ENHANCING RELIABILITY WITH DEEP KINETIC MODELS FOR SULPHUR RECOVERY UNITS

ANAND GOVINDARAJAN

THREE TEN INITIATIVE TECHNOLOGIES LLP (310i)

anandg@the310i.com

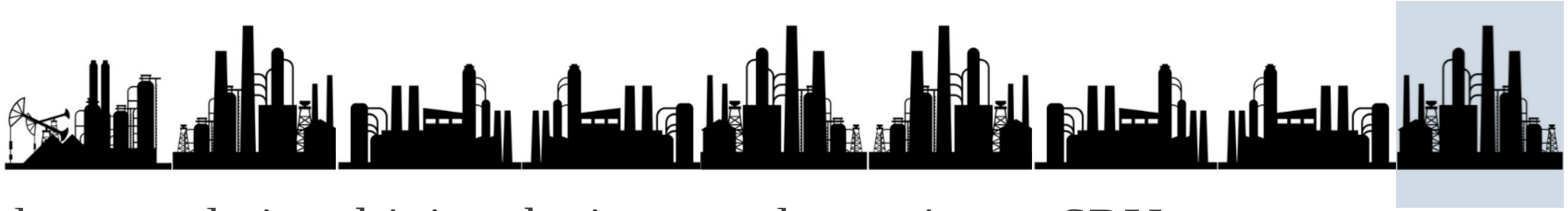
COAUTHORS: **HARI VAMSI DUGGIRALA (310i)**
PRASHANTH CHANDRAN (OPTIMIZED GAS TREATING)

PRESENTATION OUTLINE

- SRU Simulation – Significance –Background
- Simplified SRU Process Flow
- Kinetics-based INTELLIGENT simulation – DEEP and VISIBLE
- Use case-1 Catalyst degradation in Claus reactor of an SRU
- Use case-2 Evaluating the feasibility of using oxygen enrichment in the existing WHB
- Summary

SRU SIMULATION – SIGNIFICANCE

- Back end of plant, traditionally received less attention compared to other parts of the plant



- More sour crudes/tighter regulation driving the increased attention to SRUs
- Models available have largely ranged from being regression-empirical-semi-empirical

No historic data in a range or operating condition

Poor Models

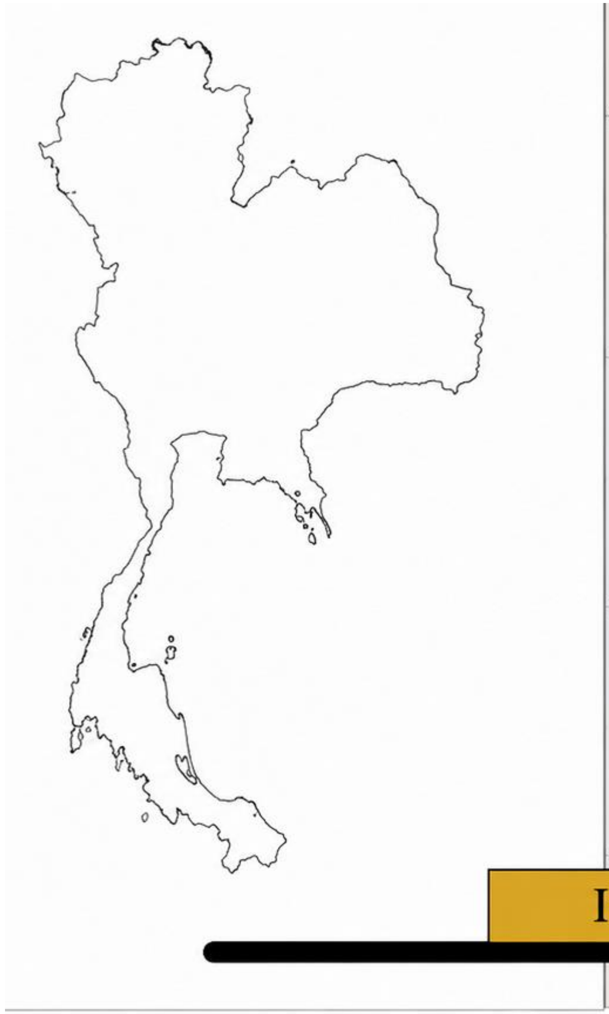
Fundamental first-principles, thermodynamics & rigorous chemistry

