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# AVEVA™ Process Simulation performance of Shell C3-MR LNG plant model

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# Introduction: Background

LNG & Cryogenics CoE (Centre of Expertise) is sponsoring a study to assess AVEVA Process Simulation(APS) as a future-proof simulation platform for the Shell Integrated Gas (IG) business needs:

- For process modelling and optimization needs; to support design, asset support, and technology development of the IG business.
- Capable of integration with Digital engineering workflows and within the Digital Twin ecosystem.

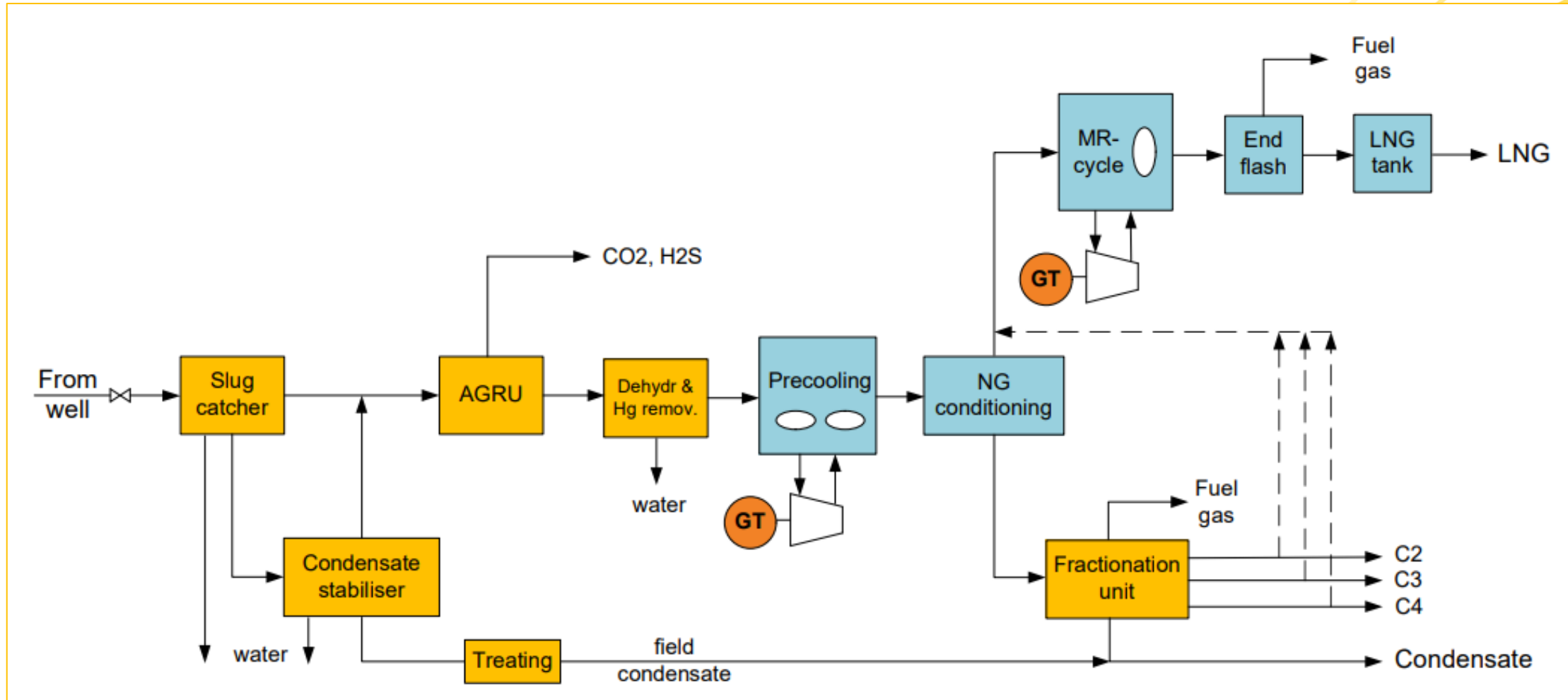
For this purpose, a detailed simulation model for a Shell C3-MR LNG plant was built in APS. The following capabilities were evaluated:

- Modelling of an Shell C3-MR LNG plant model and “closing” the precool and MR refrigerant loops
- Model Convergence, performance
- Sensitivity analysis: running scenarios with the model
- Design Optimization

