

REINHOLD ENVIRONMENTAL®



2022 Reinhold/PCUG Round Table Presentation

Hosted by Duke Energy in the Charlotte Sheraton/Le Meridien
Hotel, Charlotte, NC on June 27-28, 2022

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Exploring DSI/ACI Performance Improvement using Chemistry-Based CFD Simulations

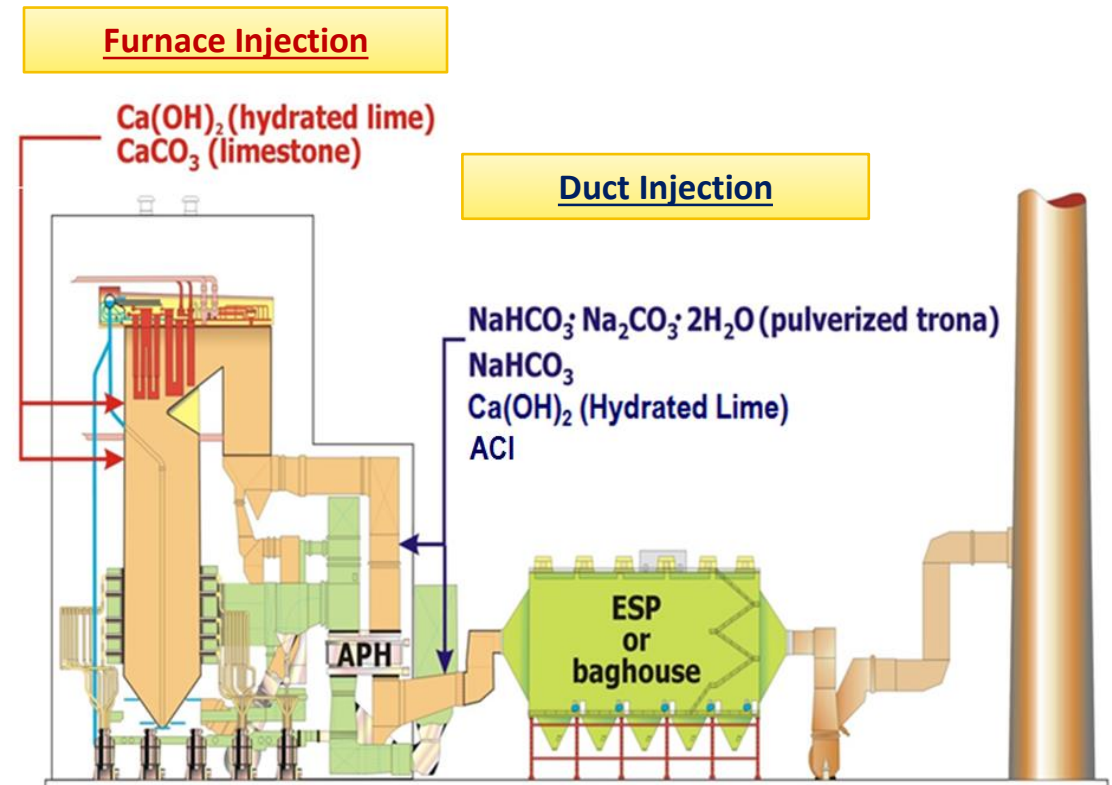
Presented at 2022 REINHOLD/PCUG Conference, June 27-28, 2022

Ron Hurst and Guisu Liu

Reaction Analytic Solutions Corp.

Sorbent Injection Technology Overview

- Sorbents
 - Limestone
 - Hydrated lime
 - Trona
 - Sodium bicarbonate (SBC)
 - Activated carbon
- Locations
 - Furnace injection
 - Duct injection (before or after AH)
- Pollutants
 - SO₂, SO₃, HCl, Hg
- Sorbent injection performance is affected by
 - Temperature
 - Residence time
 - Particle size distribution
 - Physical properties
 - Coverage/dispersion
 - Injection rate
 - PM collection device



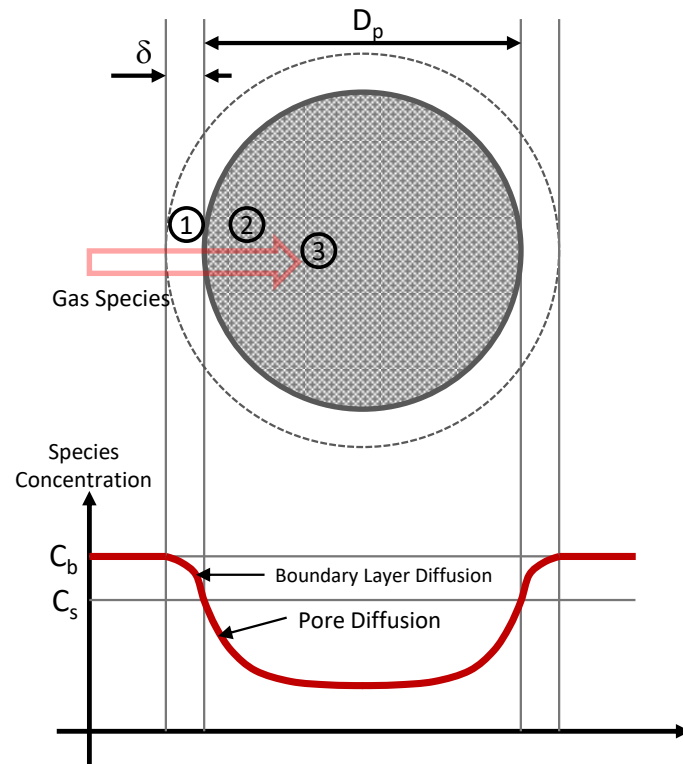
Basics - Sorbent Reaction Process

- Thermal decomposition
 - $\text{CaCO}_3 \rightarrow \text{CaO}$ >1500°F
 - $\text{Ca(OH)}_2 \rightarrow \text{CaO}$ >1000°F
 - $\text{Na}_2\text{CO}_3 \cdot \text{NaHCO}_3 \cdot 2\text{H}_2\text{O} \rightarrow \text{Na}_2\text{CO}_3$ >130°F
 - $\text{NaHCO}_3 \rightarrow \text{Na}_2\text{CO}_3$ >130°F
 - Particle porosity and surface area increase
- Sintering characteristics
 - CaO >1470°F
 - Na_2CO_3 >750°F
 - Porosity and surface area reduction
- Absorption chemistry and kinetics
 - CaO reacts with SO_2 , SO_3 , HCl
 - Na_2CO_3 reacts with SO_2 , SO_3 , HCl
- Boundary layer diffusion and pore diffusion
 - Particle size, surface area and porosity
- All processes are governed by rate equations



Fundamentals of Sorbent Reacting with Pollutants

4



Liming Shi, Guisu Liu, Lewis Benson, "An Enhanced CFD Based Chemistry Model for SO_3 Mitigation by Dry Sorbent Injection", Paper 117, MEGA Symposium, Baltimore, MD, August, 2012

- Sorbent chemistry mechanism
 - **Process 1:** Gas species transports from bulk gas phase to particle surface through boundary layer diffusion
 - **Process 2:** Gas species continues to transport to inside particle through pore diffusion; and
 - **Process 3:** Gas species reacts with inside particle active sites through adsorption
- Inputs
 - Sorbent property (surface area, porosity)
 - Size distribution
 - Flue gas operating conditions (flowrate, temp, species)
- Coding
 - Reaction rate parameters differ between sorbent types and gas species
 - Submodel integrated with CFD code

Chemistry-Based CFD Model vs. Flow-Only Model

	Conventional CFD Model (Flow-only)	Advanced CFD Model (Chemistry-Based)
CFD Output		
Particle Concentration Distribution	✓	✓
Particle Concentration RMS	✓	✓
Particle Trajectory	✓	✓
Pollutant Species Concentration	-	✓
Pollutant Reduction	-	✓
Evaluation Capability		
Impact of Injection Strategy	✓	✓
Impact of Residence Time	-	✓
Impact of Flue Gas Temperature	-	✓
Impact of Inlet Species Concentration	-	✓
Impact of Sorbent Type	-	✓
Impact of Sorbent Size	-	✓
Impact of Sorbent Porosity	-	✓
Impact of Sorbent Surface Area	-	✓
Impact of Sorbent Flow Rate	-	✓

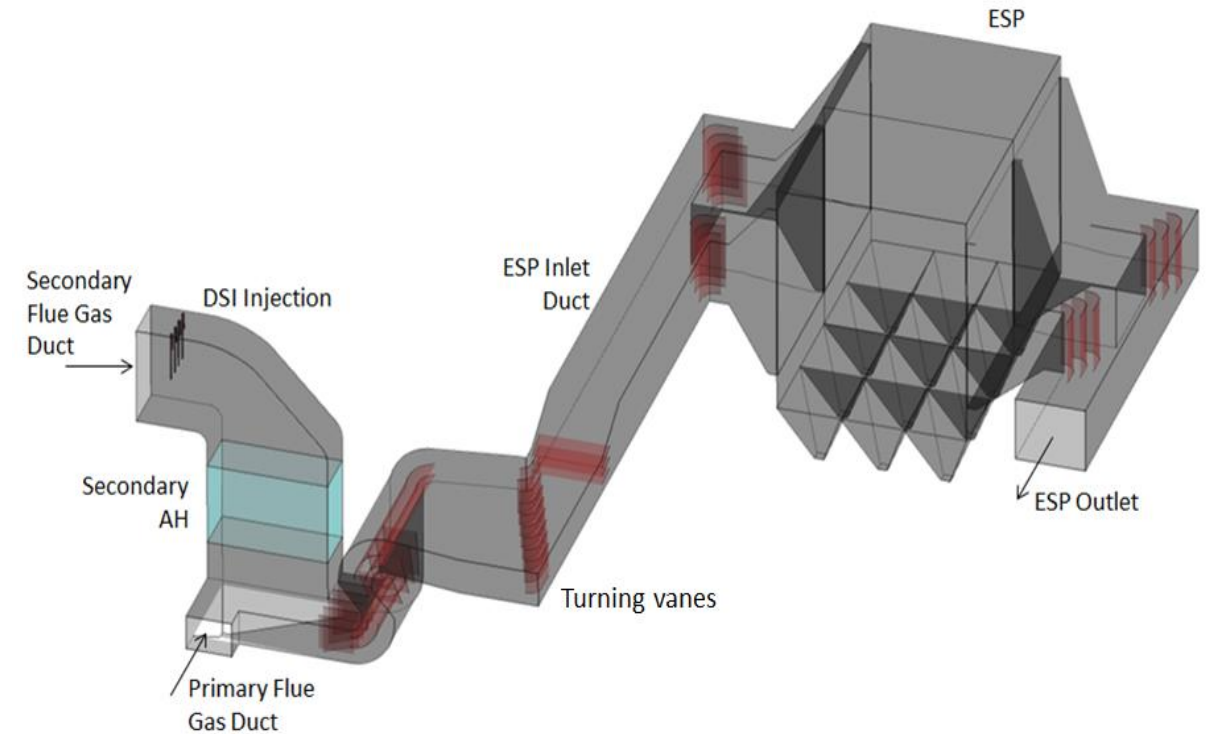
List of All Submodels

- Hydrated Lime + SO₂/HCl
- Hydrated Lime + SO₃
- Trona/SBC + SO₂/HCl
- Trona/SBC + SO₃
- ACI + Hg/HgCl₂

- Each reaction has its own set of kinetic parameters that have been validated against data