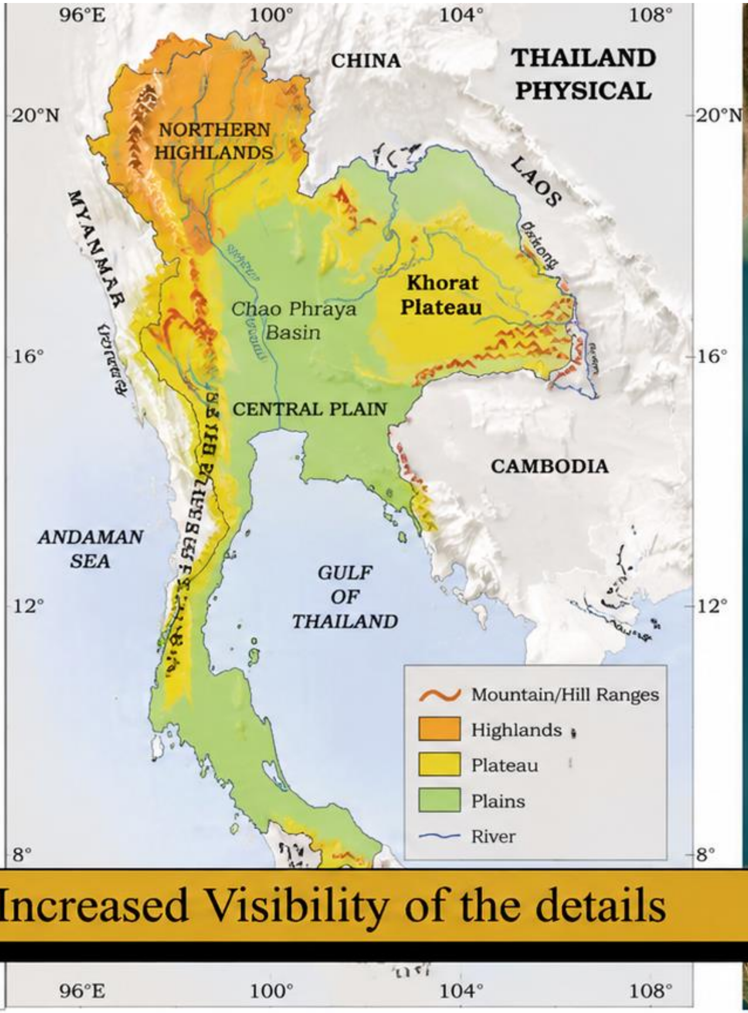
Intelligent & Predictive Models

OGT | SulphurPro®

- From the simulation suite of the industry’s most rigorous mass-transfer rate based - **ProTreat®**

DETAILS MATTER …





Increased Visibility of the details

DETAILS MATTER –IN A 500-MILLION-DOLLAR PLANT

Gibbs Energy Model

- **Gibbs Free Energy Minimization Modelling**
  - Broad View of a physical SRU - Equilibrium

Empirical Fit Model

- **Empirical Fit Models**
  - Designed for local ranges and need different models for different conditions

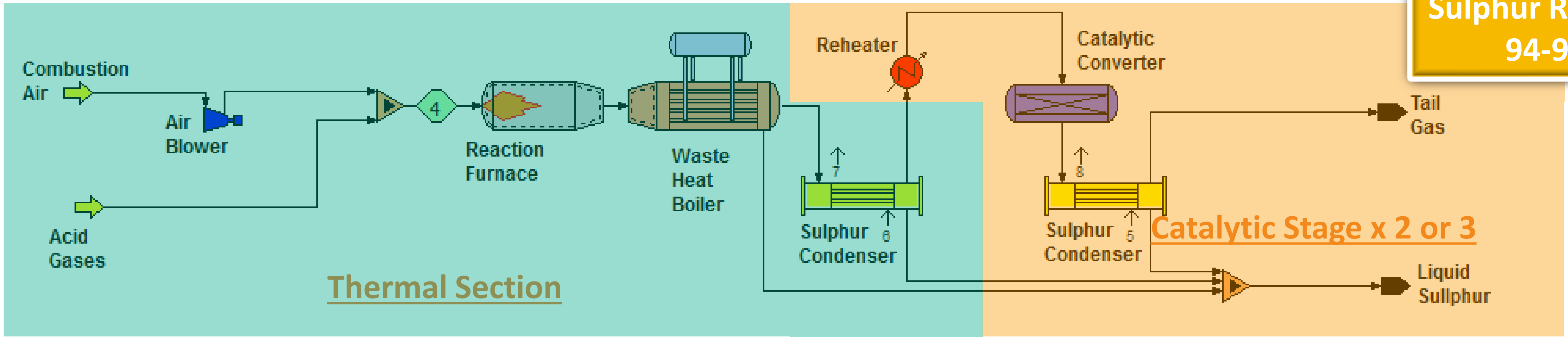
Kinetics-Based Model

- **Kinetic Model**
  - Close to the truth – Incorporates thermodynamics, reaction kinetics, hardware dimensions, mixing limitations, and all fundamental physical properties

- **All models are approximations of physical reality**
- **SOME ARE CLOSER TO THE TRUTH**