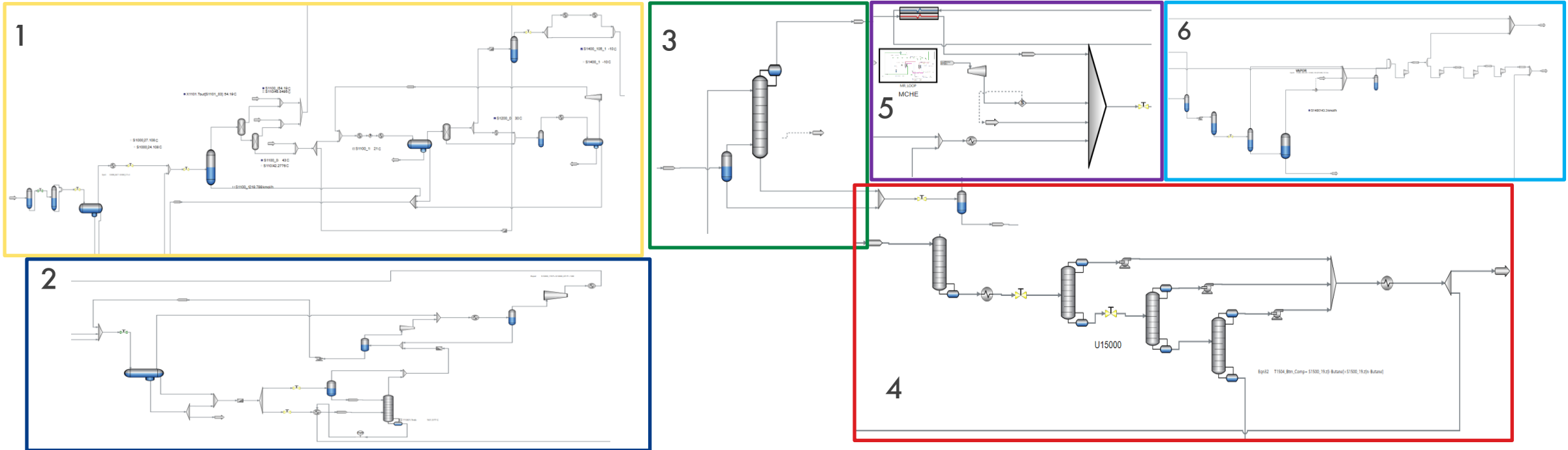
# Introduction: Why APS ?

- Next generation open-equation based platform that has the capability to combine steady-state, dynamics, and hydraulics into one simulator.
- Enables faster convergence of complex simulation models with multiple closed process loops/recycles, inherent in LNG process schemes.
- Potential to do design/operation optimization and what-if studies with features like PI Integration and real-time system (RTS).
- Integration with AVEVA Engineering for integrated digital workflows: design, simulation, training, and operations. Build an integrated digital twin for your entire plant lifecycle and use the same process model throughout every engineering phase.

# Shell C3-MR LNG Process Flow Scheme



# Simulation Process Scope



- 1: Feed gas receiving facilities
- 2: Stabilization Section
- 3: Scrub Column
- 4: Condensate Units

- 5: MR (Mixed Refrigerant) Loop
- 5: C3 (Propane) Loop
- 6: LNG/Fuel gas production unit



# Component Slate and Thermodynamics

## Thermodynamic Model Settings

- Phase behaviour, Entropy: SRK Equation of State (EOS)
- Liquid density: COSTALD
- Enthalpy: Lee-Kesler

## Pure Component Properties

- Component slate created using APS standard library based on legacy model.

## BIP: Binary Interaction Parameters

- Shell CPA (Cubic Plus Association) EOS BIP's in legacy model used as SRK BIPs in APS.

**Note:** CPA EOS reduces (no association term) to SRK EOS in absence of associating/polar molecules.

The screenshot shows the 'General' and 'Methods' tabs. In the 'General' tab, 'Fluid Type' is 'LNG', 'Library' is 'C3MR\_Reference\_Model\_17052023 - Heat Integrated', and 'Thermo Type' is 'Compositional'. In the 'Methods' tab, 'System' is 'Soave-Redlich-Kwong (SRK)', 'Binary Interaction Banks' is 'CPA\_Test:SRK\_CPA', 'Alpha Selection' is 'Default - Acentric Factor Formulation', and 'Phases' is 'Vapor/Liquid (VLE)'. Other settings include 'Apply high pressure VLE adjustments' set to 'Off', 'Vapor Enthalpy' set to 'Lee-Kesler', and 'Liquid Density' set to 'COSTALD'.