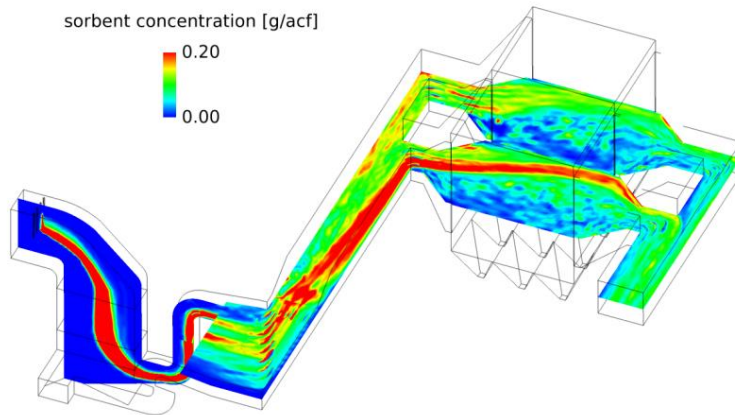
Case Study 1: Hydrated Lime/Trona to Remove SO₂

- Unit
 - Great River Energy's (GRE) Stanton station
 - Nominal 200 MWe front-wall boiler burning PRB coal
 - An annual average SO₂ at approximately 0.55 lb/MMBtu. MATS rule requires 70% SO₂ reduction
- DSI Trial
 - Hydrated Lime and Milled trona, separate trials
 - 4 angle-end vertical injection lances on horizontal duct at secondary AH inlet

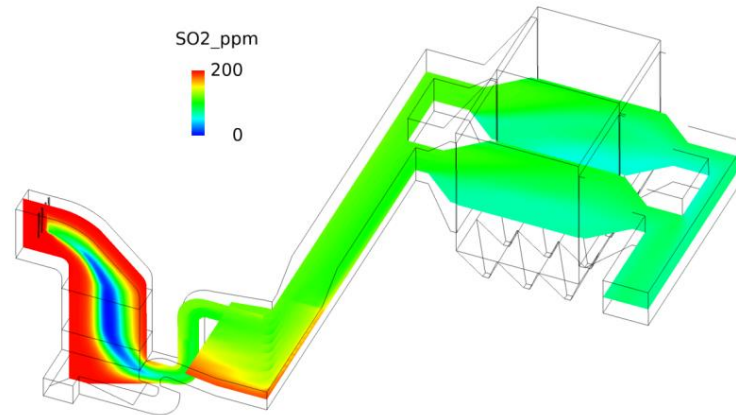


Predicted Sorbent Distribution and Performance

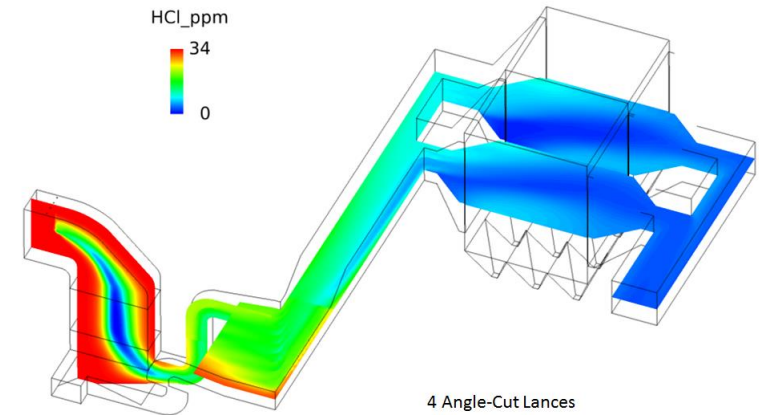
Sorbent Concentration



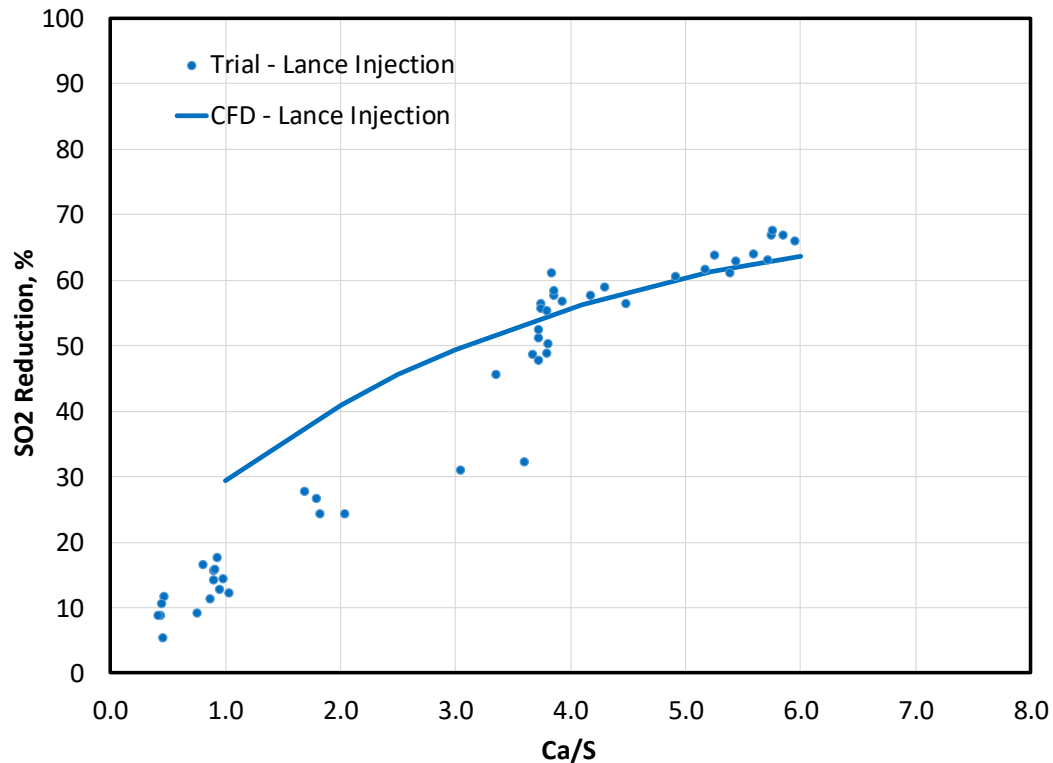
SO2 Concentration



HCl Concentration

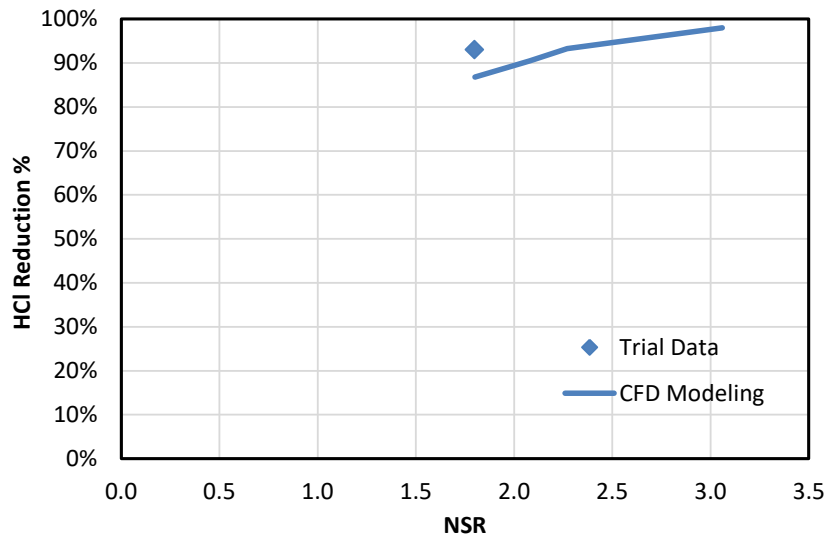
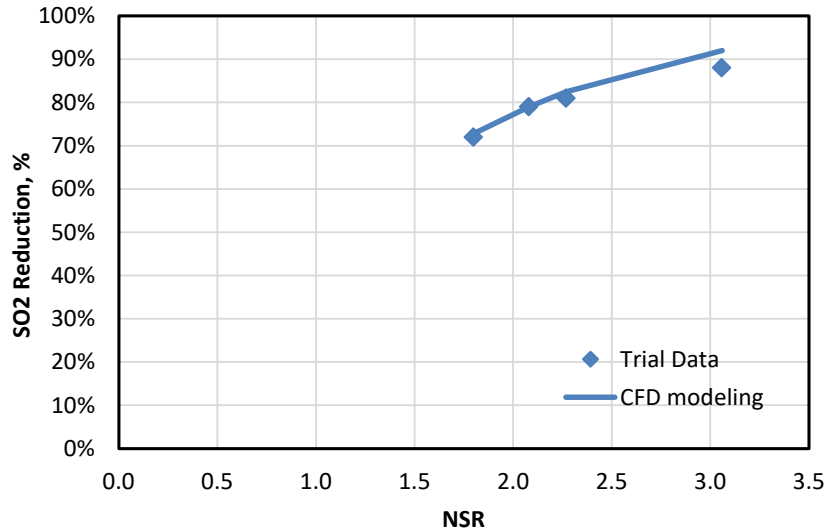


Model Validation – Hydrated Lime



- Between 60%-70% SO₂ reduction at Ca/S of 5-6 can be achieved with Enhanced Hydrated Lime.
- The chemistry model well represents the trend of SO₂ reduction at higher Ca/S, but over predicted the SO₂ reduction at Ca/S below 3.5.

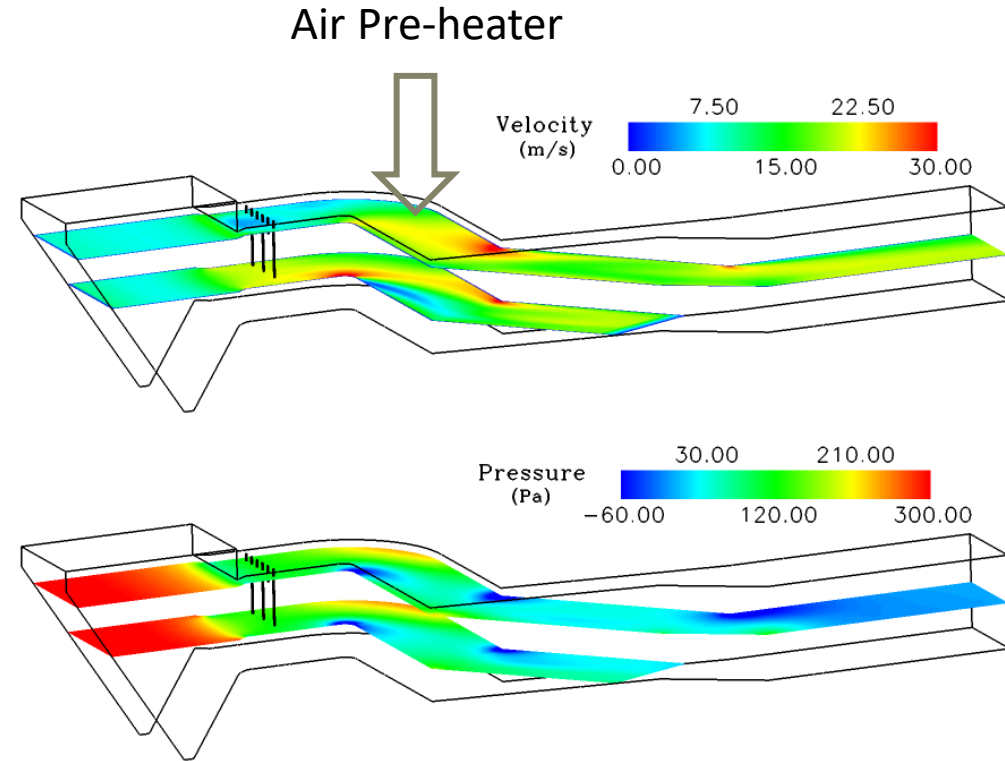
Model Validation - Trona



- Over 72% SO₂ reduction at NSR of 1.8. As NSR increased to 3.1, 88% SO₂ reduction was achieved
- 92% HCl reduction was achieved with trona injection at an NSR of 1.8
- The chemistry model well represents the trend of SO₂ reduction as function of NSR
- There is a discrepancy of HCl between measurement and prediction, although one HCl data point was obtained