SIMPLIFIED SRU PROCESS FLOW

Standard Claus Sulphur Recovery 94-97%



Reaction Furnace – Combustion and thermal reactions

WHB – Recovery of reaction heat

Condenser - S vapour condensed and drained

Reheater – Improve Claus kinetics

Catalytic Converters - $2H_2S + SO_2$ -> 3S + H2O

Condensers - S vapour condensed and drained

INTRODUCTION TO KINETICS-BASED INTELLIGENT SIMULATION

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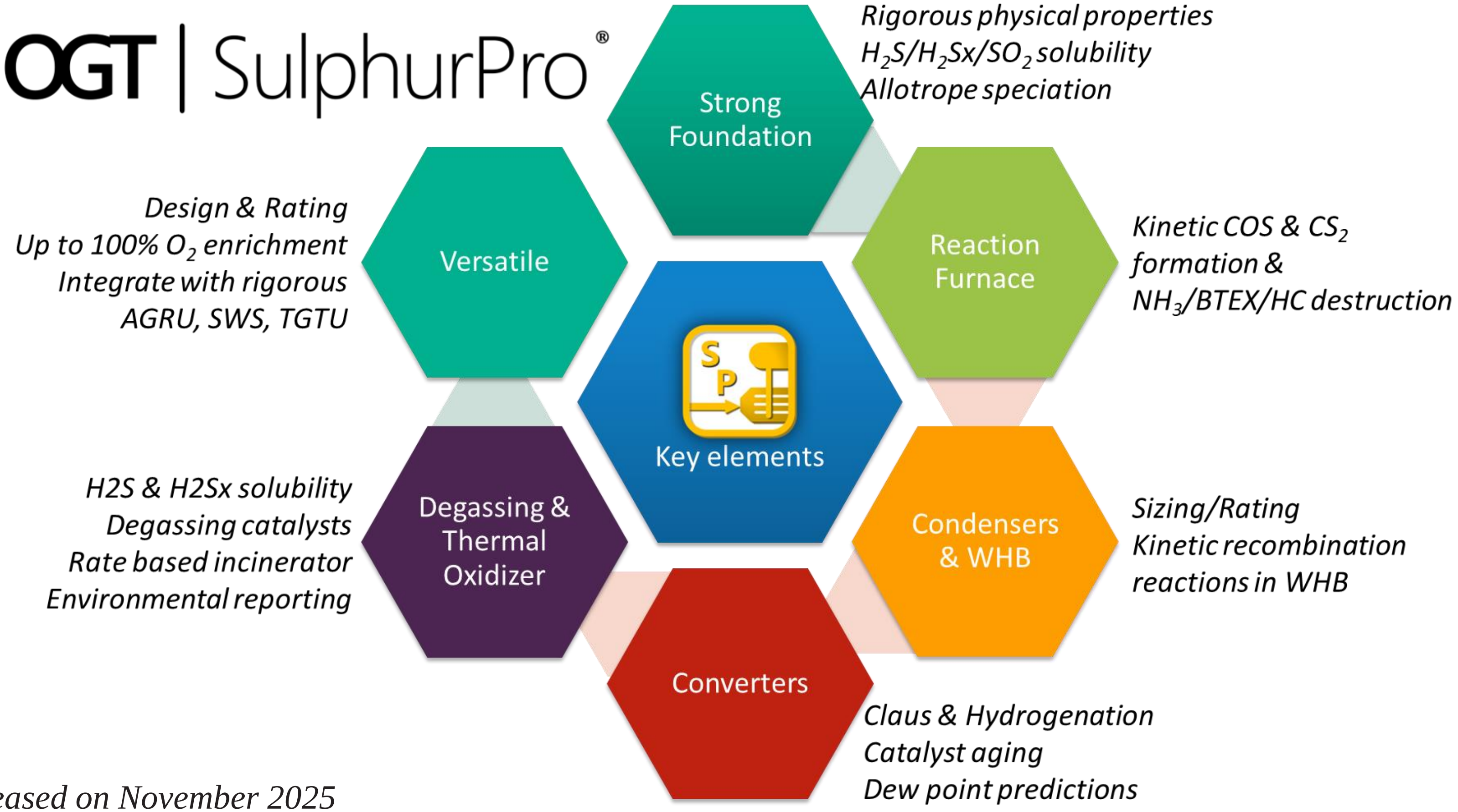
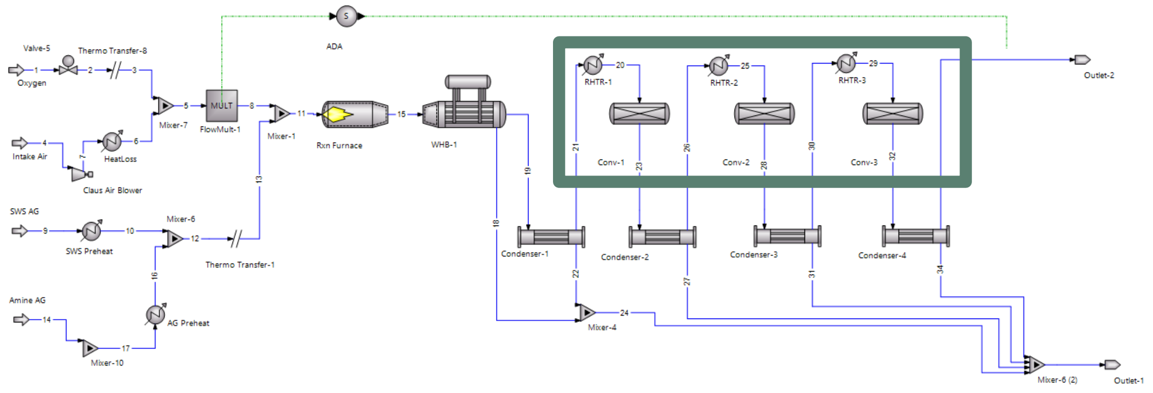