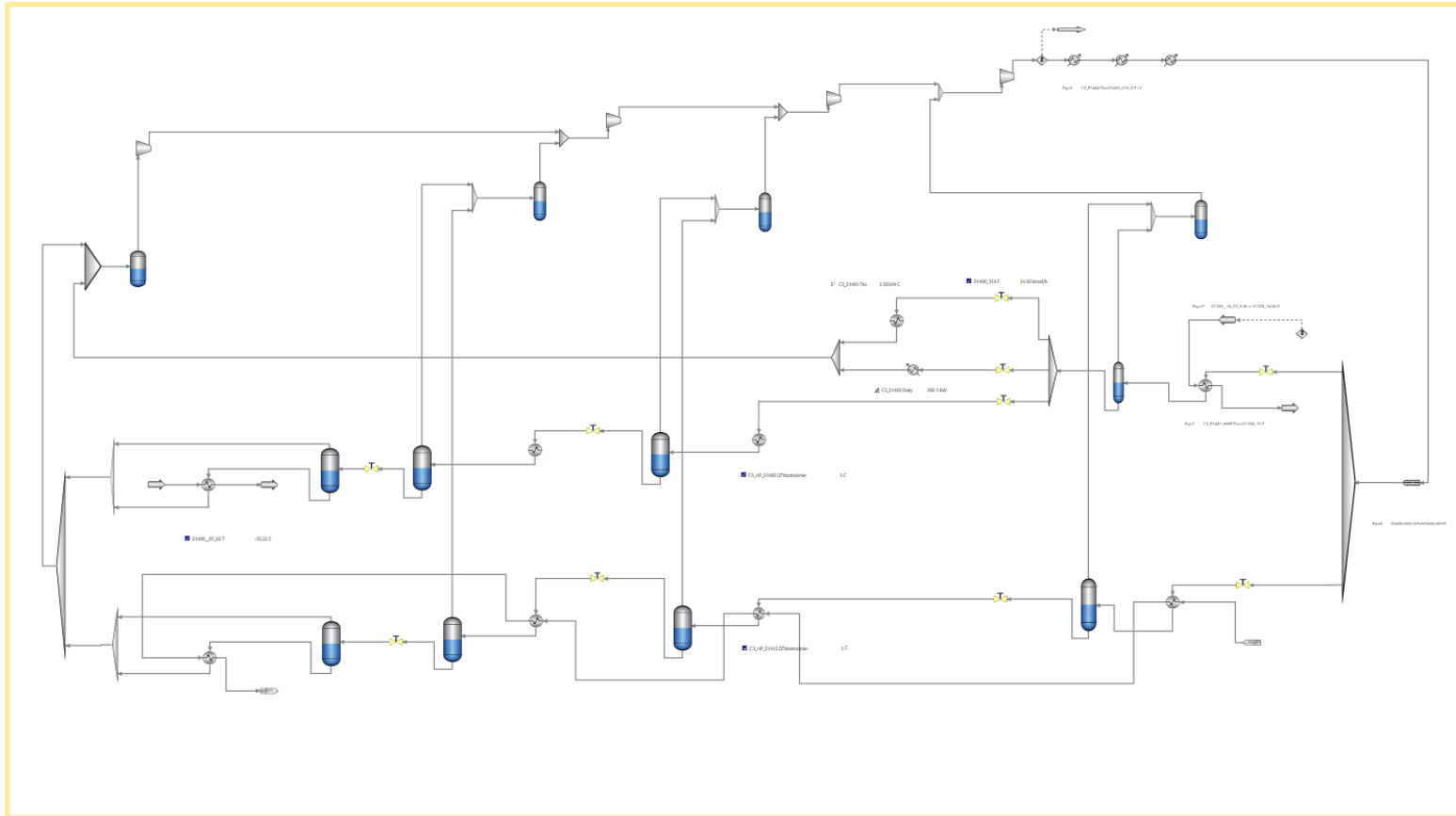
The screenshot shows the 'Component List' tab with a table of components. The table has columns for Name, Status, Type, Full Name, Bank, NBP (K), and SG60F. The components listed are:

Name	Status	Type	Full Name	Bank	NBP (K)	SG60F
H2O	<input checked="" type="checkbox"/>	●	Library Water	System:SIMSCI		
Nitrogen	<input checked="" type="checkbox"/>	●	Library Nitrogen	System:SIMSCI		
CO2	<input checked="" type="checkbox"/>	●	Library Carbon Dioxide	System:SIMSCI		
Methane	<input checked="" type="checkbox"/>	●	Library Methane	System:SIMSCI		
Ethane	<input checked="" type="checkbox"/>	●	Library Ethane	System:SIMSCI		
Propane	<input checked="" type="checkbox"/>	●	Library Propane	System:SIMSCI		
i-Butane	<input checked="" type="checkbox"/>	●	Library Isobutane	System:SIMSCI		
n-Butane	<input checked="" type="checkbox"/>	●	Library n-Butane	System:SIMSCI		
i-Pentane	<input checked="" type="checkbox"/>	●	Library Isopentane	System:SIMSCI		
n-Pentane	<input checked="" type="checkbox"/>	●	Library n-Pentane	System:SIMSCI		
C6_1	<input checked="" type="checkbox"/>	●	Library C6_1	CPA_Test:CPA_PURE		
Benzene	<input checked="" type="checkbox"/>	●	Library Benzene	System:SIMSCI		
Toluene	<input checked="" type="checkbox"/>	●	Library Toluene	System:SIMSCI		
E-Benzene	<input checked="" type="checkbox"/>	●	Library Ethylbenzene	System:SIMSCI		
m-Xylene	<input checked="" type="checkbox"/>	●	Library m-Xylene	System:SIMSCI		
O-Xylene	<input checked="" type="checkbox"/>	●	Library o-Xylene	System:SIMSCI		
124MBENZ	<input checked="" type="checkbox"/>	●	Library 1,2,4-Trimethylbenzene	System:SIMSCI		
C7_1	<input checked="" type="checkbox"/>	●	Library C7_1	CPA_Test:CPA_PURE		
C8_1	<input checked="" type="checkbox"/>	●	Library C8_1	CPA_Test:CPA_PURE		
C9_1	<input checked="" type="checkbox"/>	●	Library C9_1	CPA_Test:CPA_PURE		