Case Study 2: Hydrated Lime to Remove SO₃

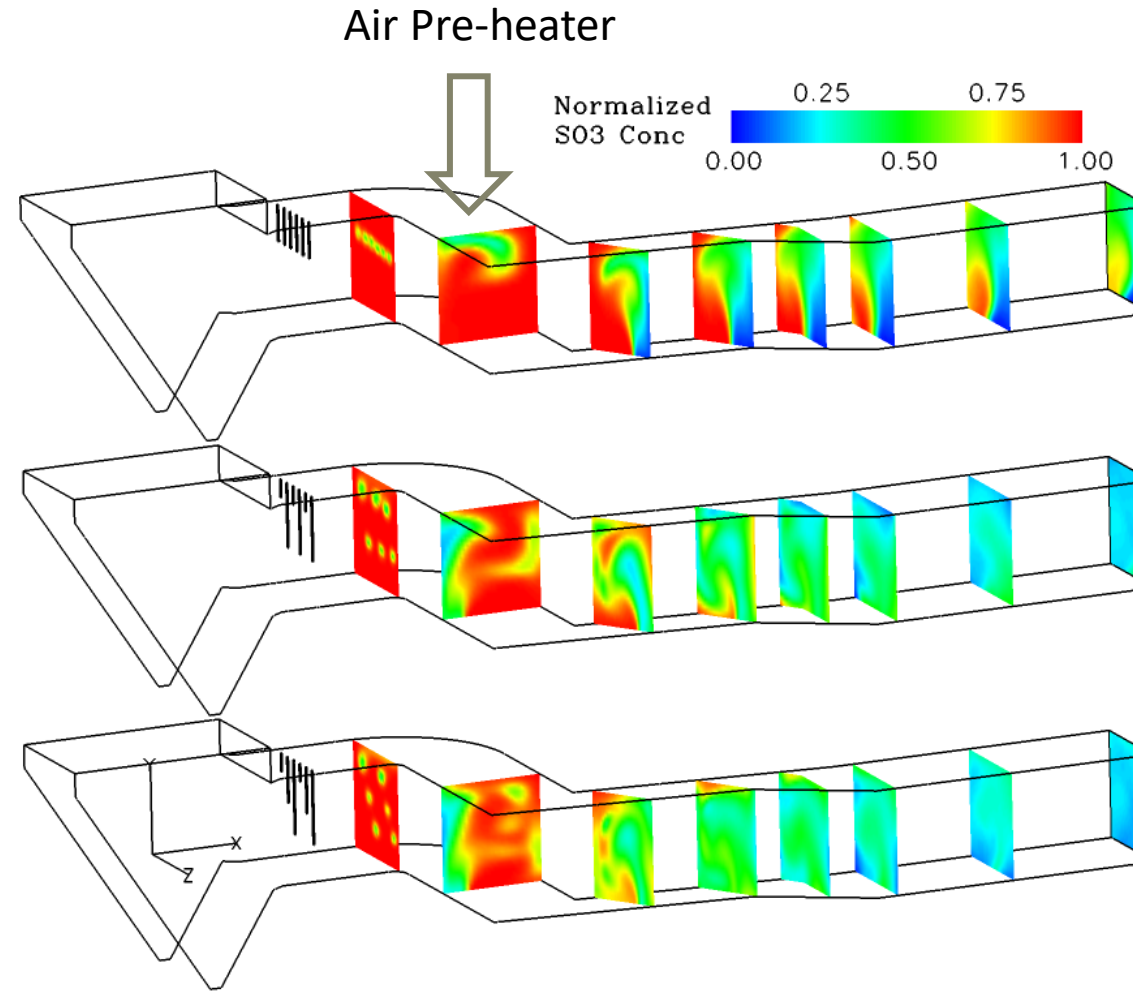
- Unit
 - 450 MW coal-fired boiler
- Velocity and Pressure Profile
 - Duct from air pre-heater inlet to ESP inlet
 - ¼ flue gas flow from a 450 MW tangentially-fired boiler
- Objective
 - Use model to optimize lance layout and SO₃ predictions



Liming Shi, Guisu Liu, Lewis Benson, "An Enhanced CFD Based Chemistry Model for SO₃ Mitigation by Dry Sorbent Injection", Paper 117, MEGA Symposium, Baltimore, MD, August, 2012

SO3 Reduction at Different Lance Depth

- Case 1: 1-depth
- Case 2: 2-depth
- Case 3: 3-depth



SO3 Red. %

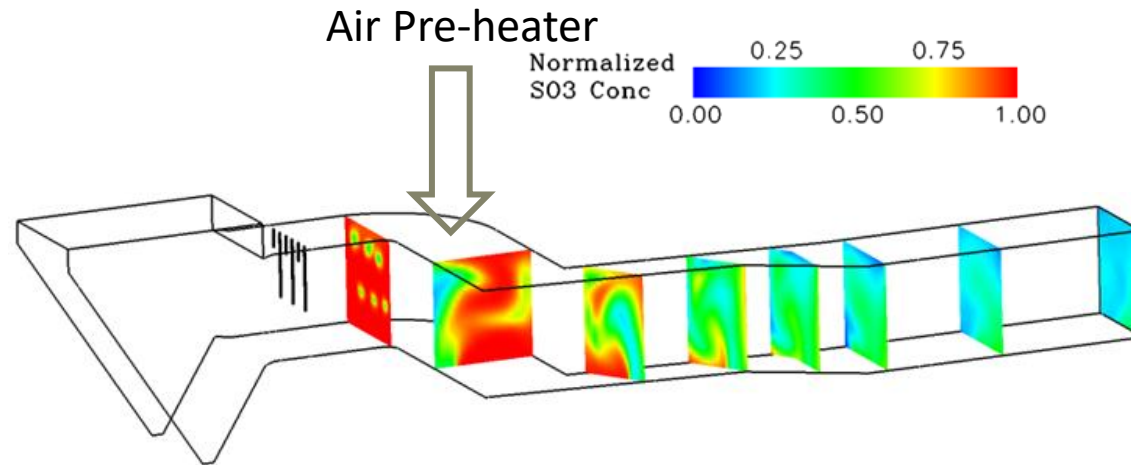
61%

75%

77%

SO3 Reduction at Different Number of Lances

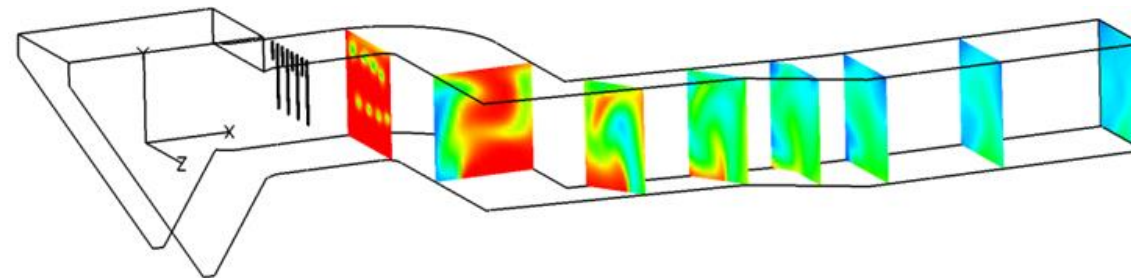
- Case 2: 6-lances



SO3 Red. %

75%

- Case 4: 8-lances

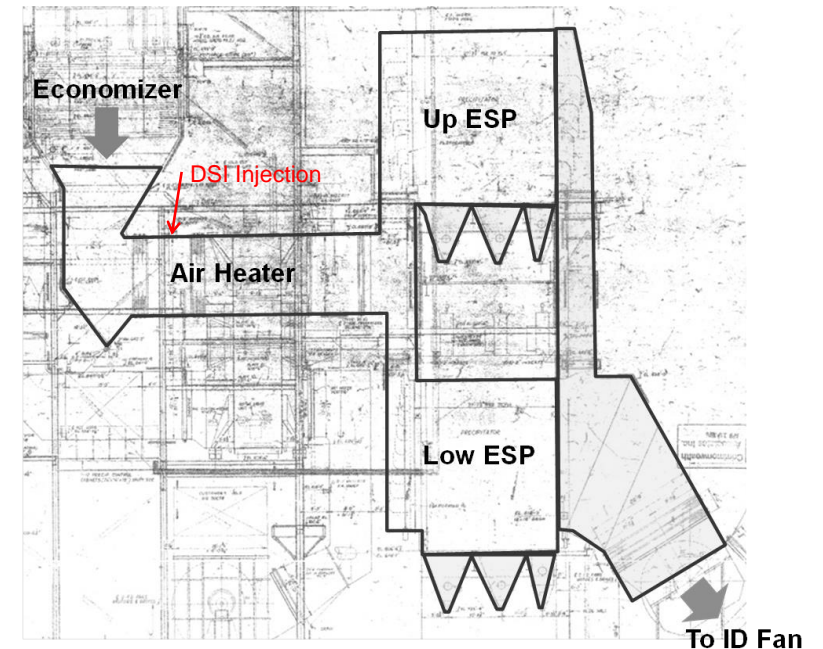


77%

Case Study 3: Trona to Remove SO₂/HCl

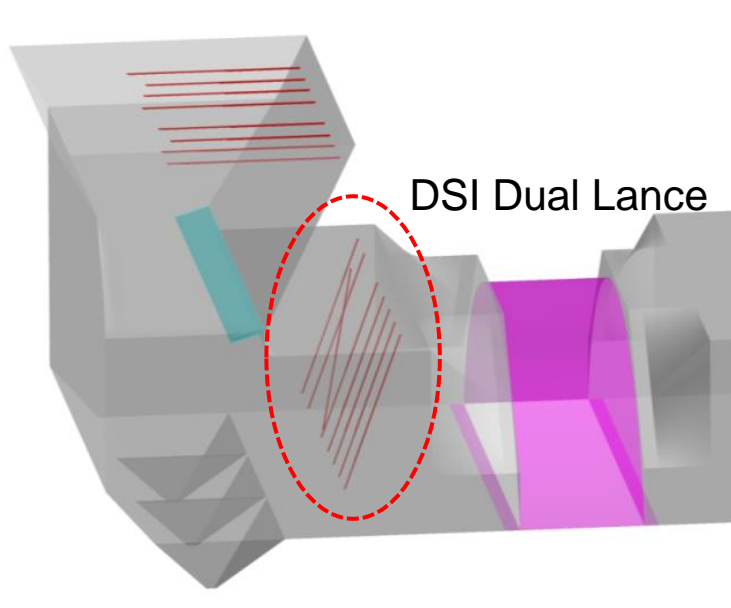
- Sponsored by DTE
- Unit
 - 370 MWe front-wall boiler burning PRB coal
 - Inlet HCl: 10 ppm
 - Inlet SO₂: 400 ppm
 - DSI trona injection to remove HCl and SO₂
 - ACI to remove Hg
- DSI
 - Milled trona
 - 8 dual injection lances per duct
 - Right upstream of AH
- Project Goal
 - Use the model to explore performance improvement

Presented at: XV International Conference on Electrostatic Precipitation (ICESP), October 9- 11, 2018 - Charlotte, North Carolina



