# INTEGRATION OF COAL-FIRED POWER PLANT FIRESIDE OPTIMIZATION TOOLS WITH THE IDAES PLATFORM

*(Award No. DE-SC0020803)*

## DOE NETL'S 2021 SIMULATION BASED ENGINEERING MEETING

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# Agenda

- Introductions
- Project Goal and Objectives
- Accomplishments
  - Plant Performance Database Development and Review
  - Ash Generator Modifications
  - Ash Vaporization/Condensation (FactSage) Modeling
  - Deposit Properties (Sintering) Model Development
  - Deposit Thermal Properties Predictions
  - Modified Heat Transfer Coefficients in IDAES
  - Steam Outlet Temperature Predictions in IDAES
- Next Steps
- Questions

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# Opportunity

- The IDAES platform BoilerHeatExchanger model offers the opportunity to utilize mechanistic ash prediction tools and experimental information to predict resistance to heat transfer for boiler heat exchangers in sub-critical and super critical power plants.
- The model provides the ability to couple fireside and water/steam side boiler models for water walls, primary superheater, secondary superheater, finishing superheater, reheaters and economizers.
- The IDAES computational framework also provides the ability to develop simplified models that can be run in 1-2 minutes. Developing IDAES simplified models that can be used in conjunction with the CSPI-CT framework would significantly enhance the ability to predict the impact of changing plant operating conditions on plant performances.

# Project Goal

The main goal of the project is the development of a computer-based tool (model) for use by coal-fired power plants to predict heat transfer losses in the water wall and convective pass sections of the boiler.

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# Phase I Technical Objectives

- IDAES-AGM Prototype – Technology proof-of-concept to predict plant heat rate
  - Incorporate Coyote Station's design and operating parameters into the BoilerHeatExchanger model
  - Identify operational databases for testing
  - Use data from the AGM model in the BoilerHeatExchanger model to predict heat rate/plant performance.
    - heat transfer resistance for the water walls and convective pass heat exchange surfaces as a function of changing operating conditions and coal properties
  - Compare predicted heat rate to actual measured heat rates.

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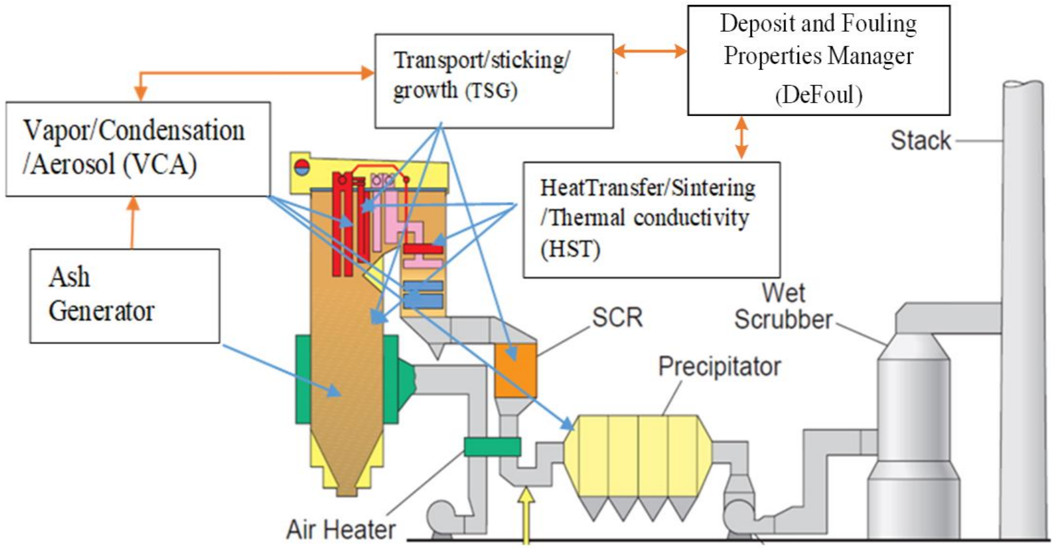
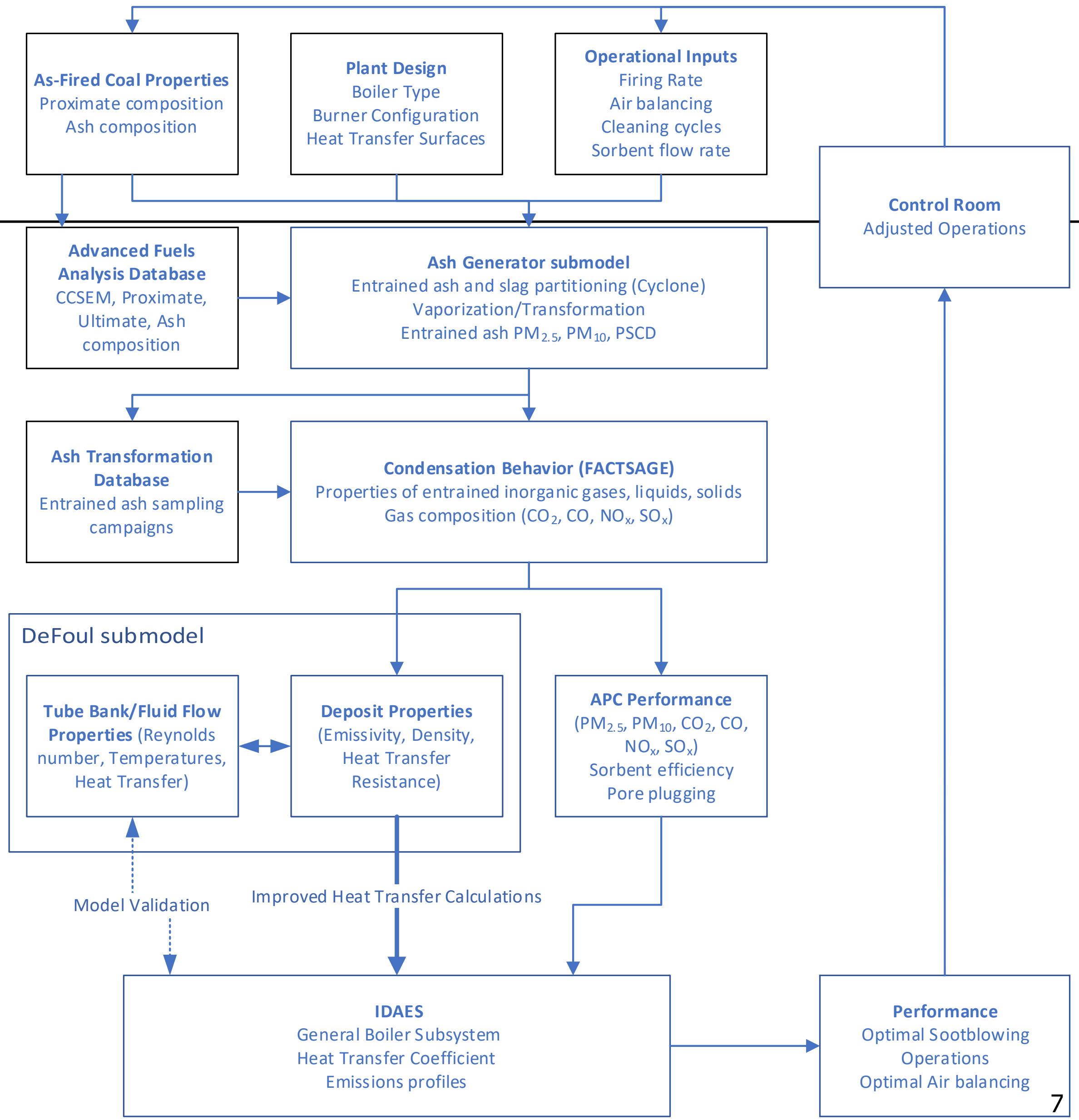
# Phase II – Technical Objectives




- Further integrate –
  - Ash generation, vapor condensation and aerosol formation (VCA)
  - Ash transport sticking and growth (TSG)
  - Heat transfer/sintering/thermal conductivity (HST)
- Implementation and Testing in IDAES platform
- Optimize power plant performance testing
- The information from the IDAES platform will be used to develop simplified relationships for use in CSPI-CT on-line at power plant
- Extent application to gasification and hydrogen production – slag flow and syngas cooler fouling

# Overall Configuration of IDAES Boilerheatexchanger On-line At Power Plants

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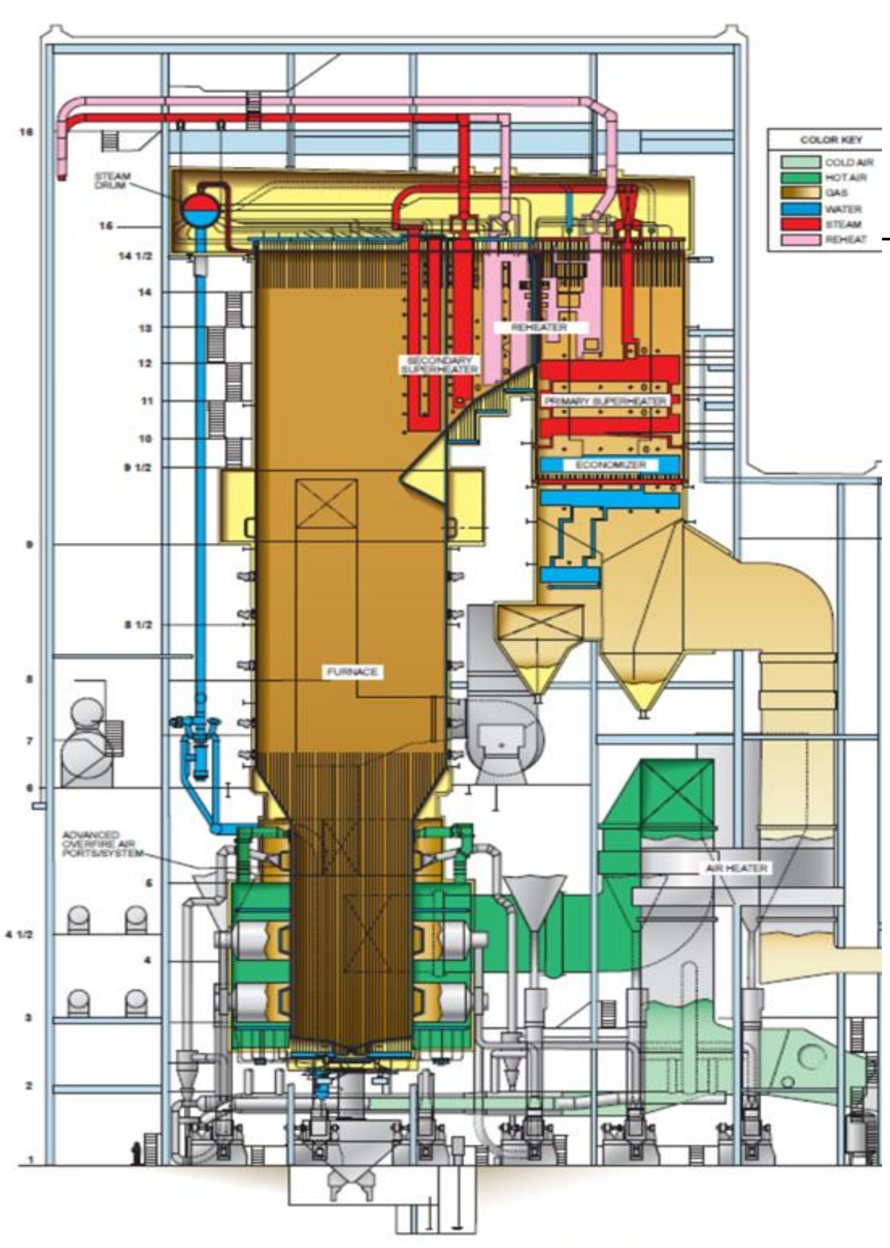
# Coyote Boiler