Number of Components: 29

# C3 Loop: Propane Condensing Duty

- This model section simulates multi-stage compression, de-superheating and condensing of Propane, integrated with MR Loop and NG process side (through C3-MR and C3-NG kettles)

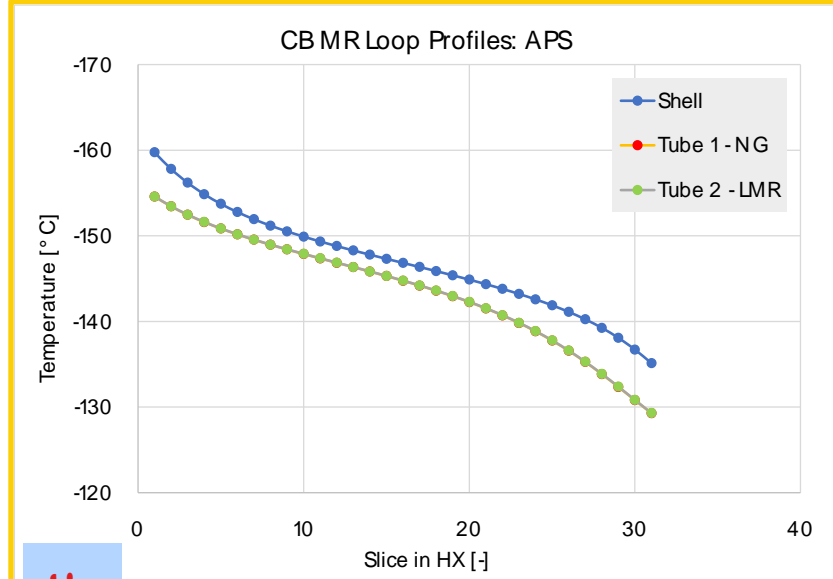
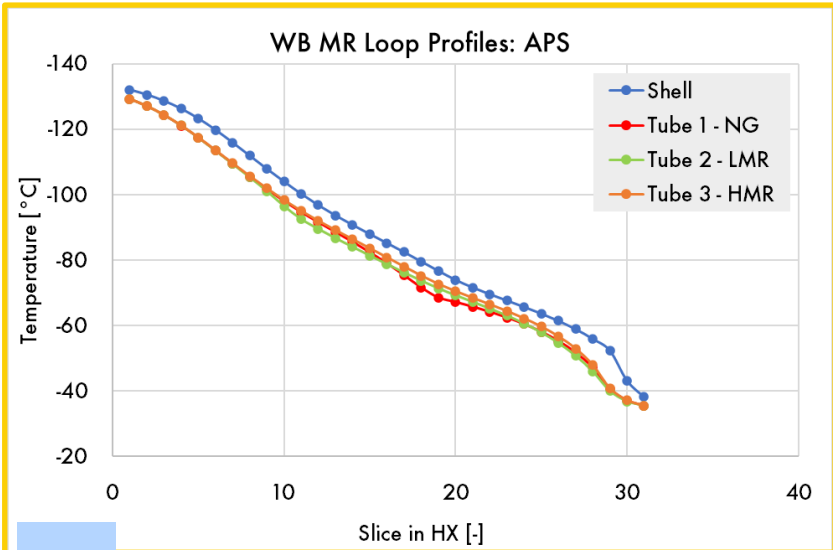