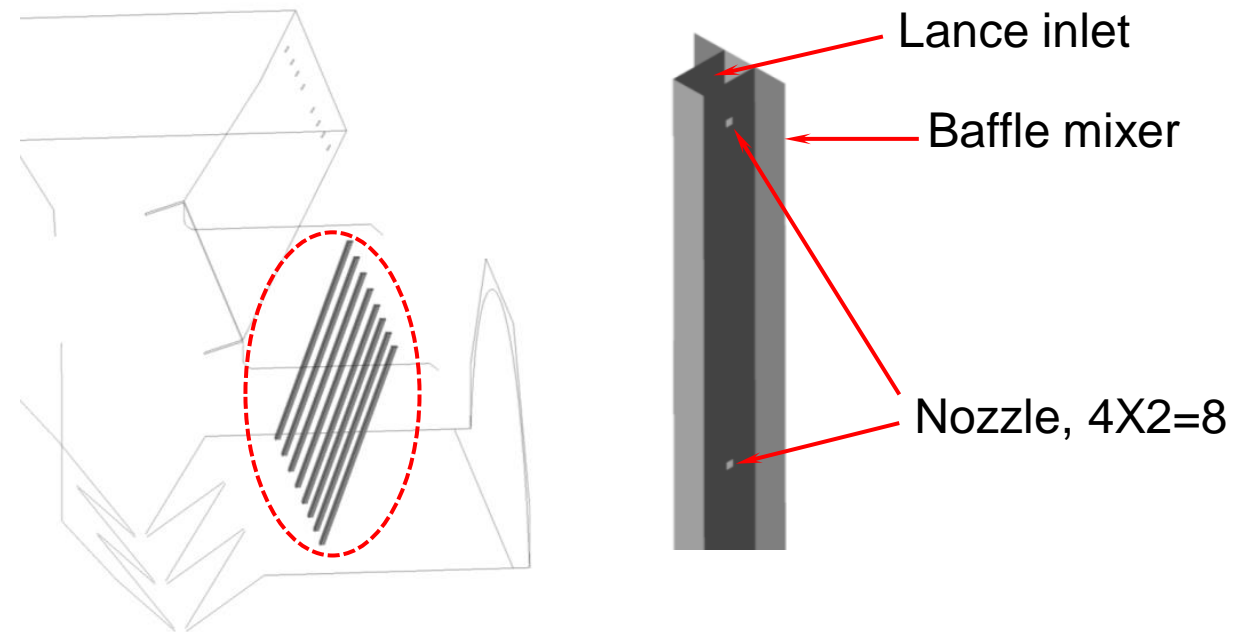
Base Injection Lance vs. Special Lances

Base Injection Lance



- Each lance has **two exit openings** at different penetration distance

Multi-Nozzle Dispersion Lance



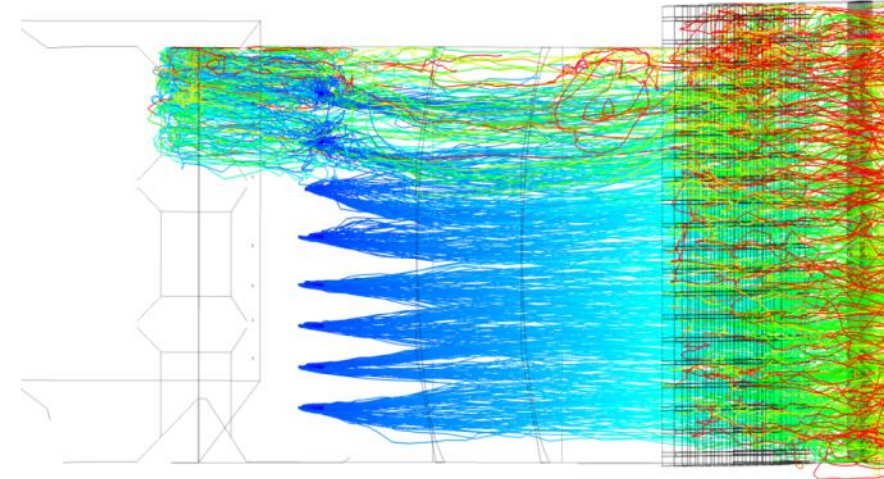
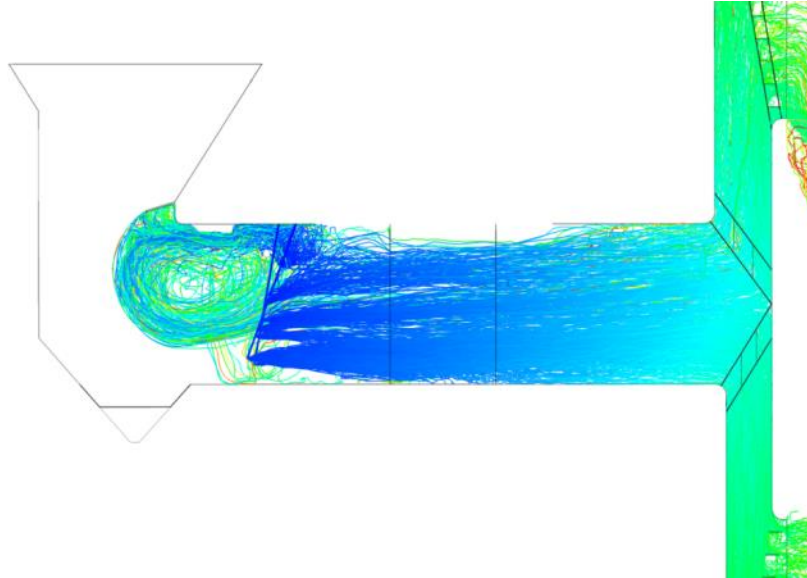
- Each lance has 4X2=8 exit openings
- Baffle mixer to enhance downstream turbulence

Field Data vs. Modeling Results – Base Lance Design

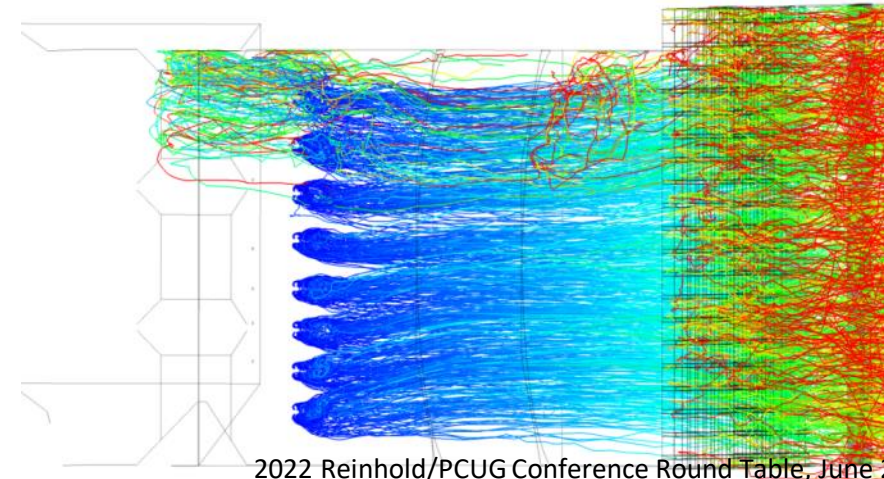
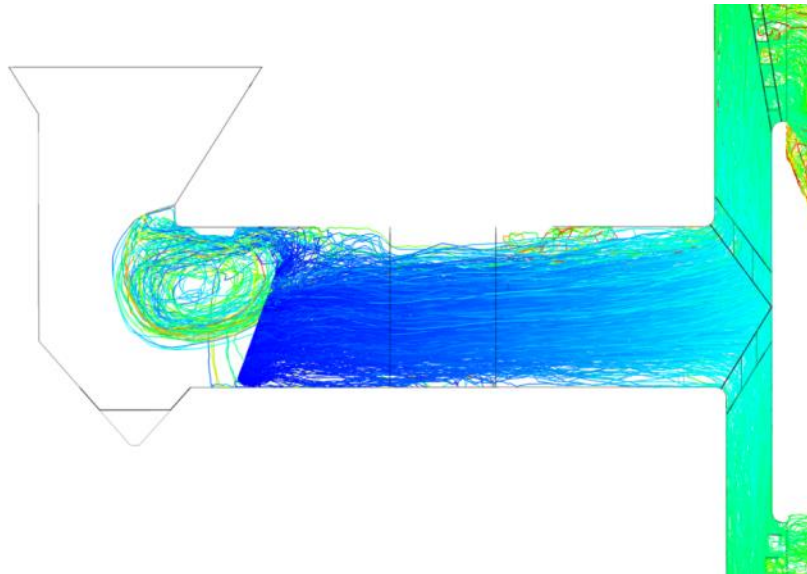
		Field Test Data	CFD Prediction
NSR _{SO2}	-	0.47	0.47
SO ₂			
In	ppmv @3% O ₂	400	357
Out	ppmv @3% O ₂	312	273
SO2 Reduction	%	23.0%	23.9%
HCl			
In	ppmv @3% O ₂	10.2	9.26
Out	ppmv @3% O ₂	1.16	1.33
HCl Reduction	%	89%	84%