- Fuel – ND Lignite
- Daily fuel delivery – 7000 – 1200 tons
- Cyclone Fired Boiler
- MW – 450
- $NO_x$ Control – Over Fired Air
- $SO_x$ Control – Dry Scrubber
- PM Control – Baghouse
- Mercury Control – Activated Carbon Injection

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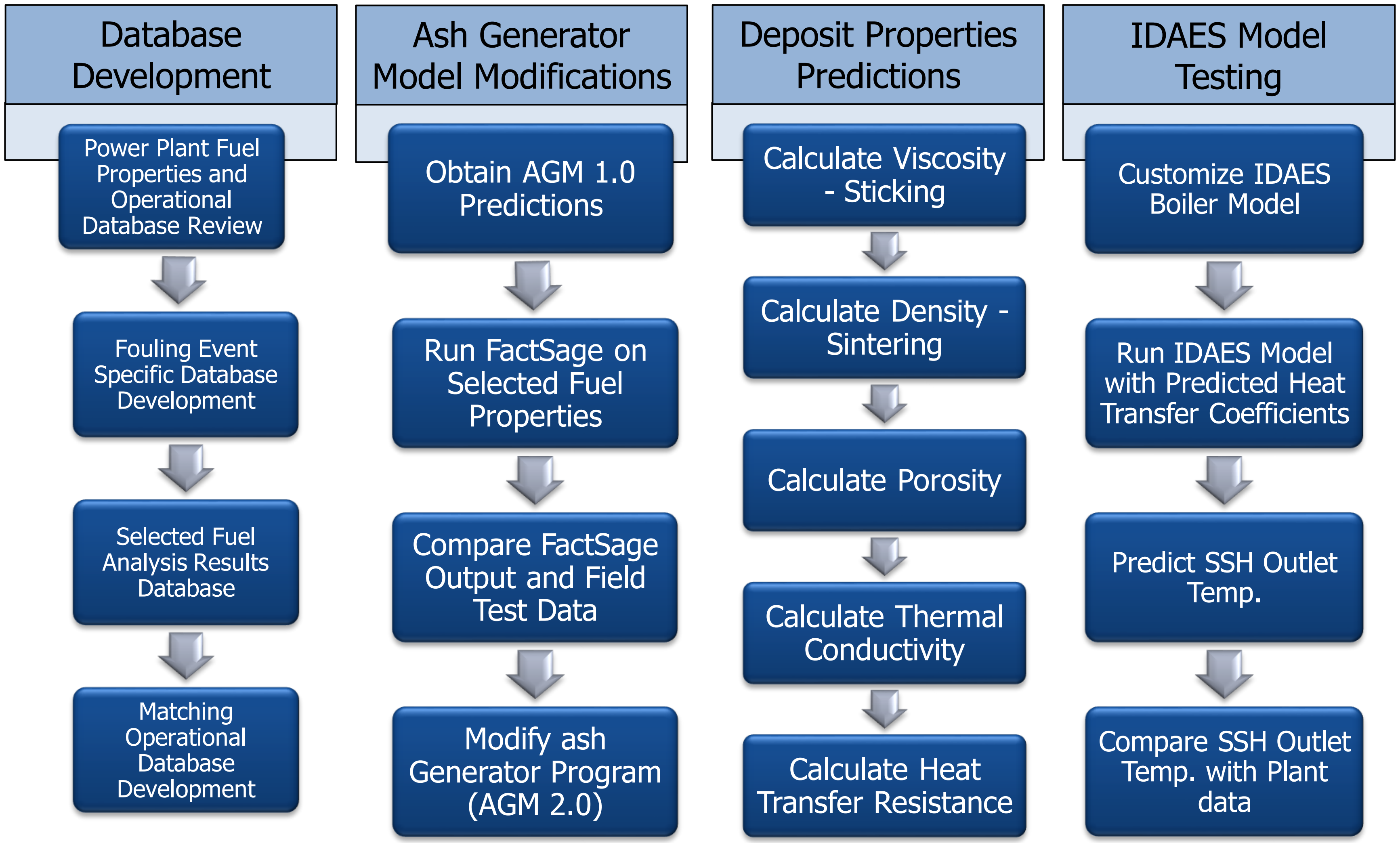
# Phase I Project Workflow



# Phase I Accomplishments

- Improved Ash Generator Model (AGM)
- Integration of AGM with FactSage to predict composition of entrained ash in different locations
- Deposit properties at each location
- Integrated into IDAES boiler model
- Compared with plant heat transfer

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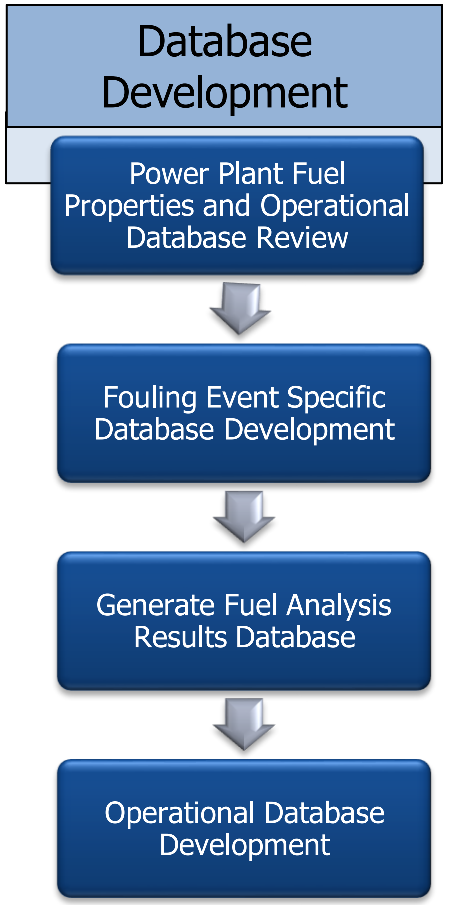
# Section 1 - Database Development

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# Operational Database Review

| Databases | Hours Running | Datapoints |
|---|---|---|
| A | 1691 | 91092 |
| B | 390 | 19761 |
| C | 337 | 18251 |
| D | 601 | 31587 |
| E | 611 | 28508 |
| F | 1294 | 69549 |
| G | 1525 | 82130 |
| H | 354 | 19167 |
| I | 83 | 4536 |
| J | 29 | 1620 |
| K | 905 | 48653 |
| L | 1428 | 77055 |
| M | 59 | 3239 |
| N | 154 | 8315 |
| O | 371 | 20033 |
| P | 168 | 9125 |
| Q | 169 | 9350 |
| R | 1739 | 95476 |
| S | 164 | 9072 |
| T | 365 | 20124 |
| U | 1899 | 88107 |
| V | 1060 | 58299 |
| W | 1217 | 66986 |
| X | 187 | 10337 |
| Y | 338 | 18529 |

# Fuel Properties Database Development

| Coal Basis | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | Case I | Case II | Baseline | D1 | D2 | D3 |
| Proximate | Moisture | 34.47 | 35.25 | 35.18 | 35.76 | 35.48 | 35.22 |
| | Volatile Matter | 28.75 | 29.04 | 28.92 | 29.14 | 29.18 | 28.35 |
| | Fixed Carbon | 26.47 | 27.92 | 28.42 | 27.87 | 27.81 | 28.44 |
| | Ash | 10.31 | 7.79 | 7.48 | 7.23 | 7.53 | 7.99 |
| | | | | | | | |
| Ultimate | Carbon | 62.93 | 67.44 | 68.42 | 68.77 | 68.06 | 67.55 |
| | Hydrogen | 4.25 | 4.53 | 4.34 | 4.36 | 4.31 | 4.27 |
| | Nitrogen | 1.02 | 0.94 | 1.02 | 1 | 1.01 | 0.99 |
| | Oxygen (diff.) | 14.97 | 13.52 | 13.49 | 13.11 | 13.86 | 13.77 |
| | Sulfur | 1.1 | 1.53 | 1.19 | 1.51 | 1.1 | 1.08 |
| | | | | | | | |
| Calorific Value | BTU/lb | 10383 | 10803 | 10847 | 10908 | 10780 | 10706 |
| | | | | | | | |
| **Ash Analysis - weight% as equivalent oxide (sulfur free)** | | | | | | | |
| | SiO2 | 4.73 | 2.60 | 2.65 | 2.14 | 2.92 | 3.41 |
| | Al2O3 | 1.59 | 0.99 | 1.00 | 0.81 | 1.02 | 1.08 |
| | TiO2 | 0.06 | 0.05 | 0.05 | 0.04 | 0.05 | 0.05 |
| | Fe2O3 | 1.05 | 1.27 | 1.07 | 1.28 | 0.94 | 0.92 |
| | CaO | 1.42 | 1.58 | 1.63 | 1.54 | 1.52 | 1.52 |
| | MgO | 0.43 | 0.44 | 0.48 | 0.48 | 0.50 | 0.48 |
| | K2O | 0.21 | 0.09 | 0.06 | 0.08 | 0.09 | 0.11 |
| | Na2O | 0.66 | 0.60 | 0.38 | 0.73 | 0.34 | 0.27 |
| | SO3 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| | P2O5 | 0.01 | 0.03 | 0.03 | 0.02 | 0.02 | 0.01 |
| | SrO | 0.04 | 0.05 | 0.04 | 0.04 | 0.04 | 0.04 |
| | BaO | 0.09 | 0.09 | 0.08 | 0.07 | 0.07 | 0.07 |
| | MnO2 | 0.00 | 0.00 | 0.01 | 0.01 | 0.01 | 0.01 |
| | **Total** | 10.31 | 7.79 | 7.48 | 7.23 | 7.53 | 7.99 |
| | | | | | | | |
| B/A Ratio | | 0.59 | 1.09 | 0.98 | 1.38 | 0.85 | 0.73 |

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# Database Development Summary

- Reviewed over two years of plant operational data
- Reviewed minute-by-minute fuel properties data to find coal quality associated with fouling events
- Developed fuel properties and plant operational database for IDAES model testing

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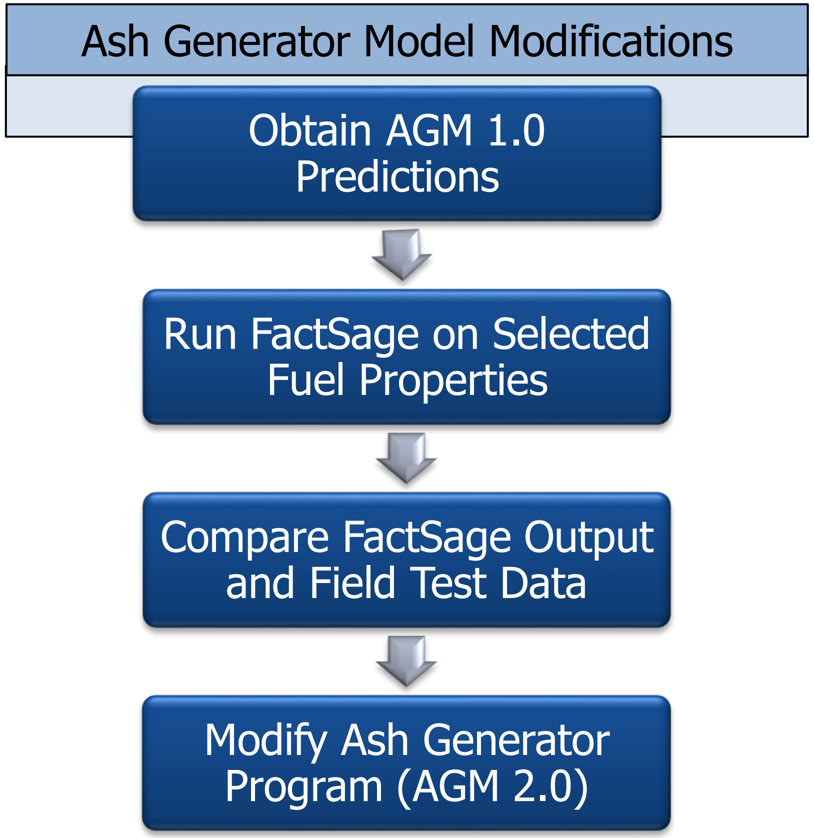
# Section 2 - Ash Generator Model Modifications