ProTreat 9.0 is out now, Released on November 2025

USE CASE-1 CATALYST DEGRADATION IN CLAUS REACTOR OF AN SRU

- Simple three bed SRU configuration in SulphurPro
- ADA maintains 2:1 H_2S:SO_2 in tail gas
- Alumina catalyst
- Study exotherms of each Claus reactor by changing the activity of first Claus bed
- Common issues encountered with catalyst degradation
  - Reduced activity of the catalyst
  - Reduced sulphur recovery efficiency
  - Higher emissions of undesired products
  - Increased maintenance/Operating cost



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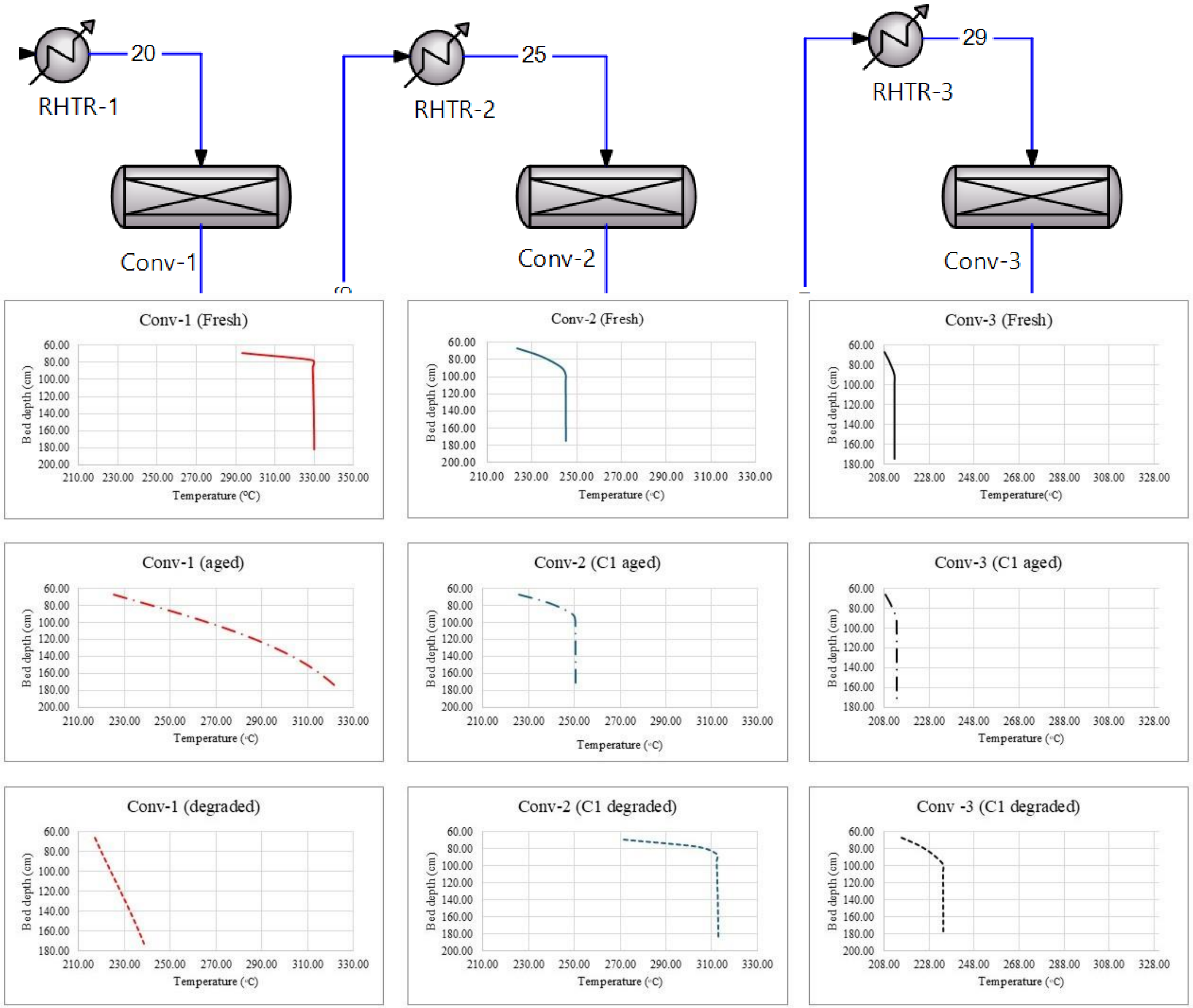