Particle Trajectory

Base Lance

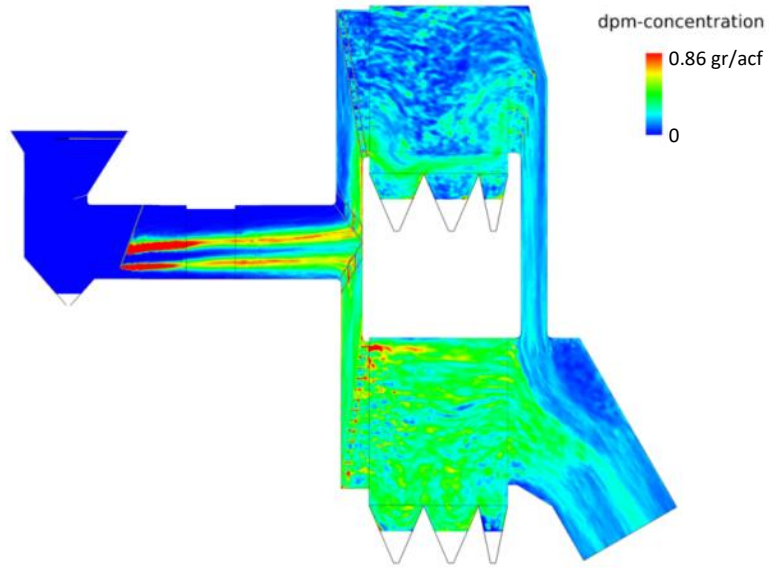


Multi-Nozzle Lance

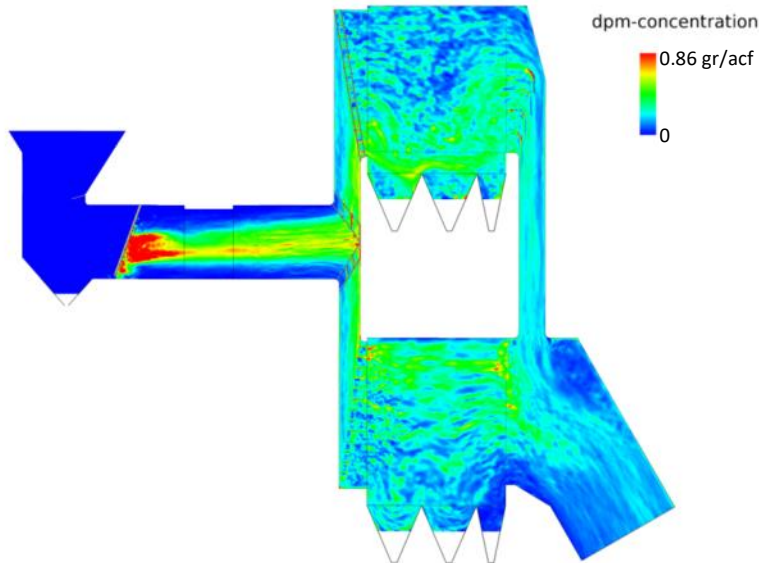


Sorbent Concentration

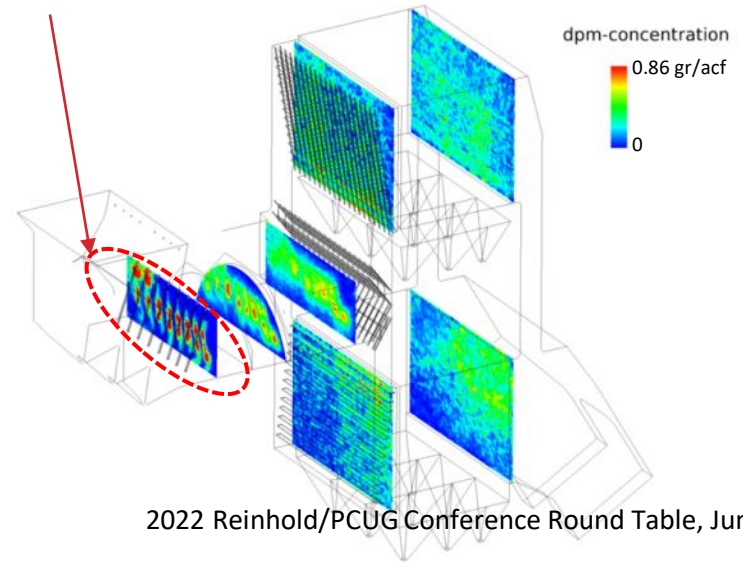
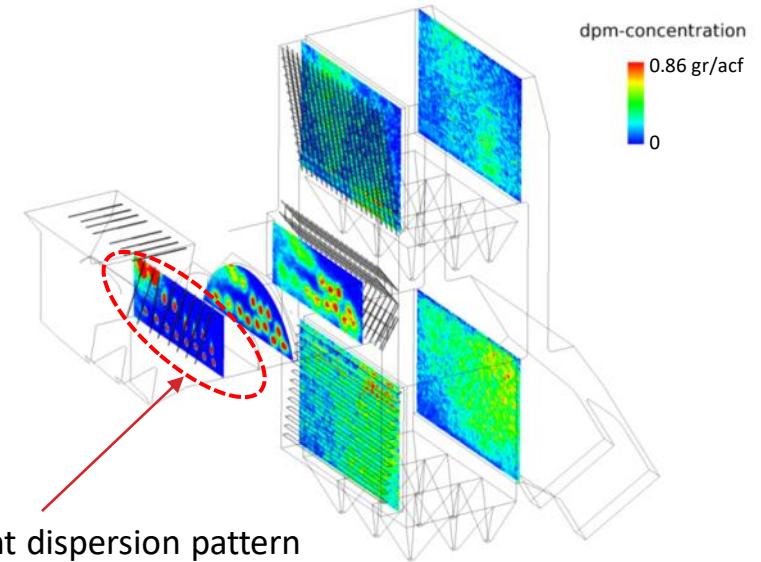
Base Lance



Multi-Nozzle Lance

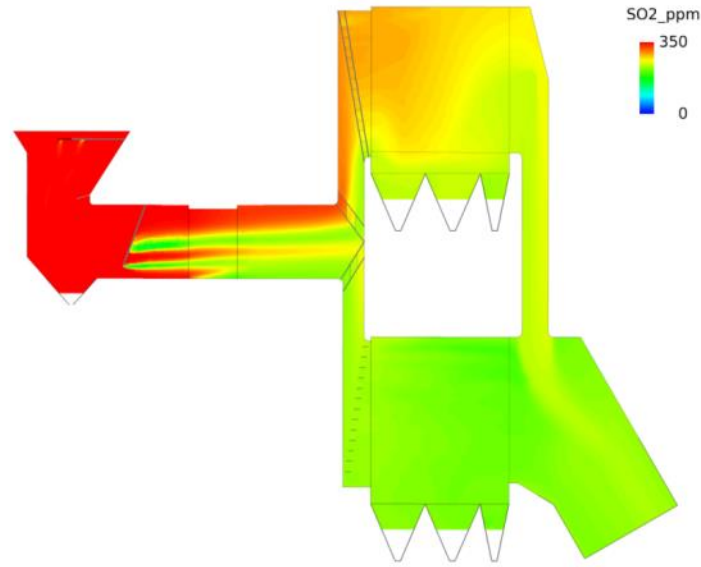


Different dispersion pattern between two lance design

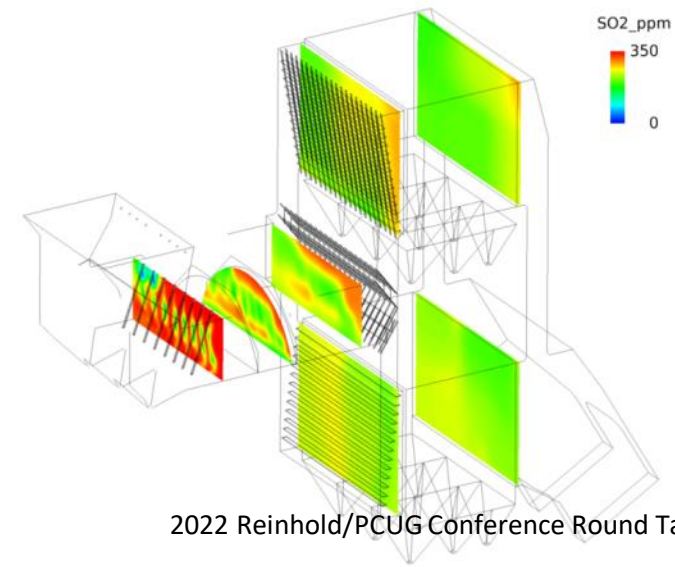
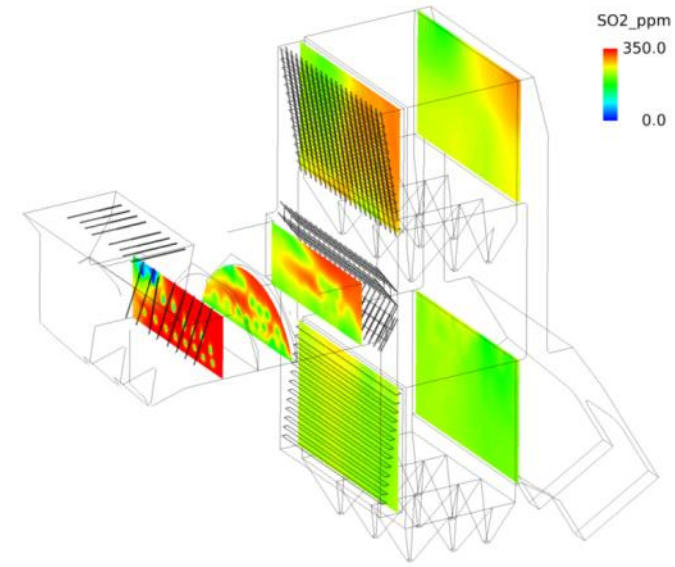
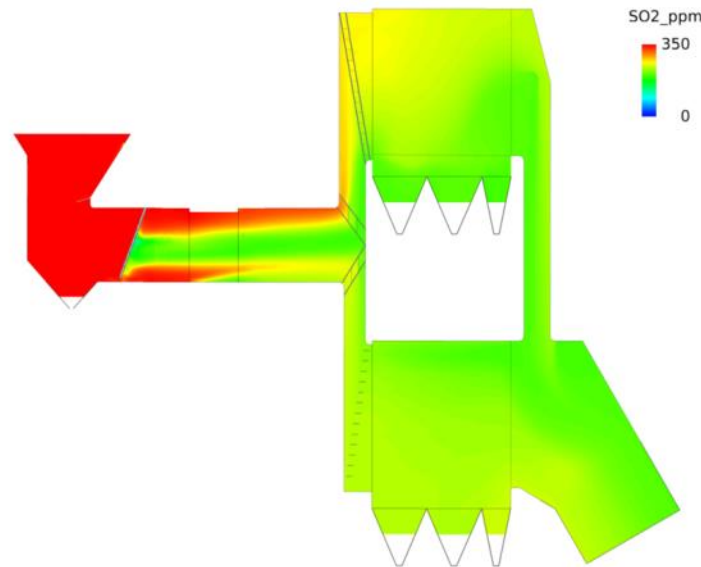


SO2 Distribution

Base Lance

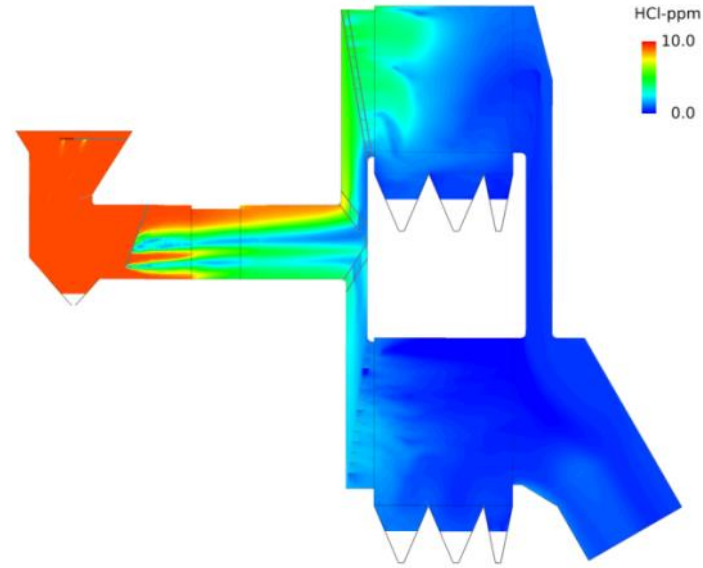


Multi-Nozzle Lance

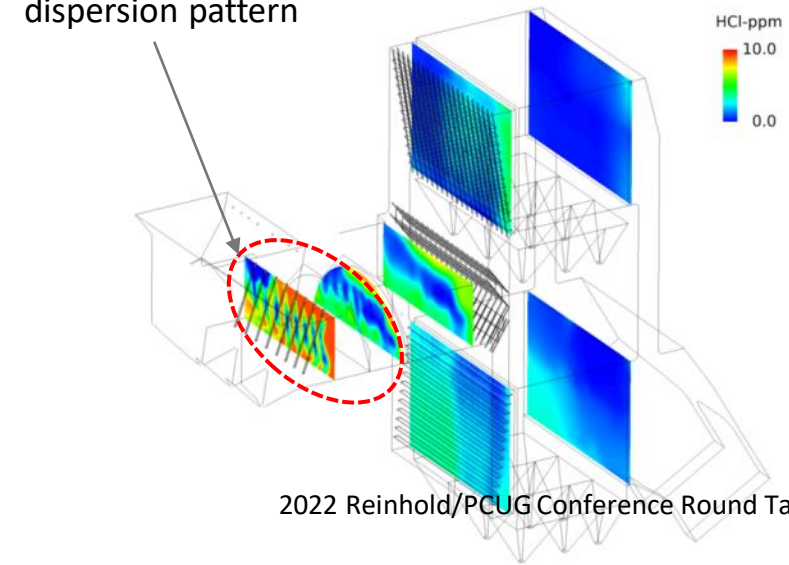
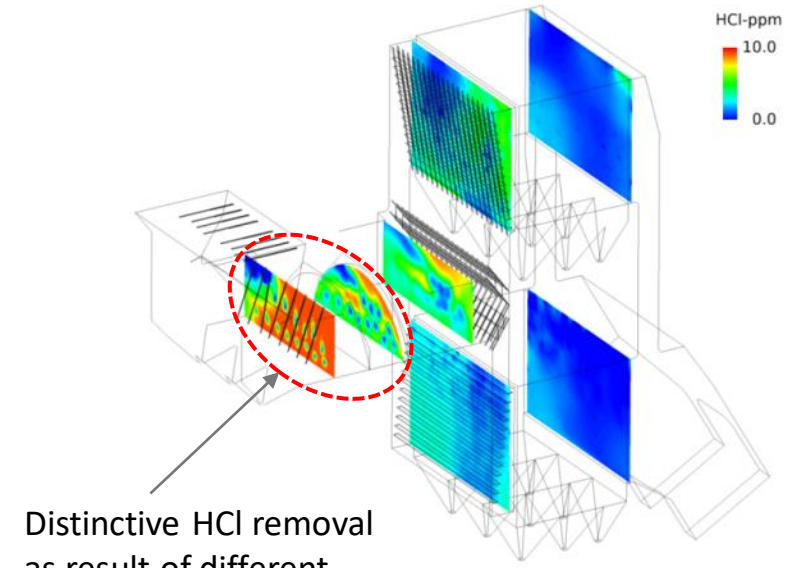
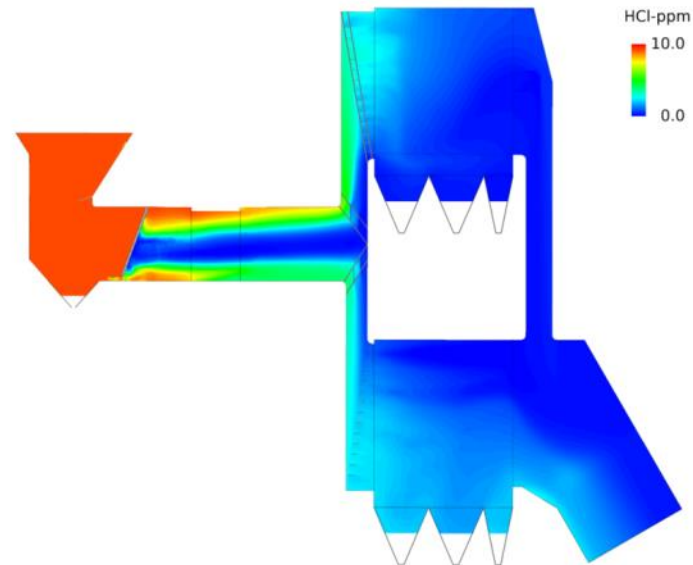