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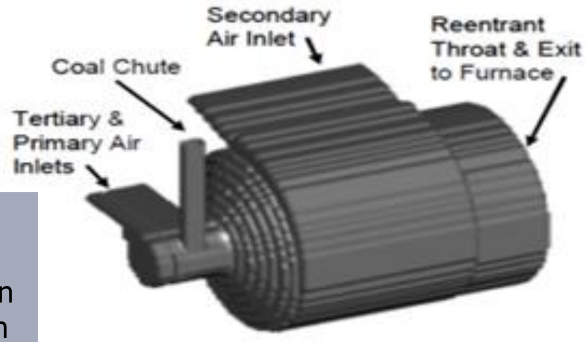
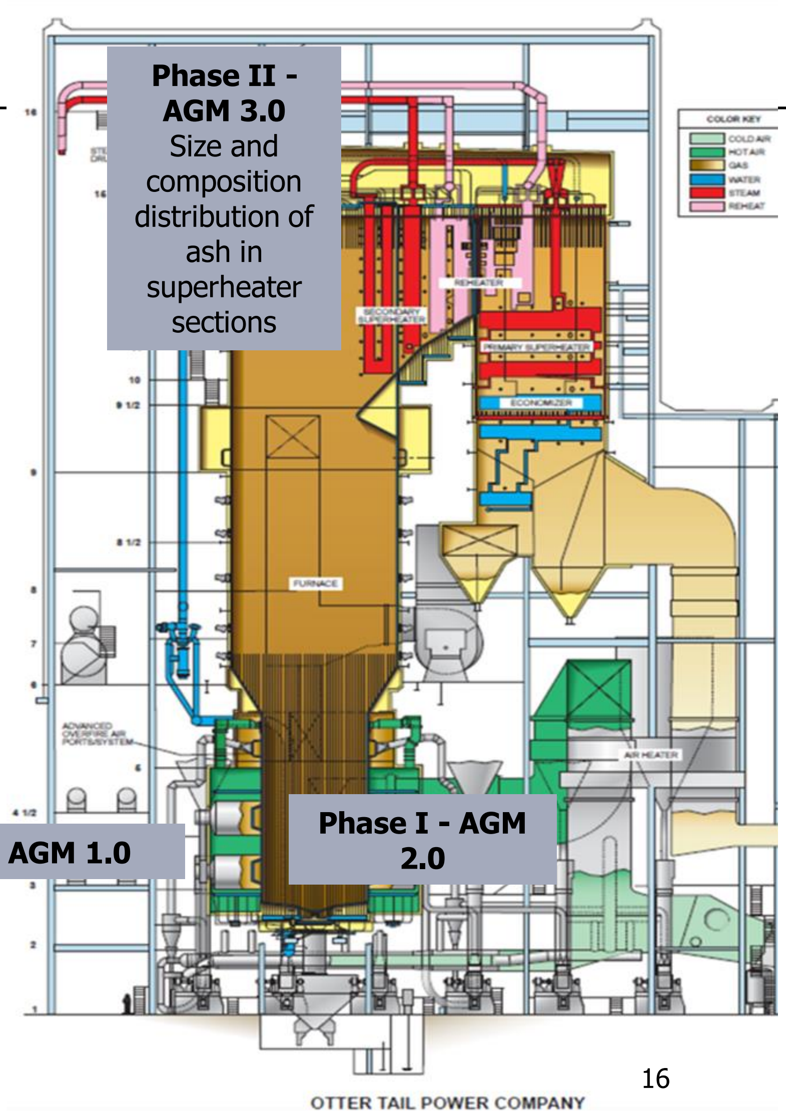
# Phase I – Ash Generator Model Modifications

- Microbeam's ash generator model was modified in order to account for transformations of different mineral species as well as slag/fly-ash partitioning in a cyclone-fired boiler.




**AGM 1.0**
Size and composition distribution of ash at cyclone inlet

**Phase I - AGM 2.0**
Size and composition distribution of ash at cyclone outlet




**Phase II - AGM 3.0**
Size and composition distribution of ash in superheater sections

**AGM 1.0**

**Phase I - AGM 2.0**

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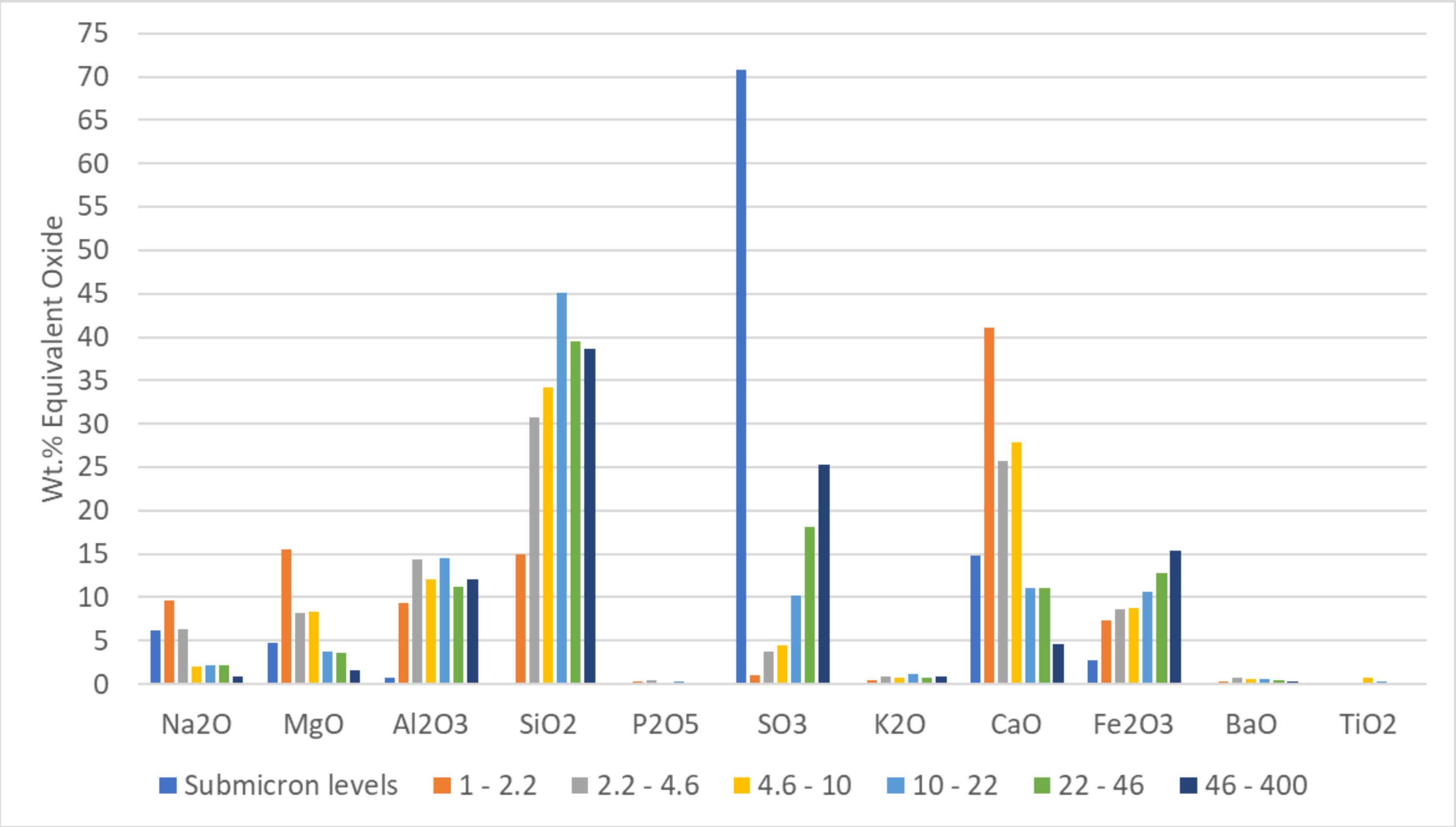
# Ash Generator Model 1.0 Output
## (D2 Coal)

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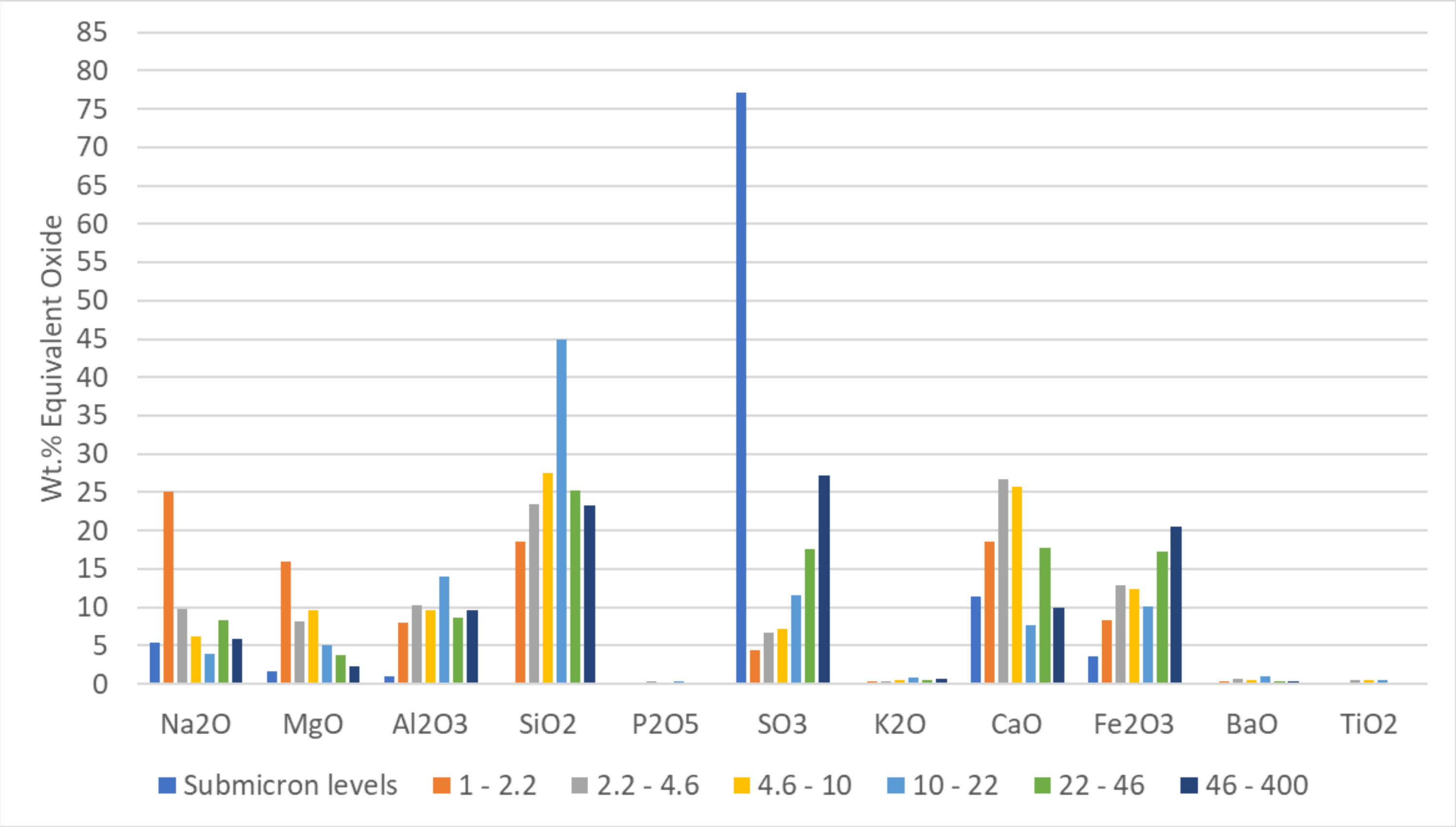
# Output of the Initial AGM for Day 1