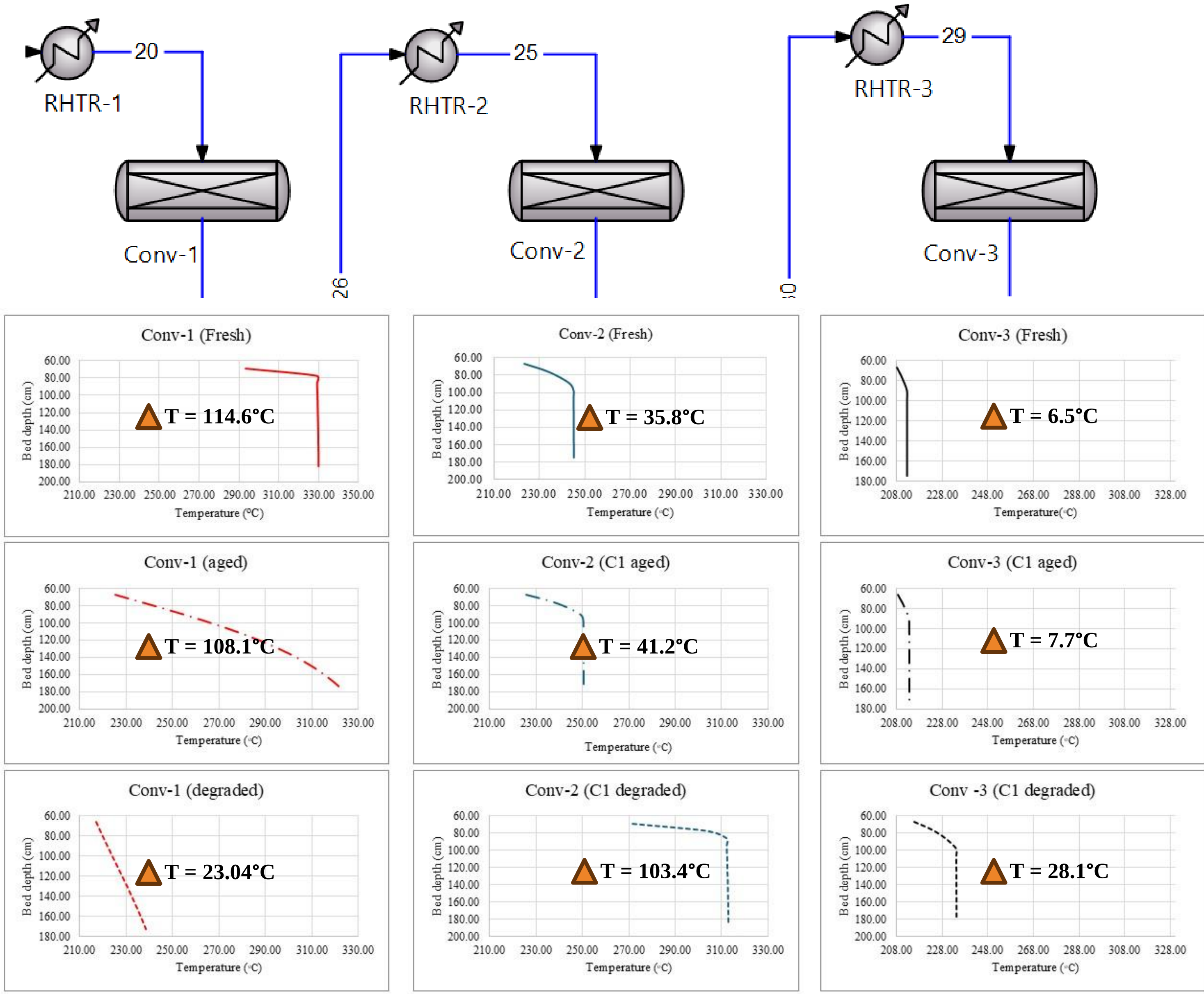
USE CASE-1 RESULTS

- Three Bed Claus – 1st bed activity is altered to study the effect on bed 2 and bed 3
- In the fresh catalyst case, we can see that there is a sharp rise in temperature at a short bed depth – as anticipated
- In the aged catalyst case, the 1st bed goes through a similar change in temperature but uses the entire bed
- In the degraded catalyst case, the 1st bed barely achieves a 41°C rise in temperature
- Altering the activity of catalyst in 1st reactor significantly affects the performance of 2nd and 3rd reactors