## APS vs Reference Model Deviations

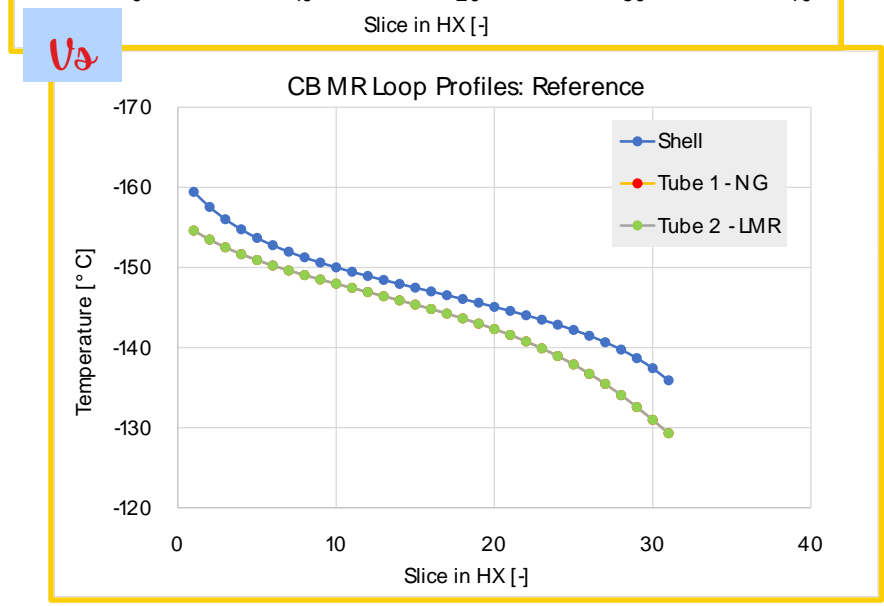
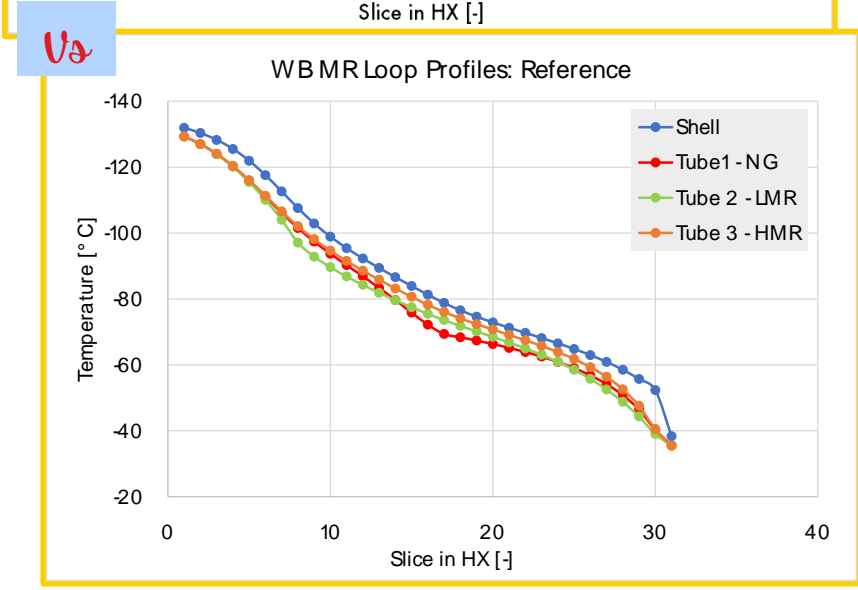
C3 Loop	% Rel. Dev. [APS-Reference]
<b>HHP compressor exit</b>	
Pressure, bar	-0.01%
Temperature, °C	0.02%
Flow rate, kg/h	-0.52%
<b>Desuperheater</b>	
Duty, MW	-0.99%
T <sub>in</sub> , °C	0.02%
T <sub>out</sub> , °C	0.05%
Pin, kPa	-0.01%
dP, kPa {Spec}	0.00%
<b>Condenser</b>	
Duty, MW	-0.66%
T <sub>in</sub> , °C	0.05%
T <sub>out</sub> , °C	0.06%
Pin, kPa	-0.01%
dP, kPa {Spec}	0.00%