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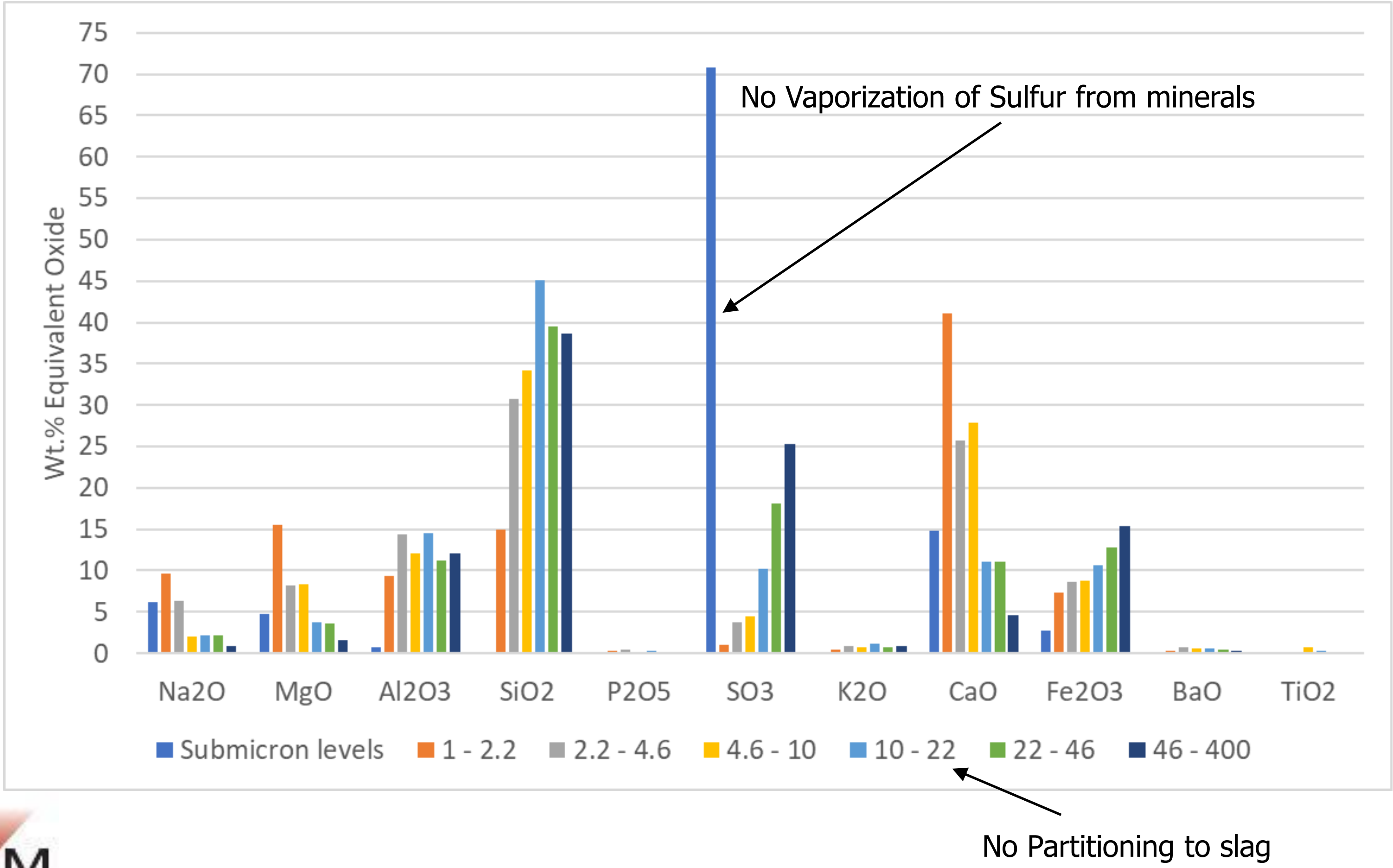
# Ash Generator Model Prediction for Day 2 Coal
# (Ash PSD and composition at the entrance of the cyclone)

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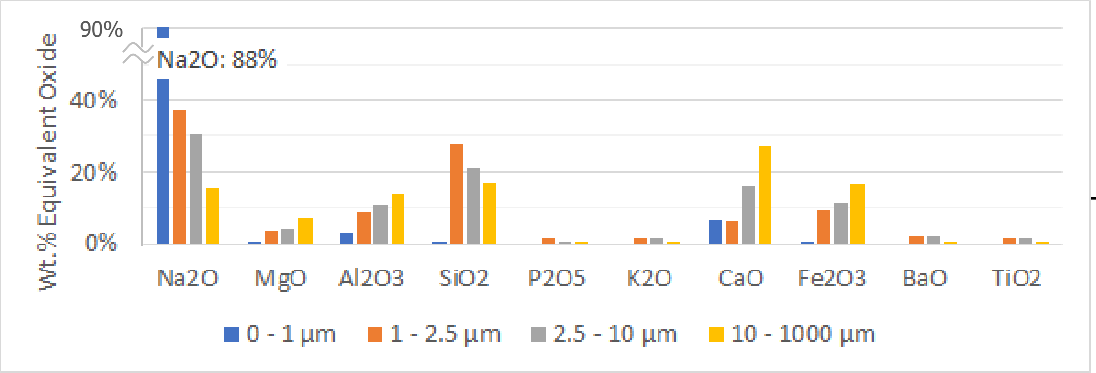
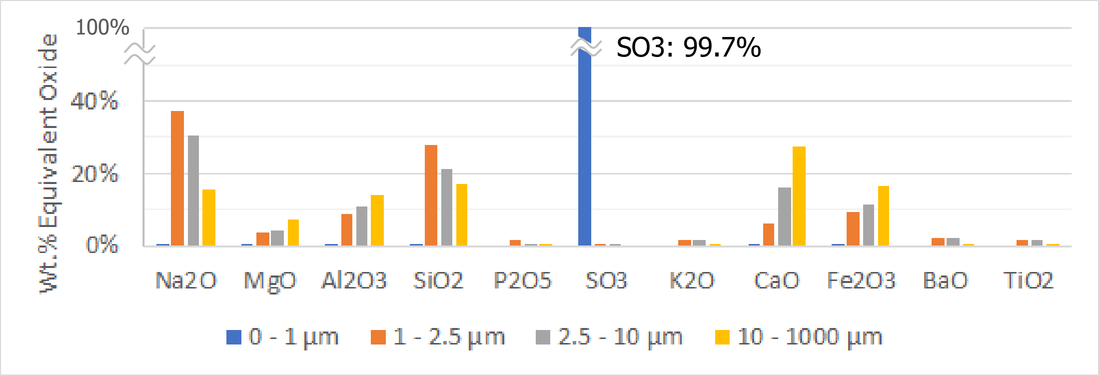
# Ash Generator Model (AGM) Prediction for Day 2 Coal

(Ash PSD and composition at the cycline exit)

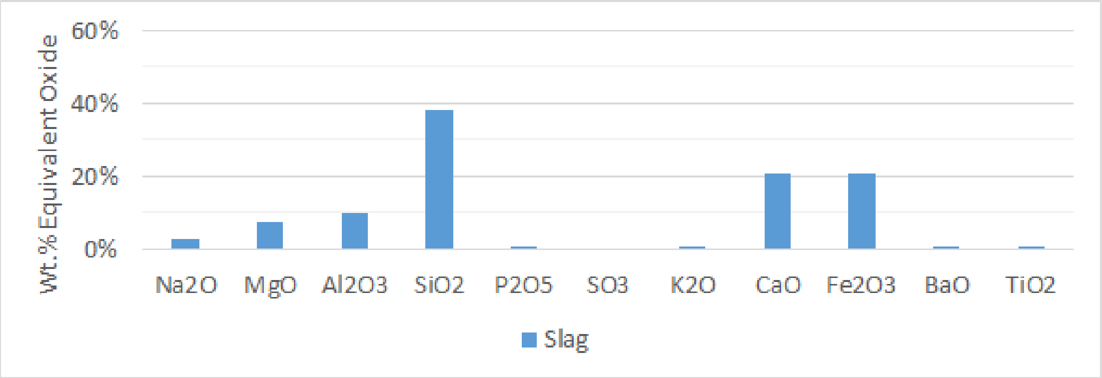
a. Fly ash composition on an $SO_3$ free basis




b. Fly ash composition including $SO_3$




c. Slag composition

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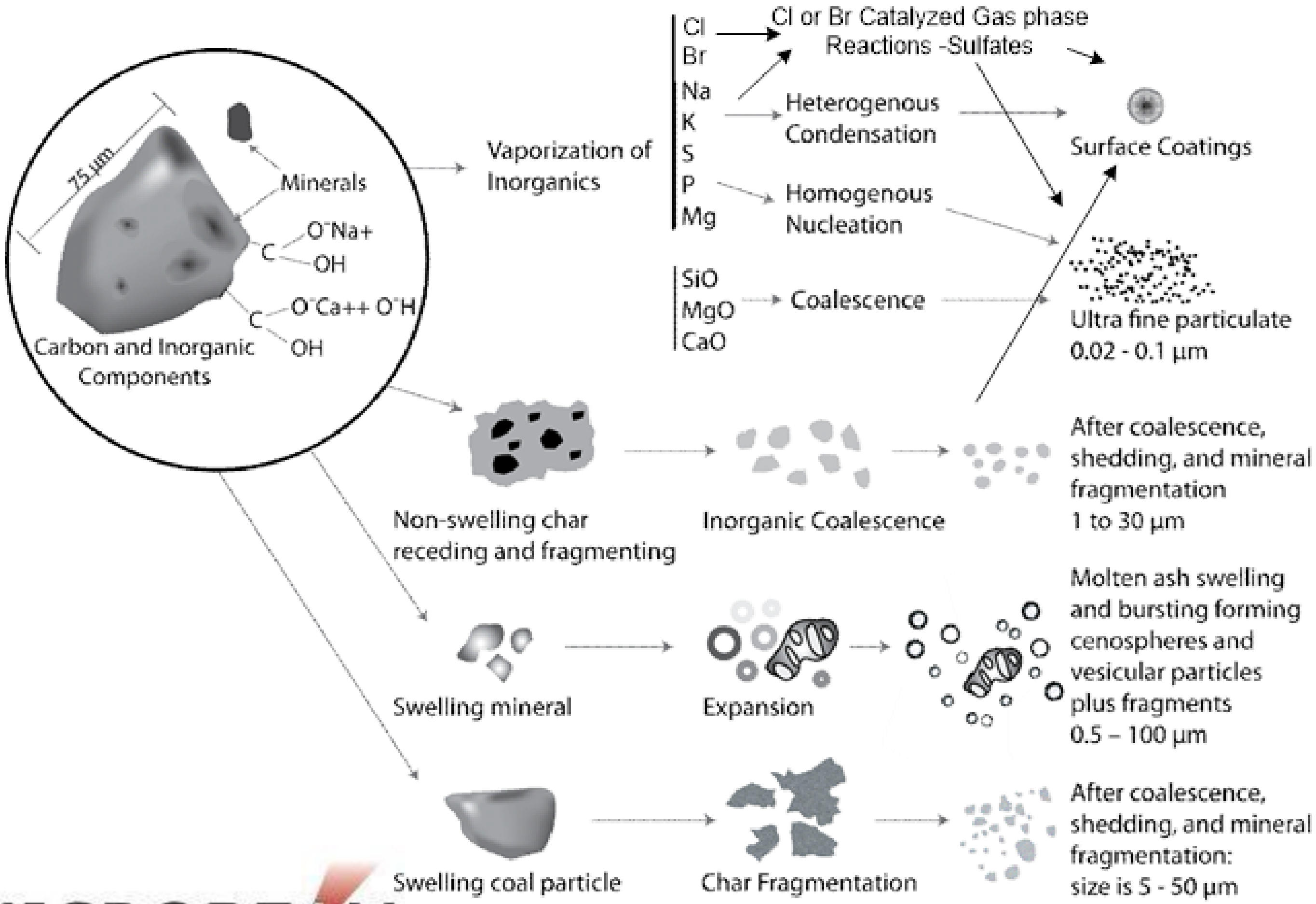
# Integration of AGM with FactSage