HCl Distribution

Base Lance

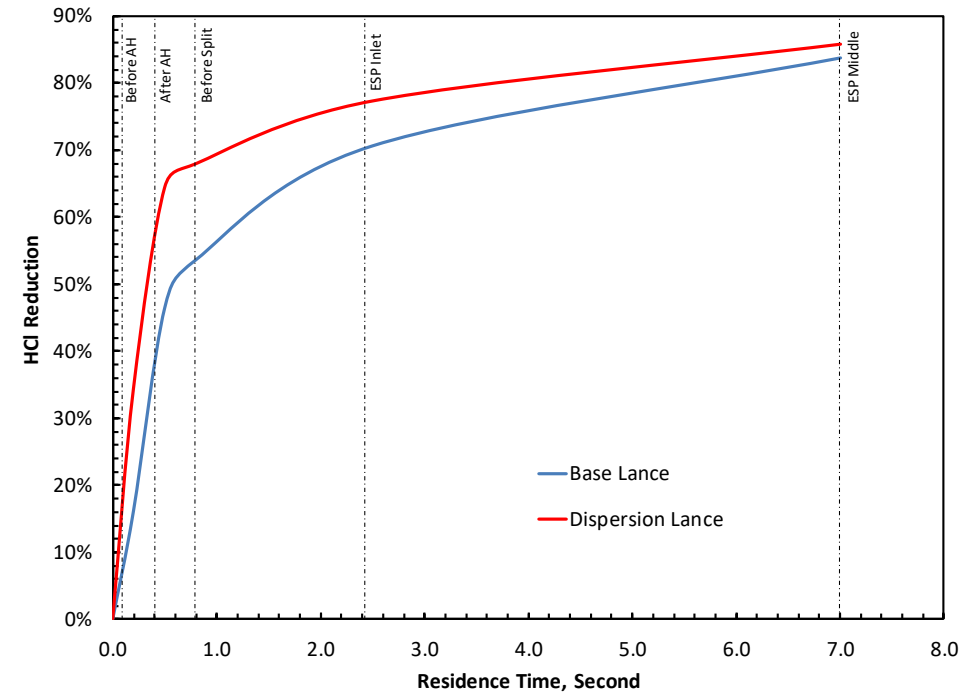
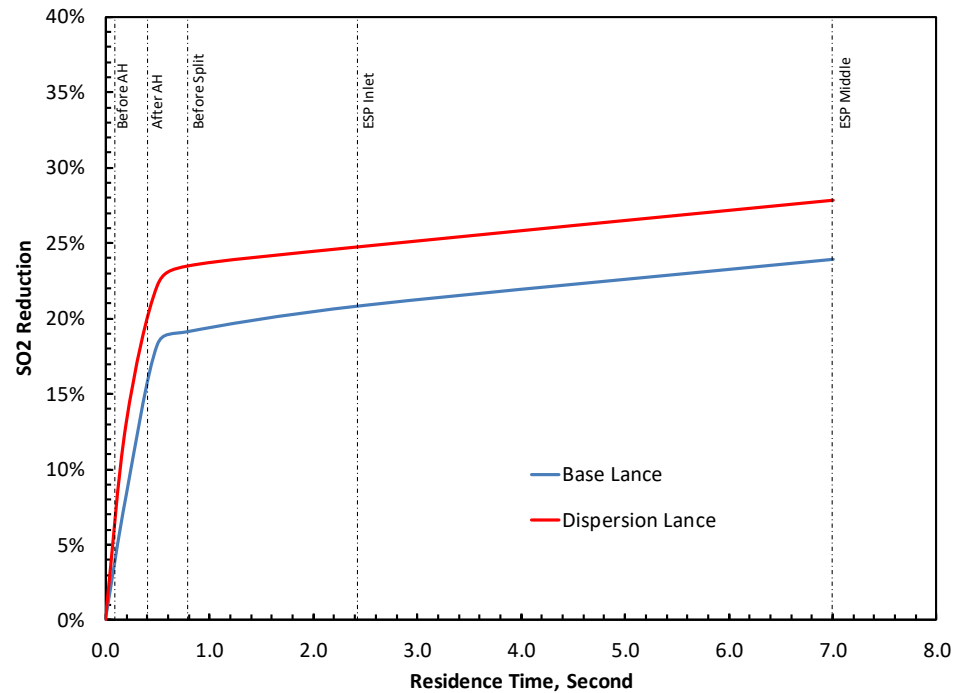


Multi-Nozzle Lance



Distinctive HCl removal
as result of different
dispersion pattern

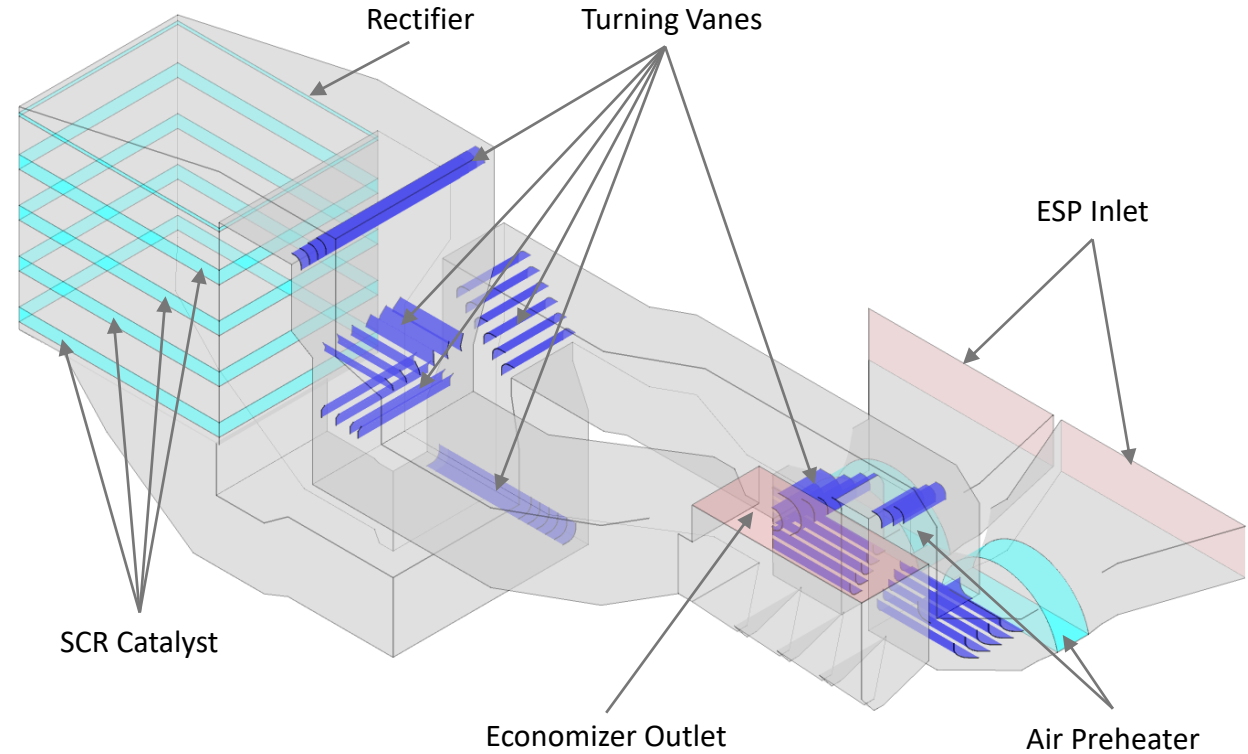
Predicted SO₂ and HCl Reduction



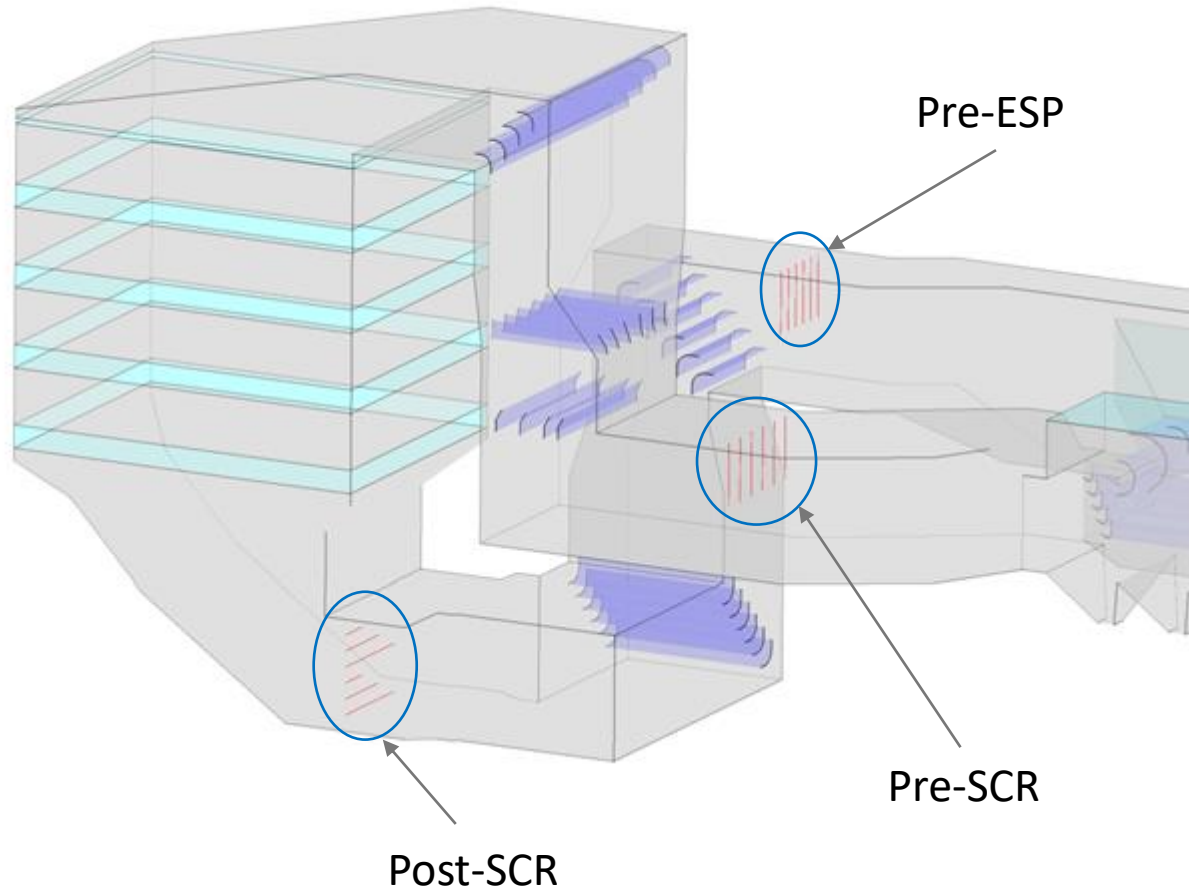
- Special designed dispersion lances enhanced mixing of sorbent particles with flue gas than standard lance
- The enhanced mixing/dispersion resulted in improvement of trona on both SO₂ and HCl removal
- The improved trona performance further resulted in roughly **15% of sorbent savings** while achieving the same HCl and SO₂ emission level.