# MR Loop MCHE Heating (Shell), Cooling (Tube) curves

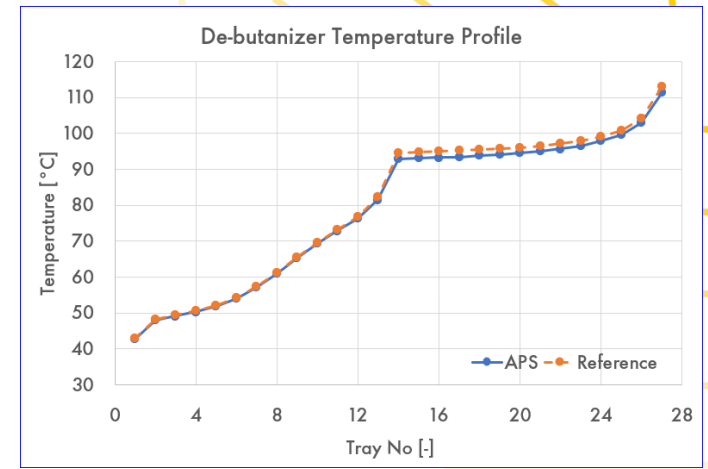
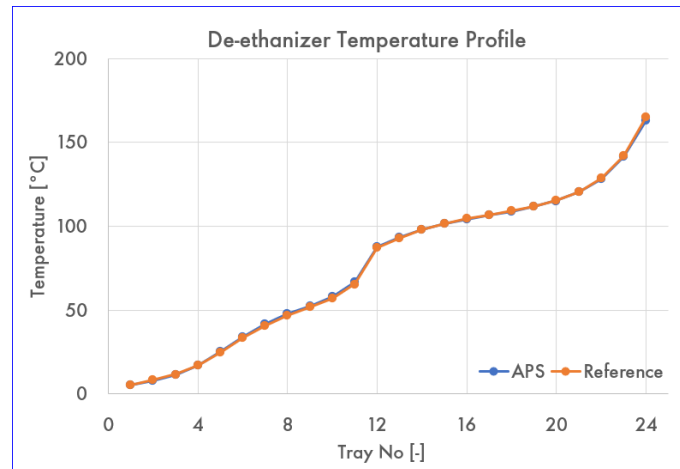
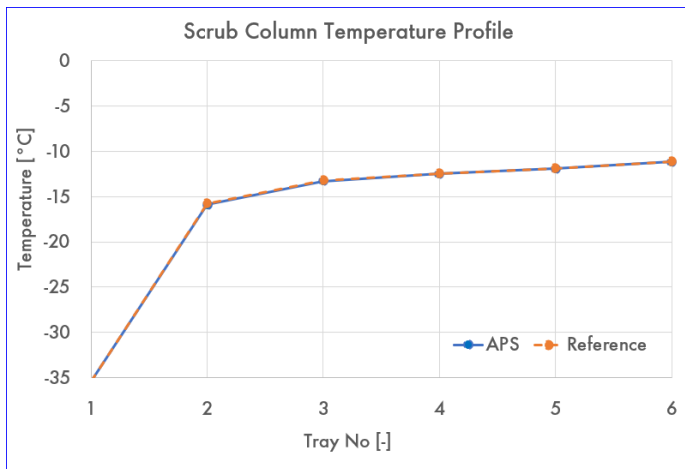
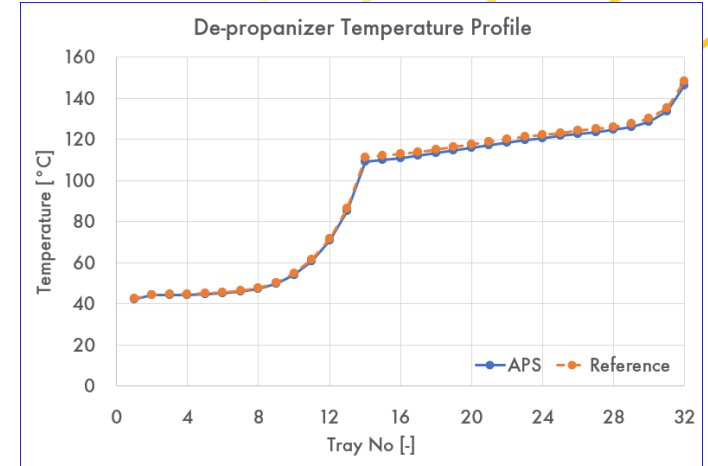
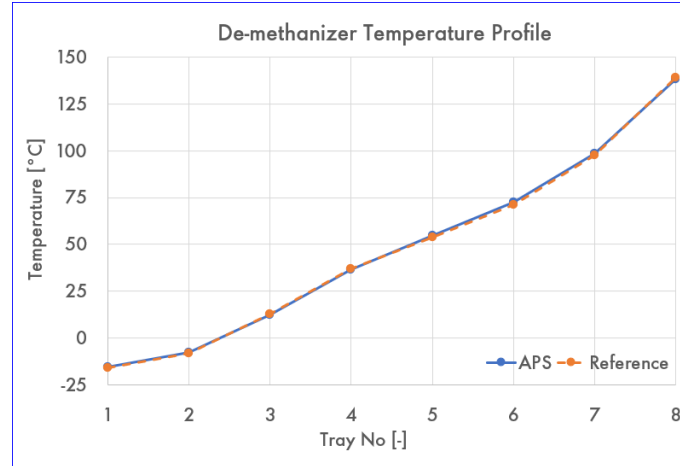
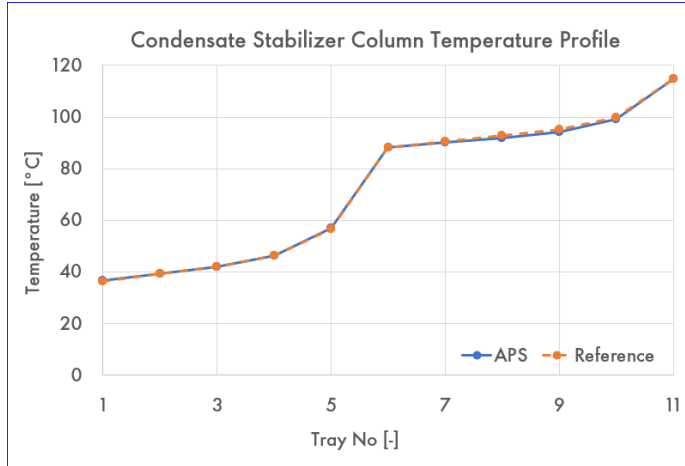