- Impact of temperature of the system
- Size-distributed fly ash condenses as particulate is transported through system
- AGM output feeds FactSage predictions of condensed phases (mostly sulfur and sodium) as a function of temperature

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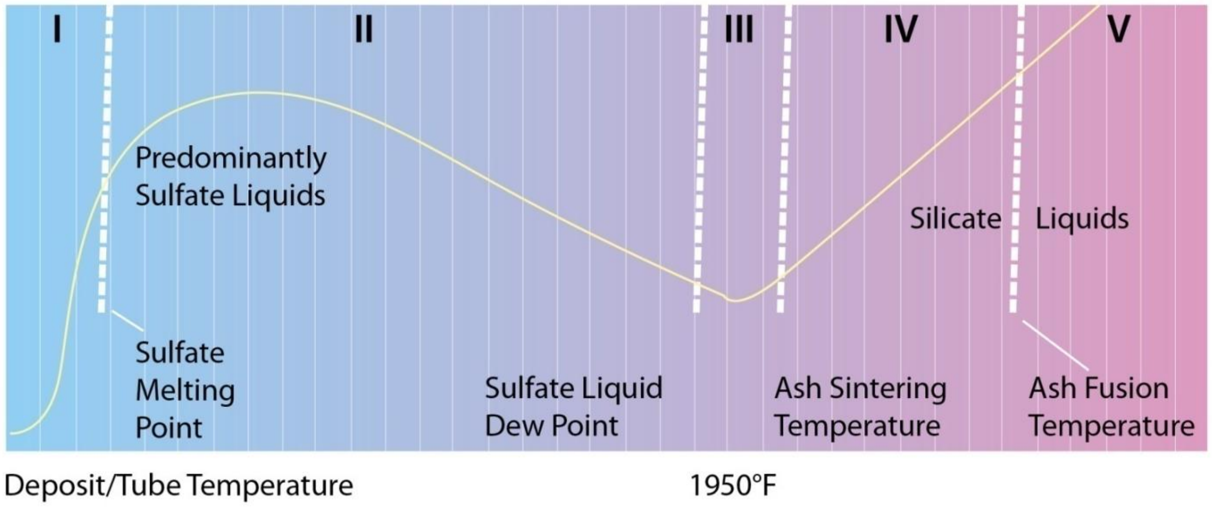
# Distribution of Bonding Phases in Combustion Systems

Low Temp Fouling | High Temp Fouling | Slagging




Deposition Regimes:

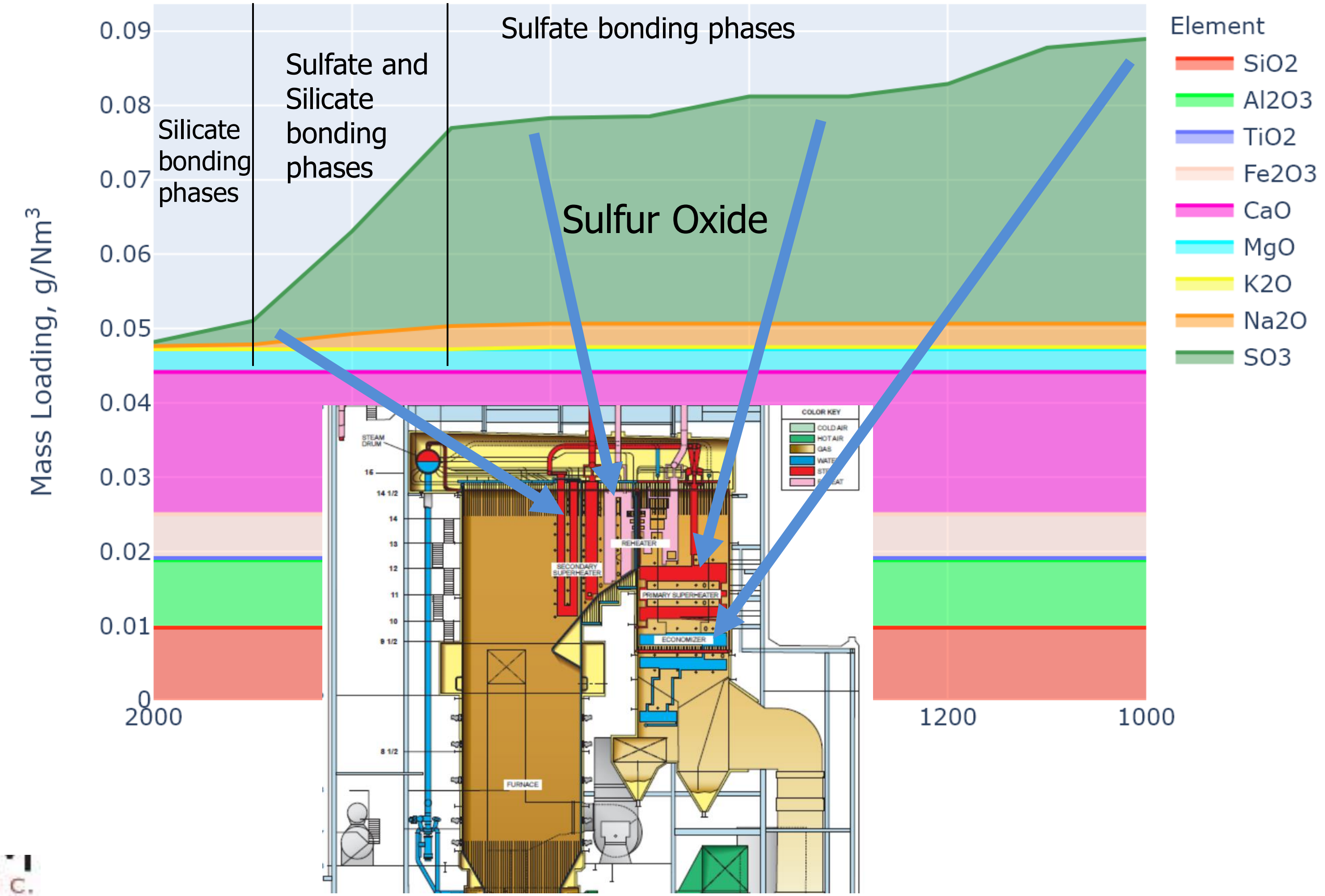
1. Dry-sticking regime: no glue
2. Vapor orthermophertically deposited liquid glue
3. Glue produced by heterogenous chemical reactions at vapor-ash interface
4. Ash particle softening on impact
5. Wet limit (sticking coefficient nearly unity)





*Modified after "Maximum Effect of vapor phase chemical reactions on cvd-rates and deposition onset conditions in the absence of interfacial kinetic barriers" Rosner, D. and Nagarajan, R.*

# Integration of AGM with FactSage Condensation as f(temperature) (Overall ash composition)

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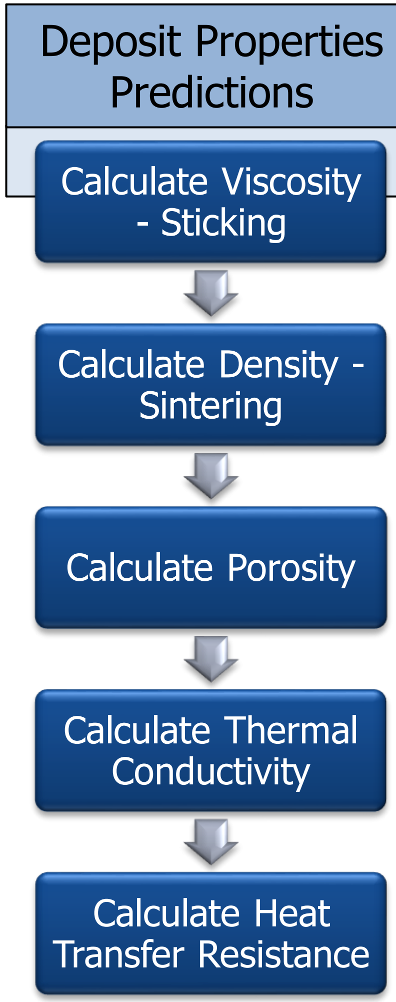
# Section 3 – Deposit Properties Predictions

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# Deposit Properties

- Simplified transport processes used to produce deposits based on particle size – diffusion, thermophoresis, impaction
- Deposit Growth - Sticking behavior
  - High temperature viscosity of particle and surface
  - Low temperature processes – sulfate base liquids (fine particle process), condensation and gas solid reactions
- Sintering processes - Densification
  - High temperature - aluminosilicate liquid phase viscosity based
  - Low temperature – sulfate liquid phase, molecular cramming due to sulfation fine
- Thermal Conductivity
  - Porosity and density of the deposit

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# Deposit and Fouling Properties Manager (DeFoul Model)

- Highly technical and detailed model incorporating both literature and experimental results to predict an array of deposit, SSH single tube, and SSH tube bank properties
- Predicts deposit growth based on coal properties and operating conditions
- DeFoul also uses a unique method of modeling deposits by dividing the deposit into radial sections (quadrants)
- Ultimately can predict whether sootblowing will be required, or recommended
  - Allows operators/users to identify optimum operating conditions and see the effect of adjust coal quality and/or operating conditions on the deposition and fouling in the convective pass
  - Efficient, “smart” sootblowing
- User friendly interface

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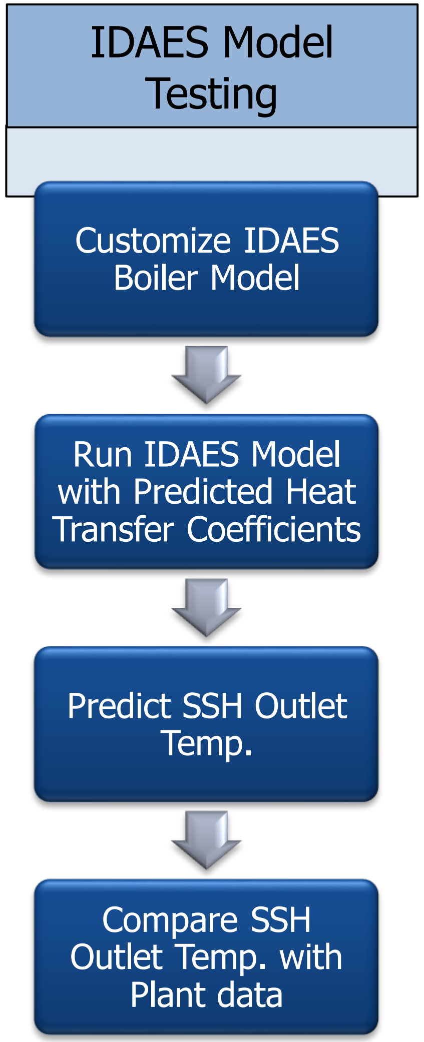
# Section 4 – IDAES Model Testing and Integration