Case Study 4: SBC to Remove SO₂ at a 330-MW Coal Boiler

- 330 MWe boiler burning PRB coal
- SCR to remove NO_x
- ESP to remove particulates
- DSI w/SBC to remove SO₂
 - Inlet SO₂: 0.45 lb/MMBtu
 - Target SO₂ reduction: 60%

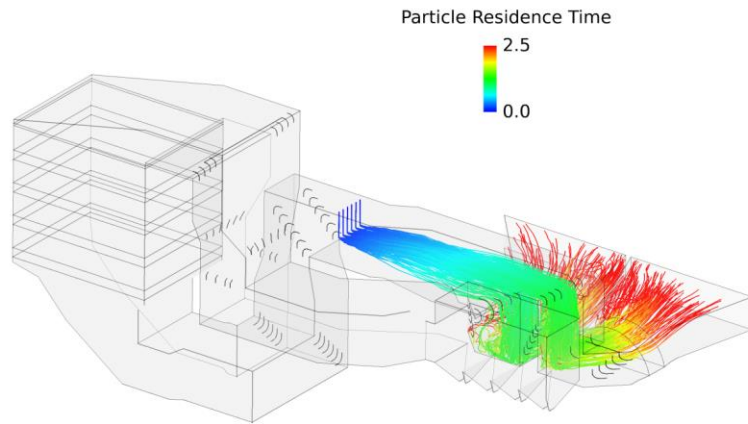


DSI Location Plan for CFD Evaluation

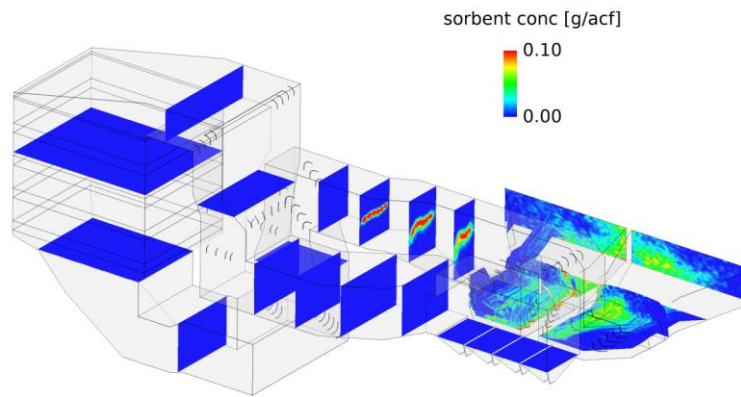


Pre-ESP Injection

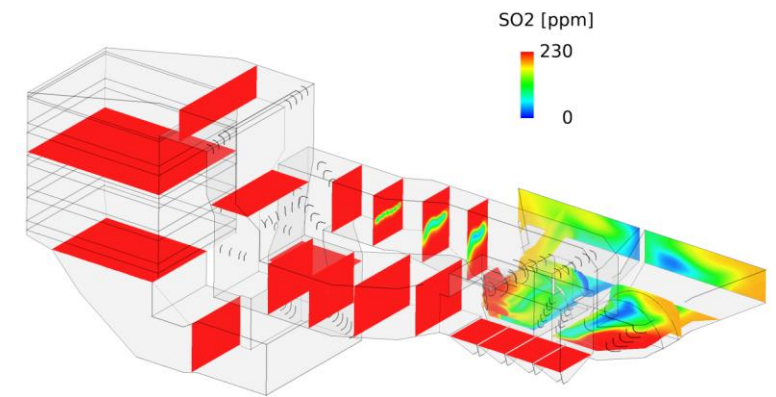
Particle Trajectory



Sorbent Concentration



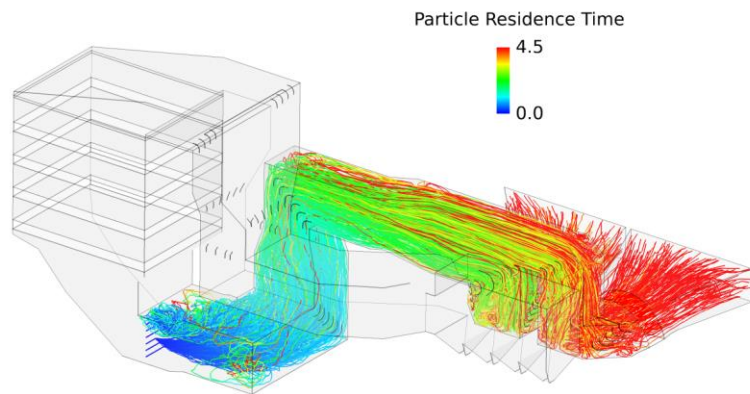
SO2 Concentration



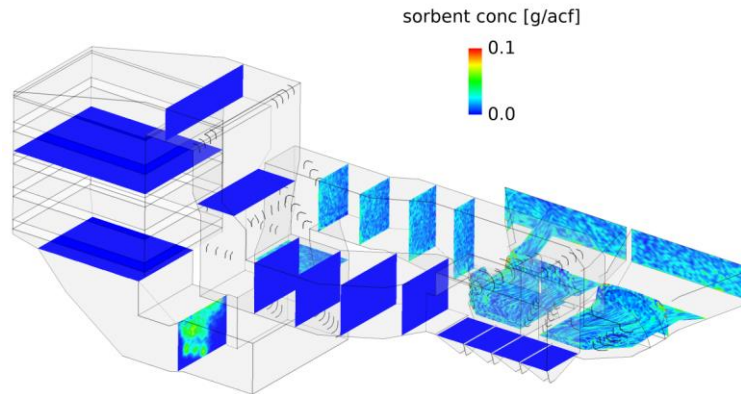
Predicted SO2 Reduction at
0.71 NSR: **34%**

Post-SCR Injection

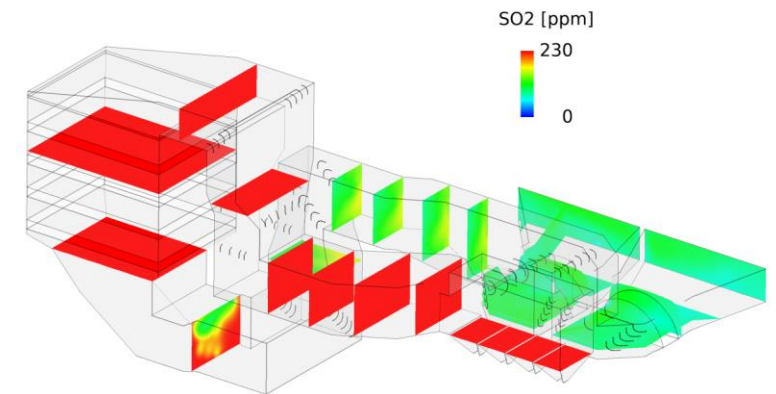
Particle Trajectory



Sorbent Concentration



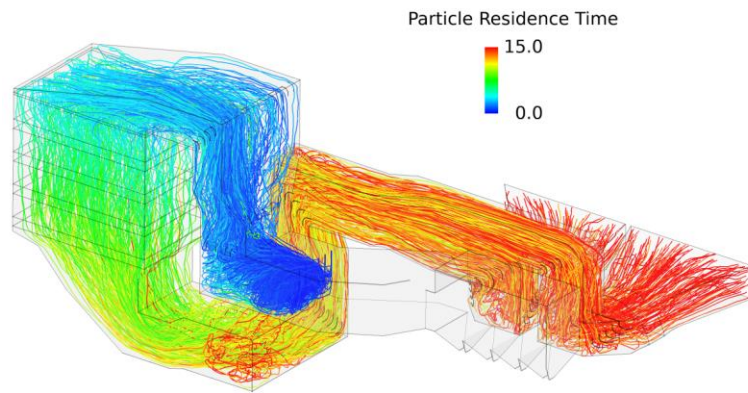
SO2 Concentration



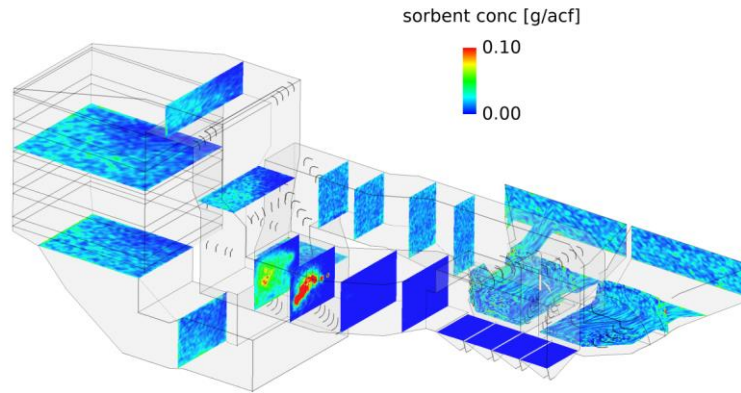
Predicted SO2 Reduction at
0.71 NSR: **54%**

