
Ashley Nguyen, Brenda Ramos Escobar, Kyle Heineken, Timothy Lucey
Compression
Benjamin Schmitz, Brandon Choi
Methanol Simulation
Alexander Dussault, Hung Chui, Austin Morey, Van Trach Giang, Jack Webster
Dimethyl Ether Simulation
Dylan Valencia, Fernando Fuentes, Nicholas Shkolnikov, Bryan Alfaro, Ahmed Monir
Utilities
Renae Munson, Jesse Campuzano
Dynamic Simulation
An Nguyen, Hunter Ross, Sydney To
HAZOP
Benjamin Inguanzo
E3D
Brian Trinh, Tyrus Vo, Aidan Agredano
XR
Brian Do, Aidan Agredano

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!

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