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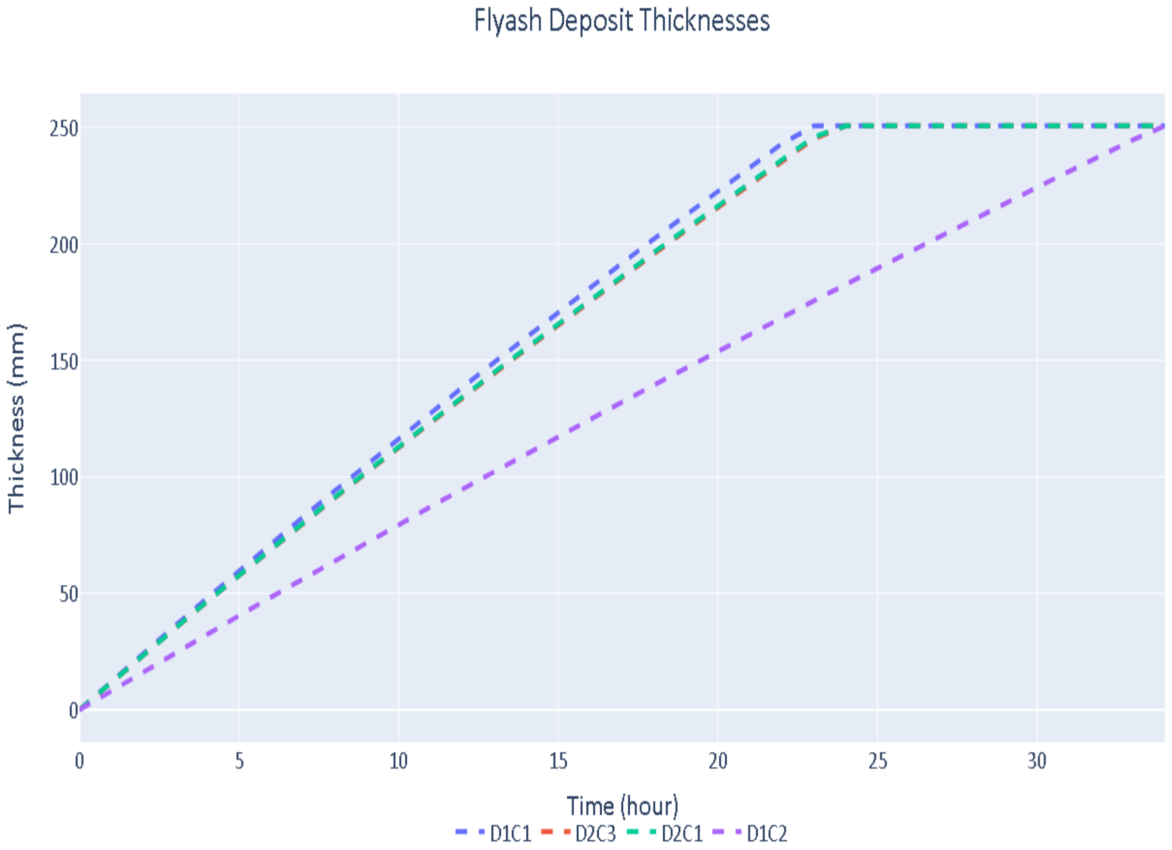
# Integration into IDAES boiler model

- Used deposit properties to calculate fouling resistance as a function of deposit thickness
- Ran IDAES BoilerHeatExchanger model for secondary superheater simulating deposit thicknesses for selected conditions
- Obtained real plant data for selected conditions in the plant and compared with predictions

# Simulated Deposit Properties with DeFoul Model




| Day/Condition | Fuel B/A Ratio | Fuel Ash Content | NOx Setpoint |
|---|---|---|---|
| Day 1 Condition 1 (D1C1) | 1.18 (Average) | 6.53 | 0.45 |
| Day 1 Condition 2 (D1C2) | 1.37 (High) | 7.23 | 0.45 |
| Day 2 Condition 1 (D2C1) | 0.85 (Average) | 7.53 | 0.44 |
| Day 2 Condition 3 (D2C1) | 0.85 (Average) | 7.53 | 0.35 |

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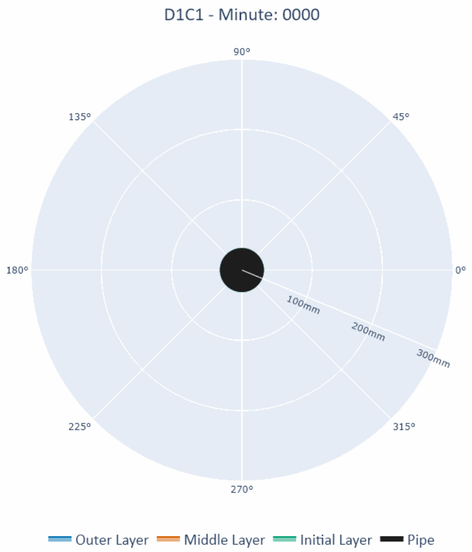
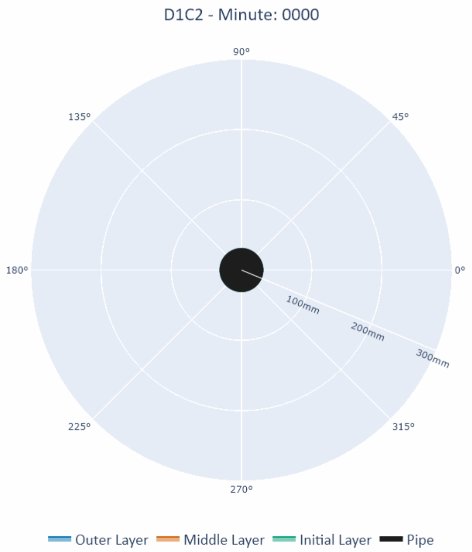
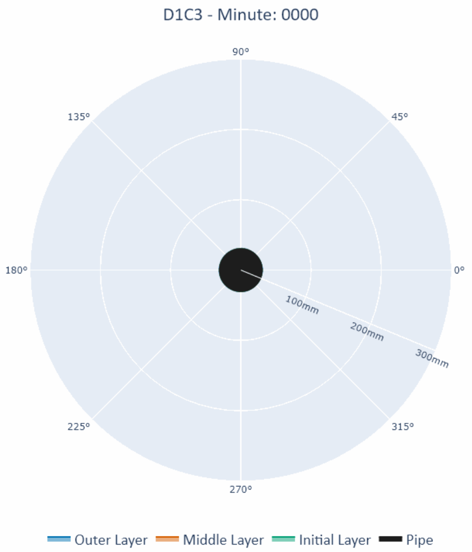
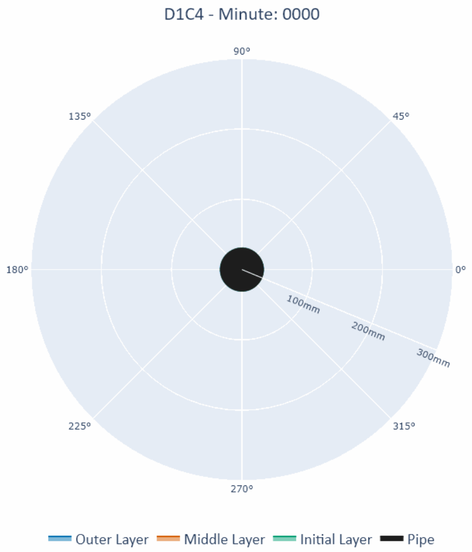
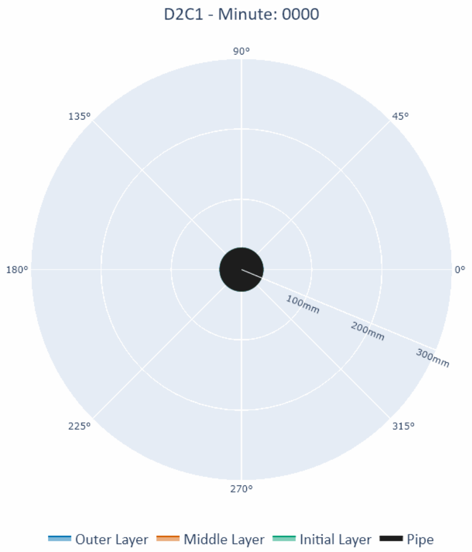
# Deposit Plots

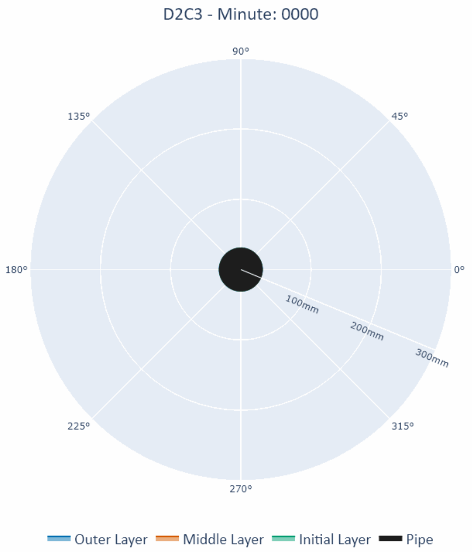
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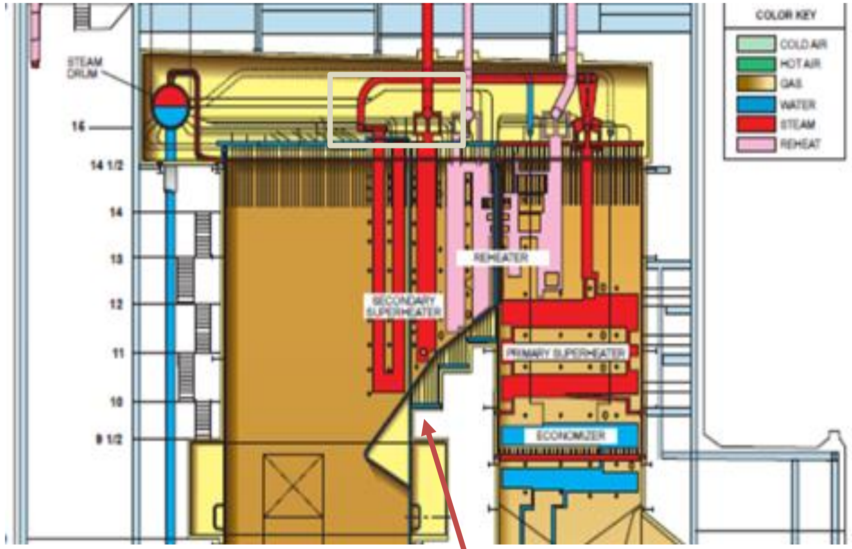
# IDAES model output comparison

- Matched fuel properties to operating conditions
- Calculated deposit properties using fuel properties
- Ran IDAES to predict outlet steam temperature
- Compared IDAES-predicted with measured plant steam temperature
- Difference between predicted and measured plant steam temperature attributed to deposit buildup