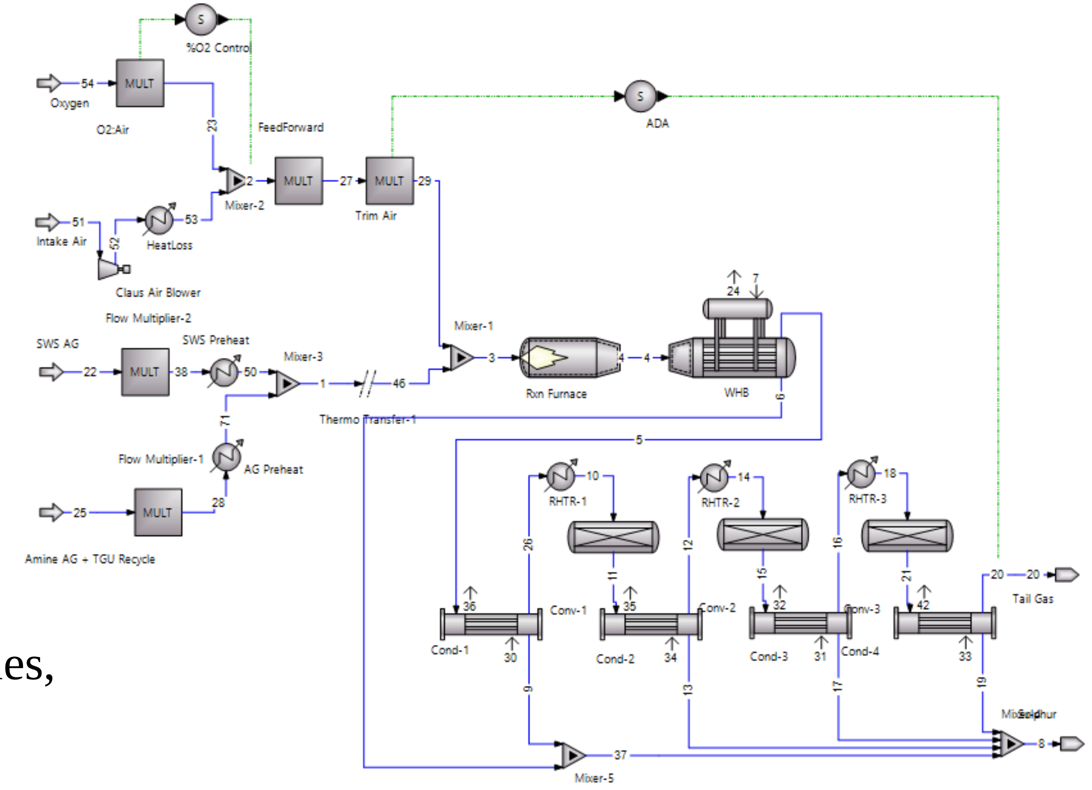
USE CASE-1 RESULTS

- The temperature rise for each bed for all the three cases have been represented in the graphs to the right side
- When the catalyst in the 1st bed is aged or degraded, the temperature rise in the second and third beds are higher.
- TAKE AWAYS
    - Simulation aids in predictive maintenance, identifying when a catalyst bed may require rejuvenation.
    - Routine physical examination of catalysts is impractical; simulation makes performance monitoring through exotherms possible - help predict catalyst degradation and guide proactive operational adjustments.



USE CASE-2 EVALUATING FEASIBILITY OF USING O2 ENRICHMENT IN EXISTING WASTE HEAT BOILER

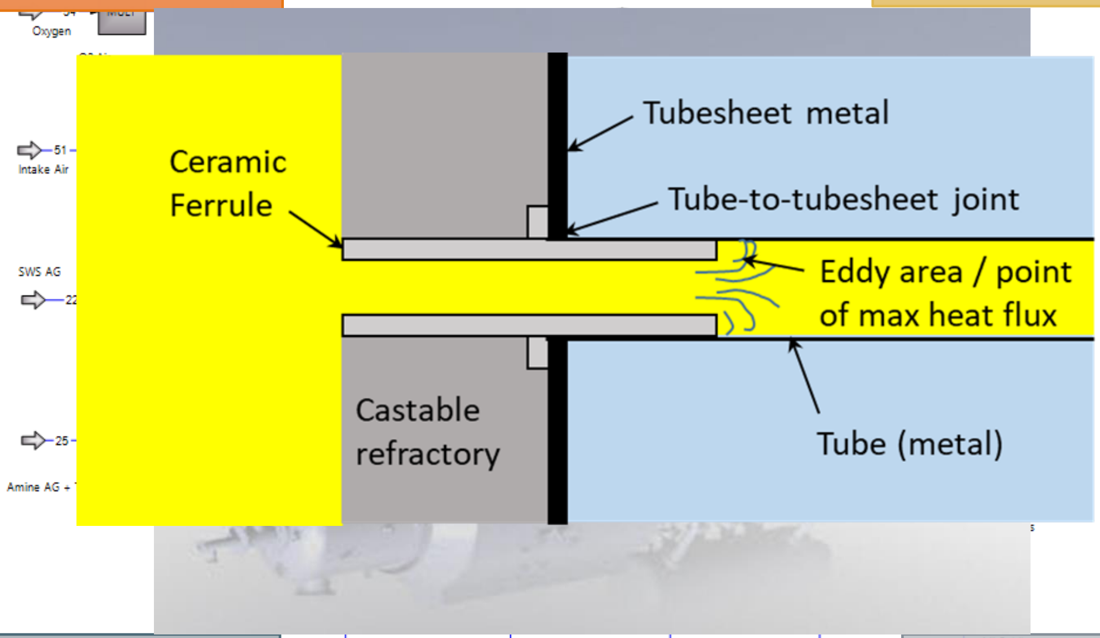
- Simple three bed SRU configuration in SulphurPro
- Base case no O_2 enrichment
- Investigated the possibility of pushing higher capacity (30% increase in feed rate) with and without oxygen enrichment
- Common issues encountered with waste heat boiler (WHB)
    - Design limitations, Fluid dynamics, Temperature profiles, Operational flexibility