○ The heating / cooling curves of the warm bundle (WB) & cold bundle (CB) generated by APS match well with the reference model.



# Column Results: Overview of Temperature Profiles

- Profiles: Temperature [shown here], match well for APS against the reference model.
- Other profiles [not shown here] such as Pressure, Column loading, Condenser duty and Reboiler duty also match well.




# Column Results: Comparison (APS vs Reference) Overview

- Most relative deviations are low (< 2.5%).
- Higher deviations such as duty condenser can be attributed to different thermodynamic methods (Ref: CPA/LKP/SMIRK) and (APS: SRK-COSTALD) and platform flash.

Parameters	Relative Deviations{APS-REF} [%]				
	Scrub Column	Demethaniser	Deethaniser	Depropaniser	Debutaniser
	Rel Dev%	Dev%	Dev%	Dev%	Dev%
Feed Rate	2.3%	0.7%	1.1%	1.0%	1.3%
Duty Reboiler	N/A	3.1%	2.3%	1.3%	0.1%
Duty Condenser	0.8%	NA	5.4%	0.9%	1.1%
Reflux Rate	6.8%	NA	6.6%	1.0%	0.5%
Bottom Product Rate	0.0%	1.1%	1.0%	1.3%	2.3%
Top Product Rate	0.0%	4.2%	1.1%	1.4%	4.5%
<b>Top Product Composition</b>					
MW	0.0%	0.3%	0.1%	0.0%	0.0%
C1, mol%	0.0%	0.2%	1.3%	0.0%	0.0%
C2, mol%	0.0%	1.3%	0.2%	0.0%	0.7%
C3, mol%	0.1%	2.1%	0.0%	0.0%	2.3%
i-C4, mol%	0.5%	3.2%	2.5%	0.1%	1.3%
n-C4, mol%	0.5%	3.8%	3.6%	1.7%	0.8%
i-C5, mol%	3.3%	6.7%	2.1%	5.9%	0.2%
n-C5, mol%	6.6%	5.8%	0.4%	9.0%	3.2%
<b>Bottom Product Composition</b>					
MW	2.0%	1.2%	1.4%	1.4%	1.4%
C1, mol%	3.8%	1.0%	0.0%	0.0%	0.0%
C2, mol%	1.2%	1.4%	1.1%	3.5%	1.3%
C3, mol%	0.8%	1.2%	1.1%	0.0%	1.5%
i-C4, mol%	0.4%	2.3%	2.2%	2.4%	3.3%
n-C4, mol%	1.0%	4.0%	3.9%	4.1%	0.8%
i-C5, mol%	0.2%	4.1%	4.0%	4.2%	2.1%
n-C5, mol%	2.0%	3.2%	3.1%	3.2%	1.8%

# Sensitivity study

- For better understanding of model convergence and robustness of APS, selected input variables
  - NG Feed rate, temperature and Pressure
  - MR (Mixed Refrigerant) Compositionwere adjusted as given in Table 
- **Observation:** The APS model converged faster.