Example for Secondary Superheater

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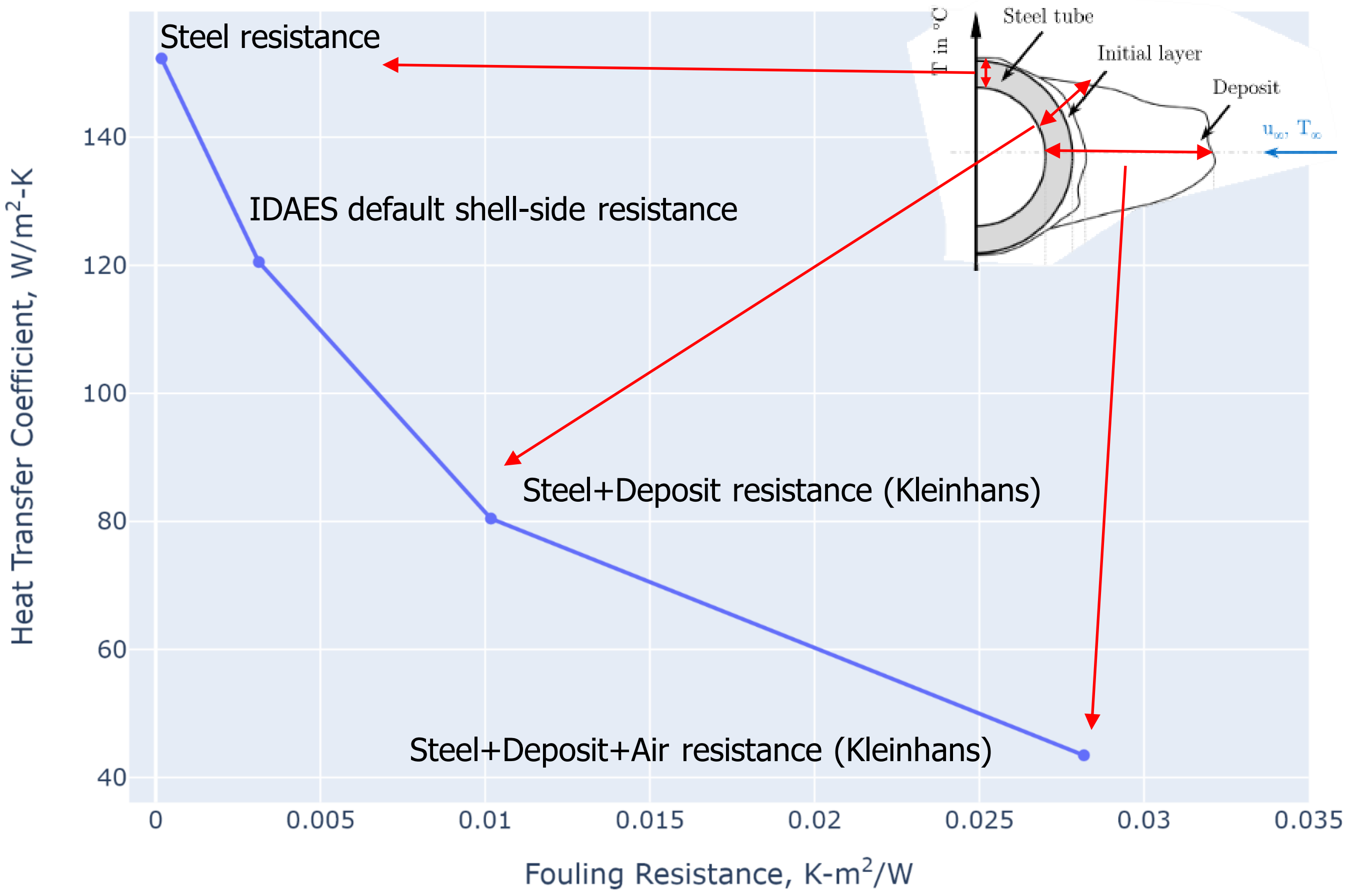
# Predicted Heat Transfer Coefficient with IDAES SSH Model (Using Literature Data)




HTC decreases from 64 W/m²·K to 15 W/m²·K – 76% decrease

U. Kleinhans, C. Wieland, F. J. Frandsen, and H. Spliethoff, "Ash formation and deposition in coal and biomass fired combustion systems: Progress and challenges in the field of ash particle sticking and rebound behavior," *Progress in Energy and Combustion Science*, vol. 68, pp. 65–168, Sep. 2018, doi: 10.1016/j.pecs.2018.02.001.

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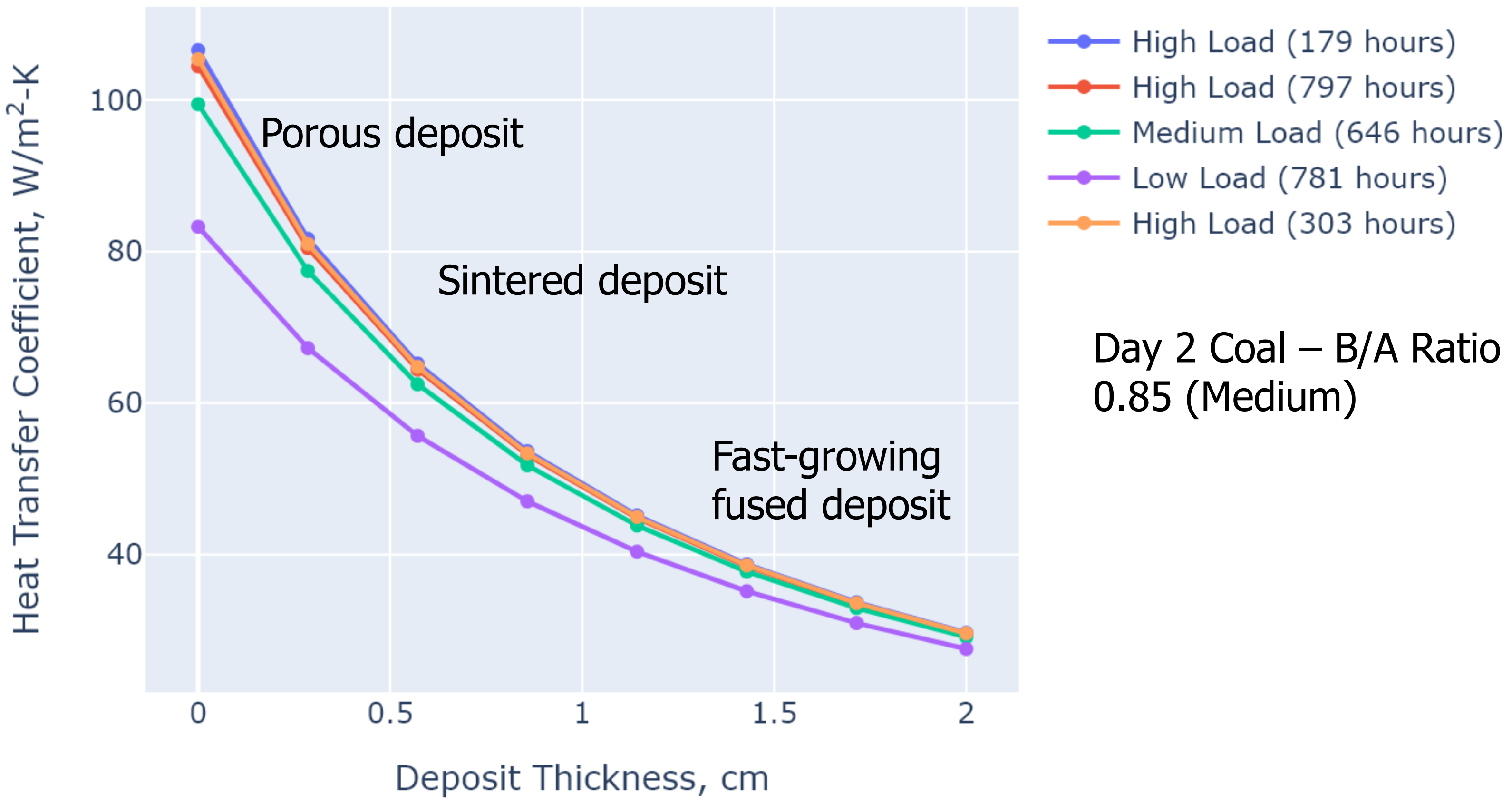
# Integration into IDAES Boiler Model – Results (Using Day 2 Coal Composition)




Day 2 Coal – B/A Ratio – 0.85 (Medium)

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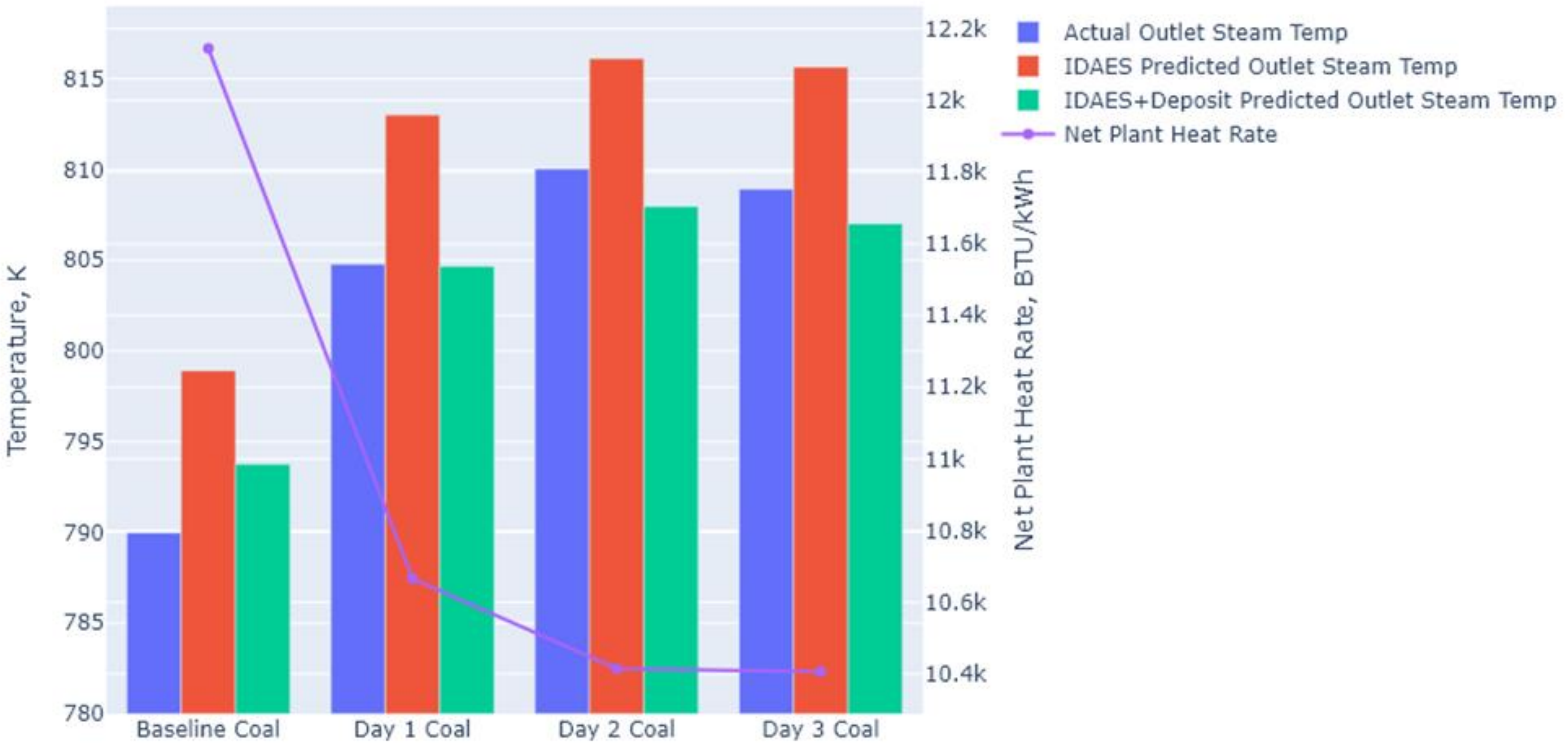
# SSH Outlet Steam Temperatures Prediction with IDAES – Effect of Coal Composition