USE CASE – 2

Part of the thermal section

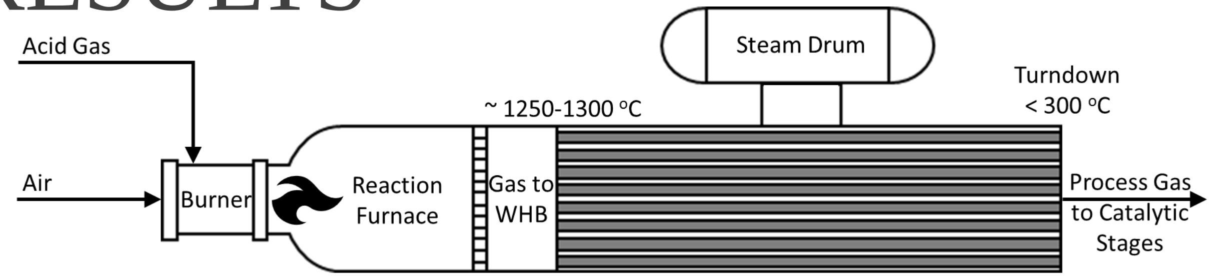
Combined assembly with RF



Specialized heat exchanger

Operates in harsh conditions

USE CASE-2 RESULTS

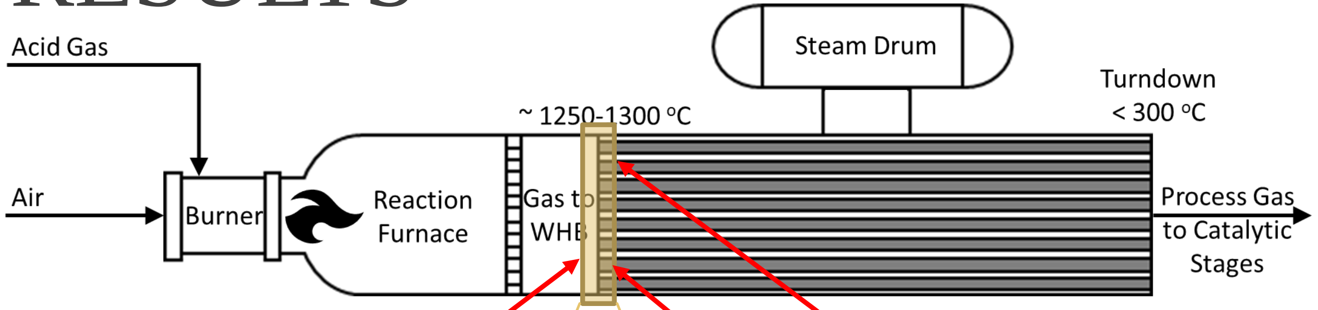


SRU current capacity – 130 MTD

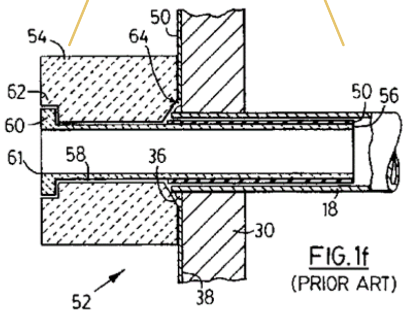
- Sulphur Recovery >97% in all cases – at the end of 3rd converter
- General guideline values for key parameters
  - Heat flux < 156 kW/m^2
  - Mass flux < 24 kg/m^2.s
  - Peak wall temperature < 343°C
  - Corrosion < 10 mpy

Parameter	Air Operation
Furnace Temperature (°C)	1292.9
Enriched air flow (kmol/hr)	335.9
H_2S in/out (mol%)	4.43 / 7.04
Temperature in/out (°C)	1293 / 303
Inlet Mass Velocity (kg/m^2.s)	22.01
Max Tube Wall Temp (°C)	322
Max Heat Flux (kW/m^2)	119
Corrosion rate in/out (mpy)	5 / 0.577

