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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Jason Montgomery – DOE NETL Project Manager
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05/24/2021
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
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.
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.
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
Coyote Boiler

- Fuel – ND Lignite
- Daily fuel delivery – 7000 – 1200 tons
- Cyclone Fired Boiler
- MW – 450
- NO\textsubscript{x} Control – Over Fired Air
- SO\textsubscript{x} Control – Dry Scrubber
- PM Control – Baghouse
- Mercury Control – Activated Carbon Injection
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
Section 1 - Database Development

- Database Development
  - Power Plant Fuel Properties and Operational Database Review
  - Fouling Event Specific Database Development
  - Generate Fuel Analysis Results Database
  - Operational Database Development
### Operational Database Review

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<th>Databases</th>
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# Fuel Properties Database Development

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<th>Case II</th>
<th>Baseline</th>
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<th>D2</th>
<th>D3</th>
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<td>Ash Analysis - weight% as equivalent oxide (sulfur free)</td>
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<td>0.03</td>
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<td>0.01</td>
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<td>0.01</td>
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<tr>
<td>Total</td>
<td>10.31</td>
<td>7.79</td>
<td>7.48</td>
<td>7.23</td>
<td>7.53</td>
<td>7.99</td>
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<tr>
<td>B/A Ratio</td>
<td>0.59</td>
<td>1.09</td>
<td>0.98</td>
<td>1.38</td>
<td>0.85</td>
<td>0.73</td>
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</table>
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
Section 2 - Ash Generator Model Modifications

<table>
<thead>
<tr>
<th>Ash Generator Model Modifications</th>
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<tbody>
<tr>
<td>Obtain AGM 1.0 Predictions</td>
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<tr>
<td>Run FactSage on Selected Fuel Properties</td>
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<tr>
<td>Compare FactSage Output and Field Test Data</td>
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<tr>
<td>Modify Ash Generator Program (AGM 2.0)</td>
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</tbody>
</table>
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.
Ash Generator Model 1.0 Output
(D2 Coal)
Output of the Initial AGM for Day 1
Ash Generator Model Prediction for Day 2 Coal
(Ash PSD and composition at the entrance of the cyclone)

No Vaporization of Sulfur from minerals
No Partitioning to slag
Ash Generator Model (AGM) Prediction for Day 2 Coal

(Ash PSD and composition at the cyclone exit)
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
Distribution of Bonding Phases in Combustion Systems

Deposition Regimes:
1. Dry-sticking regime: no glue
2. Vapor or thermophobically 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 ev 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)
Section 3 – Deposit Properties Predictions

- Calculate Viscosity - Sticking
- Calculate Density - Sintering
- Calculate Porosity
- Calculate Thermal Conductivity
- Calculate Heat Transfer Resistance
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
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
Section 4 – IDAES Model Testing and Integration

IDAES Model Testing

Customize IDAES Boiler Model

Run IDAES Model with Predicted Heat Transfer Coefficients

Predict SSH Outlet Temp.

Compare SSH Outlet Temp. with Plant data
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

<table>
<thead>
<tr>
<th>Day/Condition</th>
<th>Fuel B/A Ratio</th>
<th>Fuel Ash Content</th>
<th>NOx Setpoint</th>
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<tbody>
<tr>
<td>Day 1 Condition 1 (D1C1)</td>
<td>1.18 (Average)</td>
<td>6.53</td>
<td>0.45</td>
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<tr>
<td>Day 1 Condition 2 (D1C2)</td>
<td>1.37 (High)</td>
<td>7.23</td>
<td>0.45</td>
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<tr>
<td>Day 2 Condition 1 (D2C1)</td>
<td>0.85 (Average)</td>
<td>7.53</td>
<td>0.44</td>
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<tr>
<td>Day 2 Condition 3 (D2C1)</td>
<td>0.85 (Average)</td>
<td>7.53</td>
<td>0.35</td>
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</table>
Deposit Plots
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
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

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

- Porous deposit
- Sintered deposit
- Fast-growing fused deposit

Day 2 Coal – B/A Ratio – 0.85 (Medium)
SSH Outlet Steam Temperatures Prediction with IDAES – Effect of Coal Composition
SSH Outlet Steam Temperatures Prediction with IDAES – Effect of Run Time
SSH Outlet Steam Temperatures Prediction with IDAES – Effect of Load Condition
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
Phase II Effort

- Expand to hydrogen/biomass
- Update databases
- Integrate live onsite

**An-Fired Fuel Properties**
- Proximate composition
- Ash composition

**Plant Design**
- Boiler Type
- Burner Configuration
- Heat Transfer Surfaces

**Operational Inputs**
- Firing Rate
- Air balancing
- Cleaning cycles
- Sorbent flow rate

**Advanced Fuels Analysis Database**
- CCSEM, Proximate, Ultimate, Ash composition

**Ash Transformation Database**
- Entrained ash sampling campaigns

**Ash Generator submodel**
- Entrained ash and slag partitioning (Cyclone)
- Vaporization/Transformation
- Entrained ash PM2.5, PM10, PSCD

**Condensation Behavior (FACTSAGE)**
- Properties of entrained inorganic gases, liquids, solids
  - Gas composition (CO2, CO, NOx, SOx)

**DeFouT submodel**
- Tube Bank/Fluid flow Properties (Reynolds number, Temperatures, Heat Transfer)
- Deposit Properties (Emissivity, Density, Heat Transfer Resistance)

**IDAES**
- General Boiler Subsystem
- Heat Transfer Coefficient
- Emissions profile

**Control Room**
- Adjusted Operations

**Advanced emissions performance predictions**
- Model Validation
  - Improved Heat Transfer Calculations

**Performance**
- Optimal Sootblowing Operations
- Optimal Air balancing

**Performance**
- APC Performance
  - PM2.5, PM10, CO2, CO, NOx, SOx
  - Sorbent Efficiency
  - Pore plugging

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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
Questions

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Phone: (701)757-6202

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