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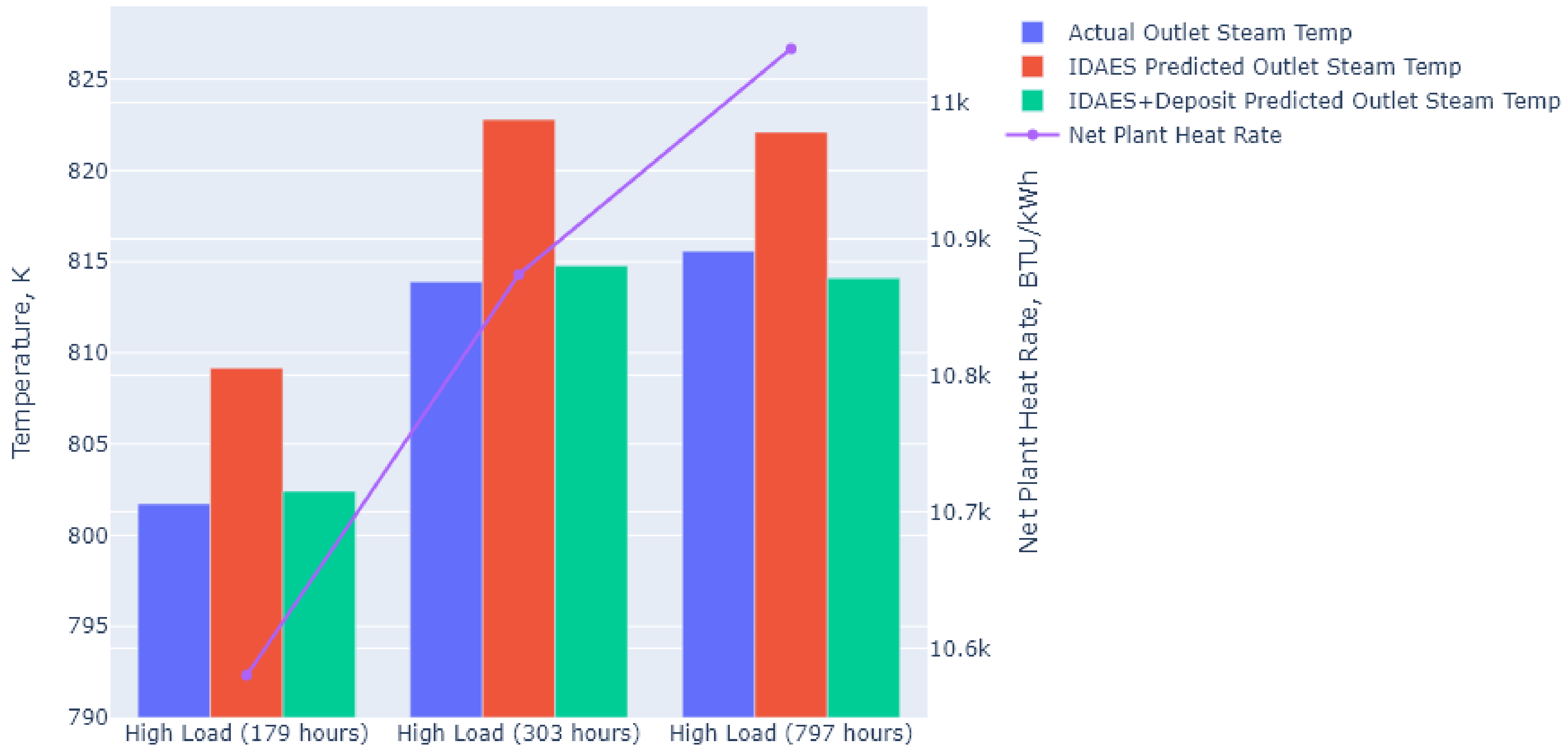
# SSH Outlet Steam Temperatures Prediction with IDAES – Effect of Run Time

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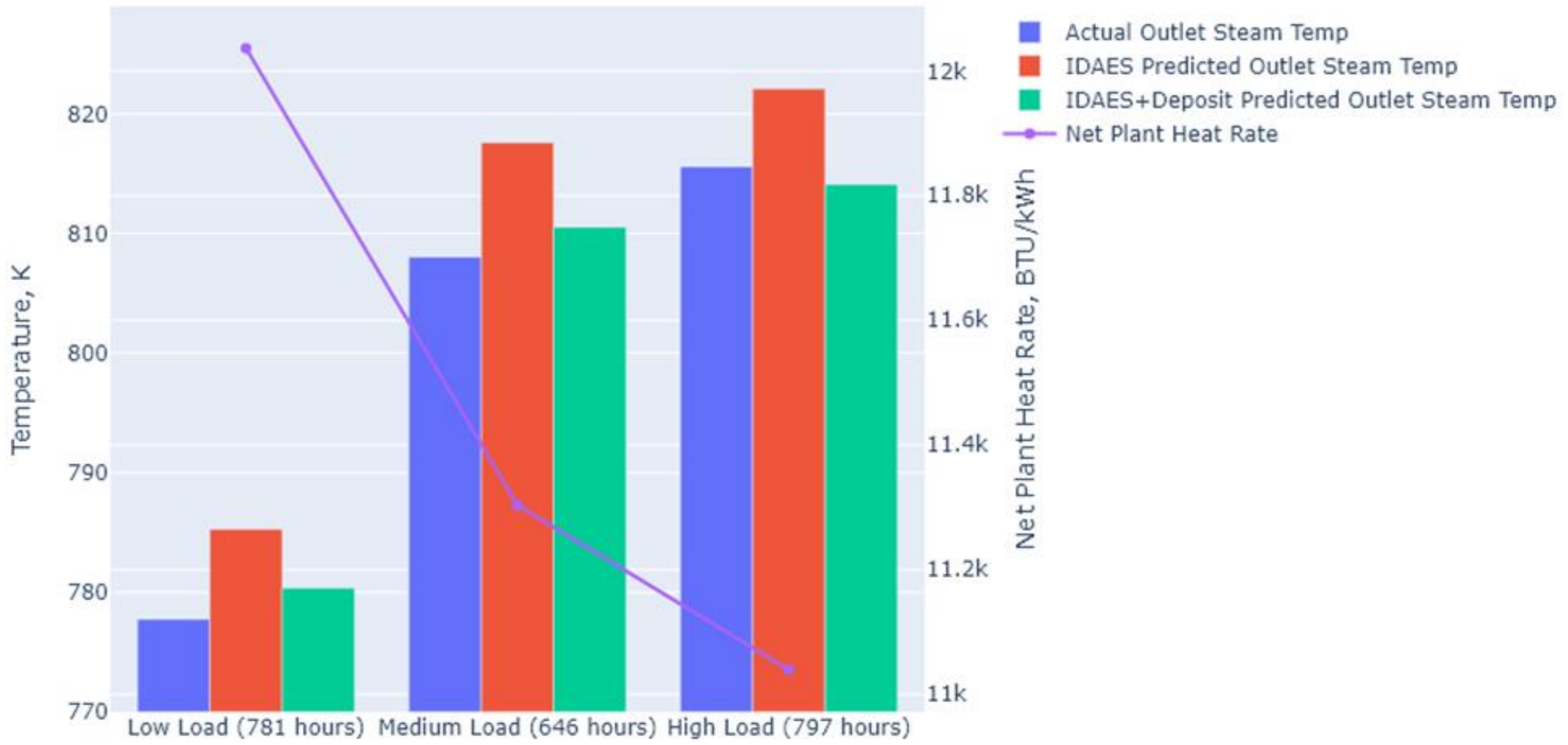
# SSH Outlet Steam Temperatures Prediction with IDAES – Effect of Load Condition

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# Phase I - Conclusions

- Ash generator model was integrated with a condensation/reaction model (FactSage) to prediction the properties of ash during gas cooling.
- A model that incorporates ash transport, sticking, growth, and sintering was developed to determine thermal conductivity of deposited ash.
- The thermal conductivity of the ash material was incorporated into the IDAES boiler model to predict outlet steam temperature for the SSH.

# Next Steps – Phase II Efforts

- Further integrate –
  - Ash generation, vapor condensation and aerosol formation (VCA)
  - Ash transport sticking and growth (TSG)
  - Heat transfer/sintering/thermal conductivity (HST)
- Implementation and Testing in IDAES platform
- Optimize power plant performance testing
- The information from the IDAES platform will be used to develop simplified relationships for use in CSPI-CT on-line at power plant
- Extent application to gasification and hydrogen production – slag flow and syngas cooler fouling

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# Phase II Effort

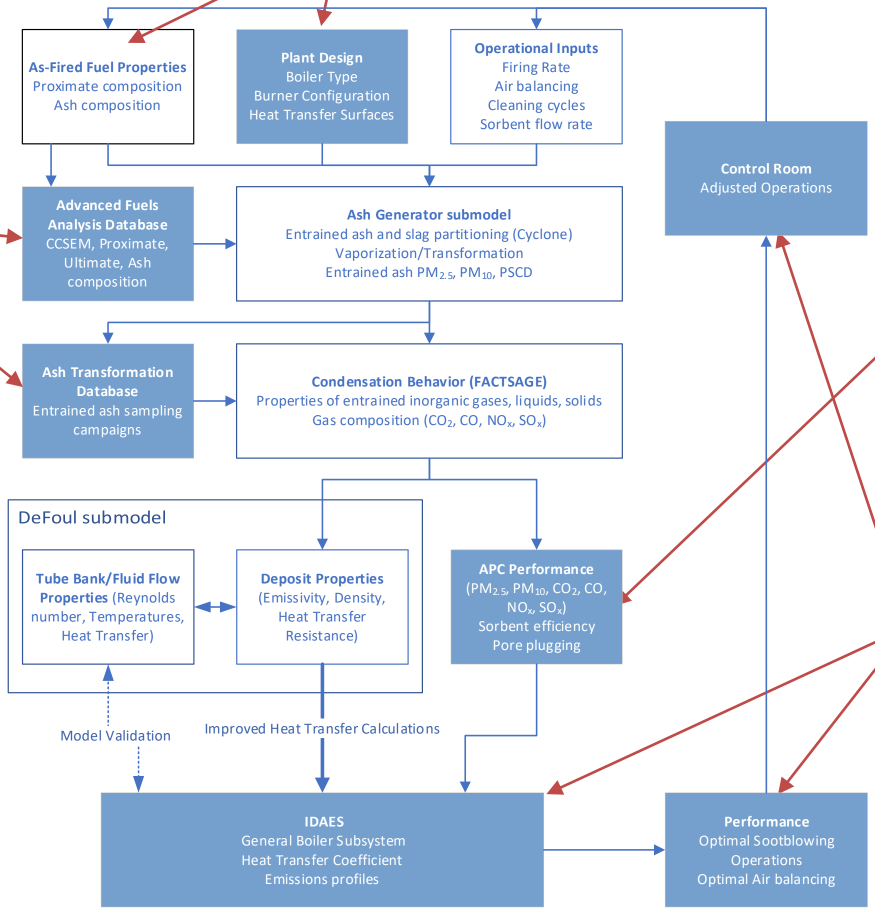
Expand to hydrogen/ biomass

Update databases

Integrate live onsite

Advanced emissions performance predictions

Simulate scenarios to optimize operations

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# Commercial Product

- IDAES model will be included in Microbeam's Combustion System Performance Indices - CoalTracker program.
- This will give an opportunity to the plant operators and engineers to run different scenarios to predict the effect of changing operational conditions on heat transfer and plant efficiency.
- On-premise license and cloud-based application
- Potential Clients
  - Coal-fired Power Plants
  - Gasifiers (Syngas/Hydrogen/Ammonia)
  - Biomass-fired systems
  - Waste-fired Systems
  - Co-firing Applications

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# Questions

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