USE CASE-2 RESULTS



- Higher Capacity (No O_2 Enrichment)
  - Furnace Temperature – 1289.9°C
  - Heat flux - 136 kW/m^2
  - Mass flux – **28.4 kg/m^2.s**
  - Peak wall temperature - 336°C
  - Corrosion in/out – 5/0.577 mpy



- 30% O2 Enrichment
  - Furnace Temperature – **1464.2°C**
  - Heat flux - **174 kW/m^2**
  - Mass flux – 23.11 kg/m^2.s
  - Peak wall temperature - **344°C**
  - Corrosion in/out – 7.69/0.693 mpy

- Sulphur Recovery >97% in all cases – at the end of 3rd converter
- H_2 concentration >2 mol% (all cases) – low SO_2 breakthrough suspicion, COS concentration in the tail gas – as expected

USE CASE-2 RESULTS

- Base case - no violation of key design factors
- Higher capacity - inlet mass velocity ⚠
- O2 enrich. - max tube wall T & max heat flux. ⚠
- So, the current configuration cannot withstand desired higher capacity with or without enrichment and must undergo a revamp (or process higher capacity only till material consideration allows – verifiable by simulation)

Parameter	Air Operation	Higher Capacity (No O_2 Enrichment)	30% O_2 Enrichment
Sulphur Recovery %	97.38	97.28	97.54
Furnace Temperature (°C)	1292.9	1289.9	1464.2
H_2 in tail gas (mol%)	2.29	2.50	2.85
COS in tail gas (ppmv)	315	366	489
WHB Specific			
Enriched air flow (kmol/hr)	335.9	433.68	301.3
H_2S in/out (mol%)	4.43 / 7.04	4.51 / 6.94	4.13 / 10.02
Temperature in/out (°C)	1293 / 303	1290 / 330	1464 / 329
Inlet Mass Velocity (kg/m^2.s)	22.01	28.49	23.11
Max Tube Wall Temp (°C)	322	336	344
Max Heat Flux (kW/m^2)	119	136	174
Corrosion rate in/out (mpy)	5 / 0.577	6.67 / 0.632	7.69 / 0.693

- TAKEAWAYS
  - SRU WHBs often fail mechanically at the front end due to improper operations and lack of reliable temperature measurements in the reaction furnace (RF). SulphurPro provides the ability to accurately assess critical parameters in the RF-WHB assembly including a detailed temperature profile of the WHB.
  - Provides critical insights into the weakest part of the SRU, allowing plant users to make operating decisions in an informed manner.

KEY VIRTUES OF SRU SIMULATION – WATCHLIST

Physical Properties

- Vapor distribution
- Liquid viscosity
- Liquid heat capacity
- Solubility of SO_2, H_2S & H_2S_x
- H_2S effect on viscosity

Reaction Furnace

- NH_3 destruction
- BTX destruction
- CS_2 formation
- Time
- Temperature
- Turbulence

Waste Heat Boiler/Condenser

- Sizing/Rating
- Kinetic exothermic COS formation
- Kinetic exothermic H_2 recombination
- Rigorous heat transfer
- Heat flux
- Radiative heat transfer
- Sulfidation corrosion

Converter

- Accurate COS, CS_2 hydrolysis
- Sulphur dew point profiles
- SOR, Aged, EOR profiles
- Temperature profiles
- Reheater options

Integration

- AGR, AGE, SWS
- Quench & TGTU
- Incinerator stack SO_2 scrubbing
- Thermal Oxidizer
- Sulphur Degassing
- Hydrogenation Reactor

SulphurPro® checks all the boxes, emphatically, providing best-in-class simulation.

SUMMARY

- Chemistry and thermodynamics of SRU processes are complex
- Capturing key elements is necessary
- Using models that rely on past experimental or plant data may not work sometimes
  - Depend on user inputs heavily to determine the right model to use in all the key equipment
- More model options – more confusion for the designer/operations engineer
  - Akin to having a GPS but asking which road to take instead of letting the GPS find the correct path to shortest travel time
- SulphurPro® - a simulator built by process engineers, for process engineers

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- JGC CORPORATION
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- TechnipFMC
- SNC • LAVALIN
- suez
- gti
- NESTE
- MiRO
- SOS Sulfur Operations Support
- Garo by Gardner Denver
- KPI Kinetics Process Improvements, Inc.
- FRAMES
- NexoSolutions
- W AMINE GLOBAL SERVICE WORLD IMAGE

Thank You!

Enhancing Reliability with Deep Kinetic Models for Sulphur Recovery Units

HARI VAMSI DUGGIRALA—THREE TEN INITIATIVE TECHNOLOGIES LLP, INDIA
HARID@THE310I.COM

ANAND GOVINDARAJAN – THREE TEN INITIATIVE TECHNOLOGIES LLP, INDIA
ANANDG@THE310I.COM

PRASHANTH CHANDRAN– OPTIMIZED GAS TREATING INC.,USA
PRASHANTH.CHANDRAN@OGTRT.COM