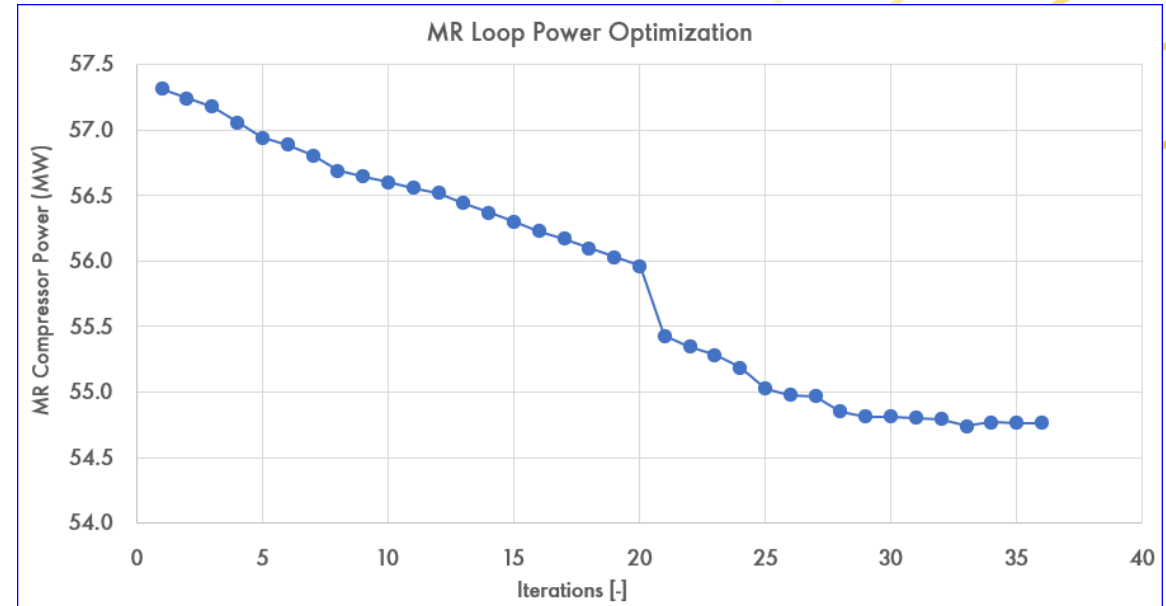
Adjusted Parameter	%Change	Convergence Time	
		Reference	APS
NG Feed Rate	0.1	~2 min	~3 s
	0.5	~4 min	~3 s
	1	~5 min	~5 s
	3	~15 min	~8 s
NG Feed Temp	0.1	~1.12 min	~4 s
	0.5	~2.32 min	~4 s
	1	~3.05 min	~4 s
	3	~7.0 min	~5 s
NG Feed Pressure	0.1	~36 s	~4 s
	0.5	~36 s	~4 s
	1	~50 s	~4 s
	3	~50 s	~4 s
MR Composition	C1 +/-2	~30 s	~20 s
	C2 +/-1	~20 s	~10 s
	N2 +/-1	~10 s	~4 s

# MR (Mixed Refrigerant) Loop Optimization

- Aim of the study is to assess APS capability for process optimization.
- Objective Function: Minimize total compressor power with MR loop composition as optimization handles.

## Results

- APS optimizer optimized the MR loop composition to minimize the compressor power.
- Optimizer achieved the solution in 37 iterations within 2 minutes.
- Optimum composition (Delta shown here) resulted in 4.6% reduction in power as compared to reference case, as shown in Table



Optimizing Variable	Unit	Optimization Setting	Low Bound	High Bound	Delta {APS-Ref}
MR Composition:Nitrogen	Mol Frac	Dependent	0	0.1	0.01
MR Composition:Methane	Mol Frac	Independent	0	0.5	-0.01
MR Composition:Ethane	Mol Frac	Independent	0	0.5	-0.04
MR Composition:Propane	Mol Frac	Independent	0	0.2	0.03
MR flow	kmol/h	Dependent			-1626.22
LMR/HMR Ratio	Frac	Dependent			0.03
Compressor Power	MW	Objective Function	52	58	-2.6



# Conclusions & Future Work

- APS evaluation of the Shell C3/MR LNG model was positive in terms of performance and functionality.
- Next phase assessment: integration of Shell thermodynamic methods in APS and carry out similar studies.
  - Separate Shell-AVEVA R&D project to integrate Shell Thermodynamic package (SPPTS) with APS, commenced in September 2023.
  - Outcome of study would be further reviewed by LNG & Cryogenics CoE TA-2, TA-1 (technical authorities) for steer.

## Other APS Features

- Capability to **integrate with PI Server** and provide PI Data filtering, as well as read and write access to PI system.
- Real time sequence (RTS) console capabilities for Real Time Optimization (RTO), offline and online studies.
- Convert design to rating model: match model to plant data.
- Currently limited number of Shell users have hands-on experience in APS or even EO modelling.
  - A face to face APS course arranged in Shell WoodCreek Center, Houston to increase interest, familiarity with features of new release: v2023.2.
- This study lays foundation for APS as future platform for LNG dynamic model-Digital Twin integration applications. [Separate Shell-AVEVA PoT (Proof of Technology) commenced in September 2023 to integrate DYNMIM Model with Digital Twin environment for what-if scenarios, troubleshooting, shadow plant modelling for wider user base]
- **Potential Future Use Case: Trigger APS with API using LLM models (GPT-3) driven process model benchmarking, design, optimization studies.**

# Q&A