Pre-SCR Injection

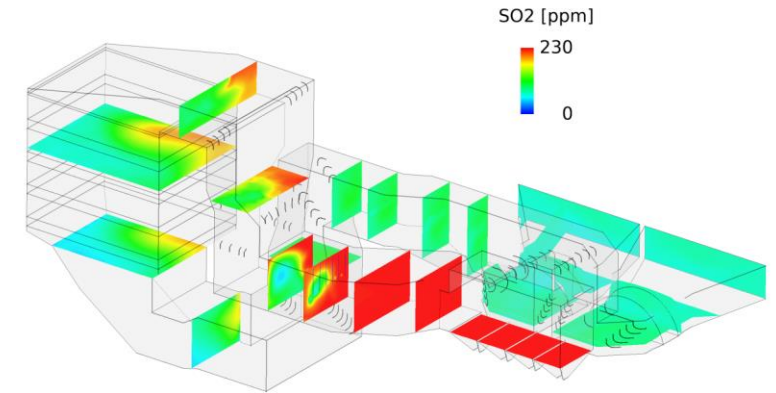
Particle Trajectory



Sorbent Concentration

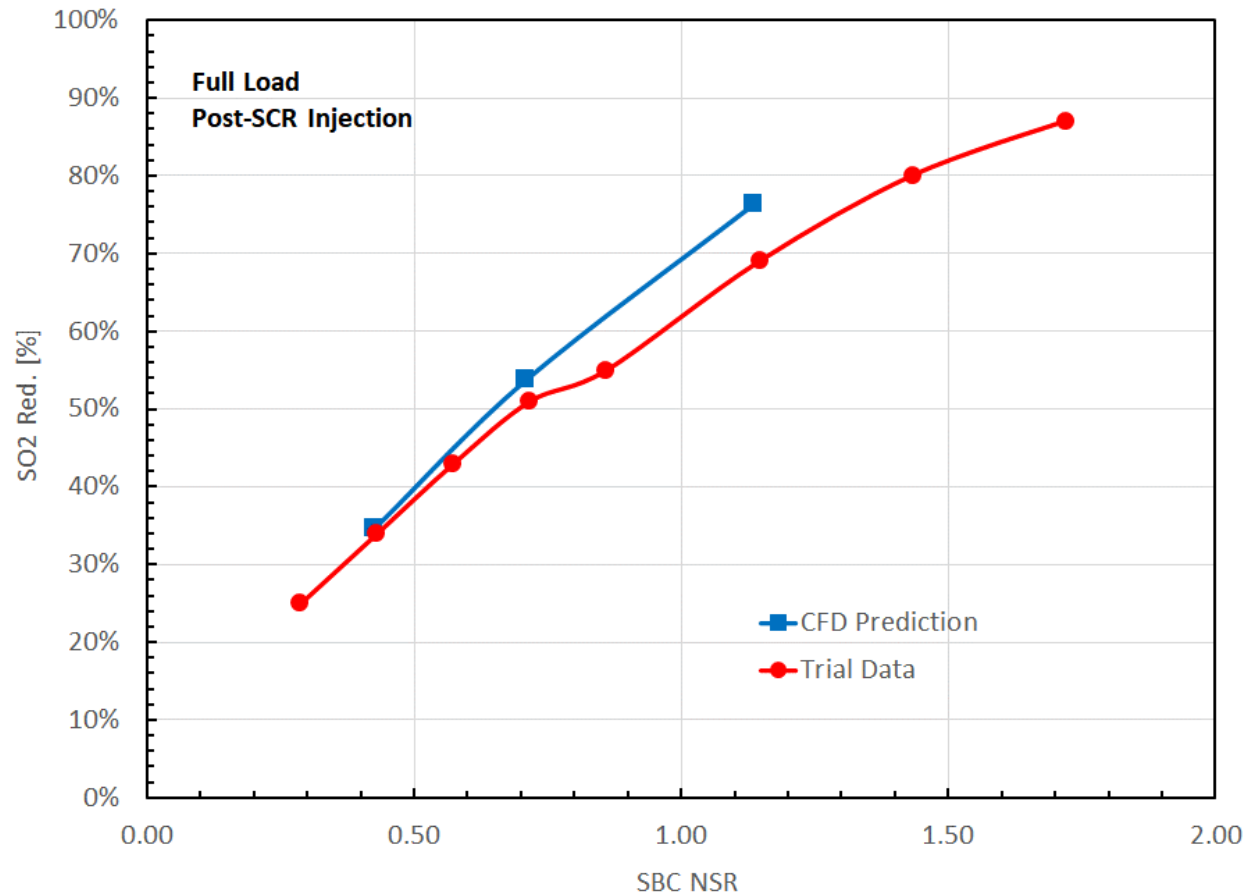


SO2 Concentration



Predicted SO2 Reduction at
0.71 NSR: **64%**

Comparison with Trial Data

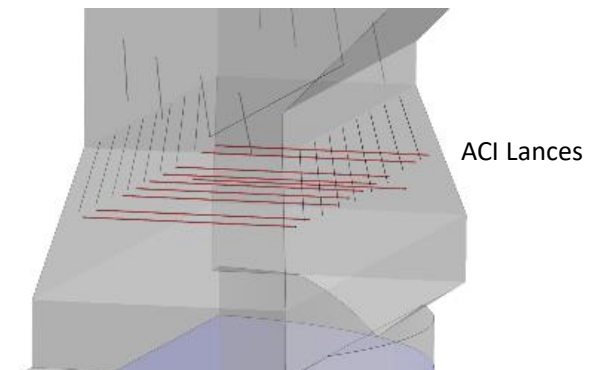
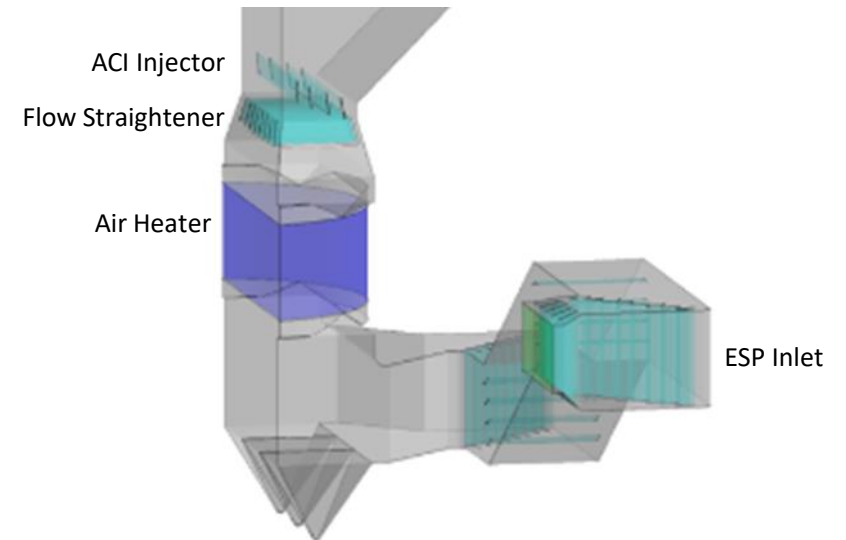


- Trial was successful – it achieved the SO2 reduction goal
- DSI decreased opacity
- SCR outlet injection is the better option
- Trial performance was well predicted by CFD simulations with chemistry submodels.

Case Study 5: ACI to Remove Hg at a 750-MW Coal Boiler

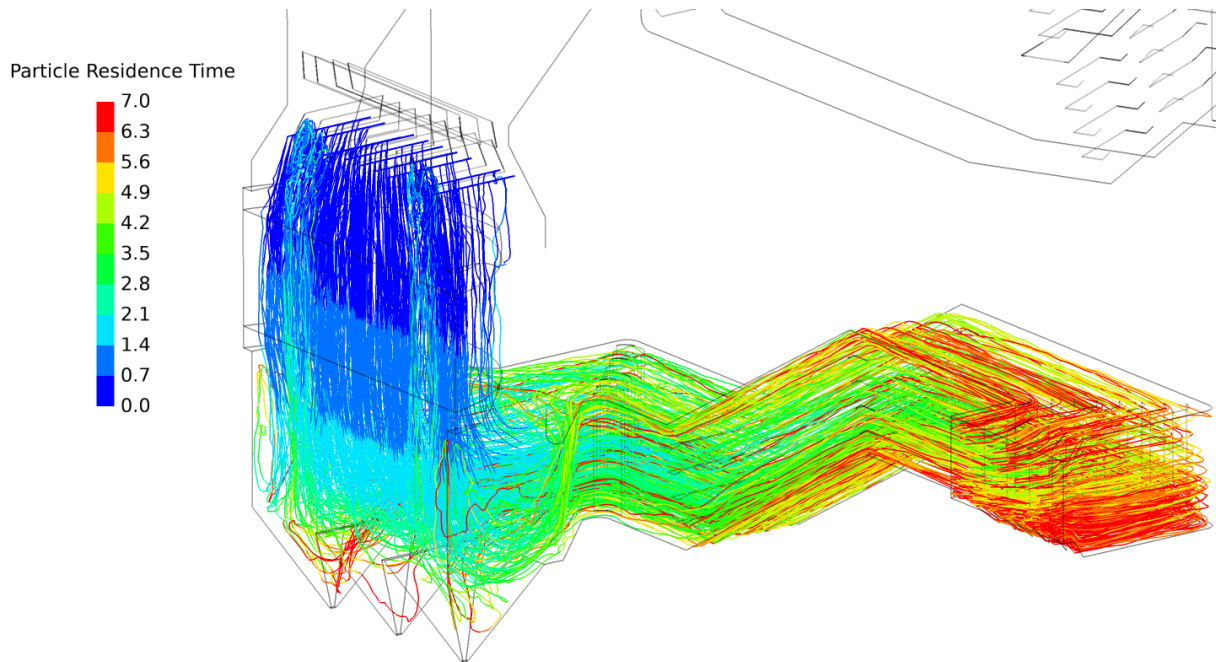
- 750 MWe coal-fired boiler burning PRB coal
- Inlet Hg emission: 6.04 lb/TBtu
- ACI Injection before AH: 350 lb/hr (3.46 lb/MMSCF)
- Multi-nozzle lances
- Stack Hg: 0.7 lb/Tbtu
- Hg reduction: 88.4%

- CFD model has been developed to explore optimization strategy to improve performance

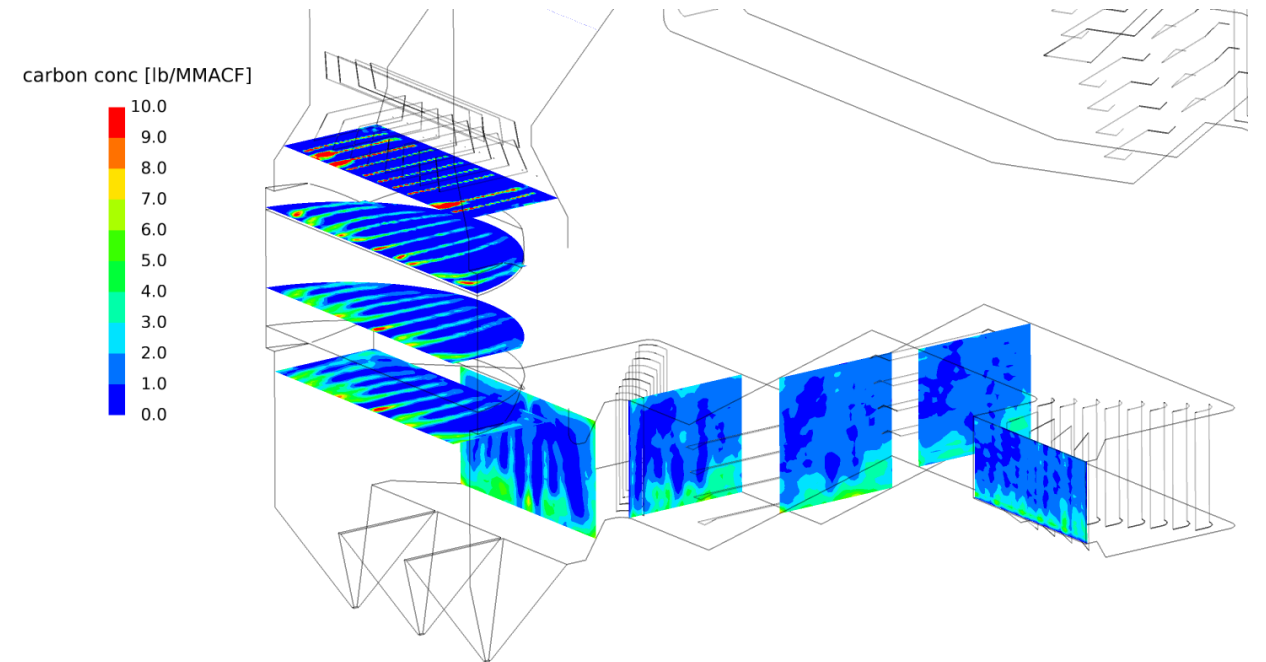


ACI Particle Dispersion

Particle Trajectory



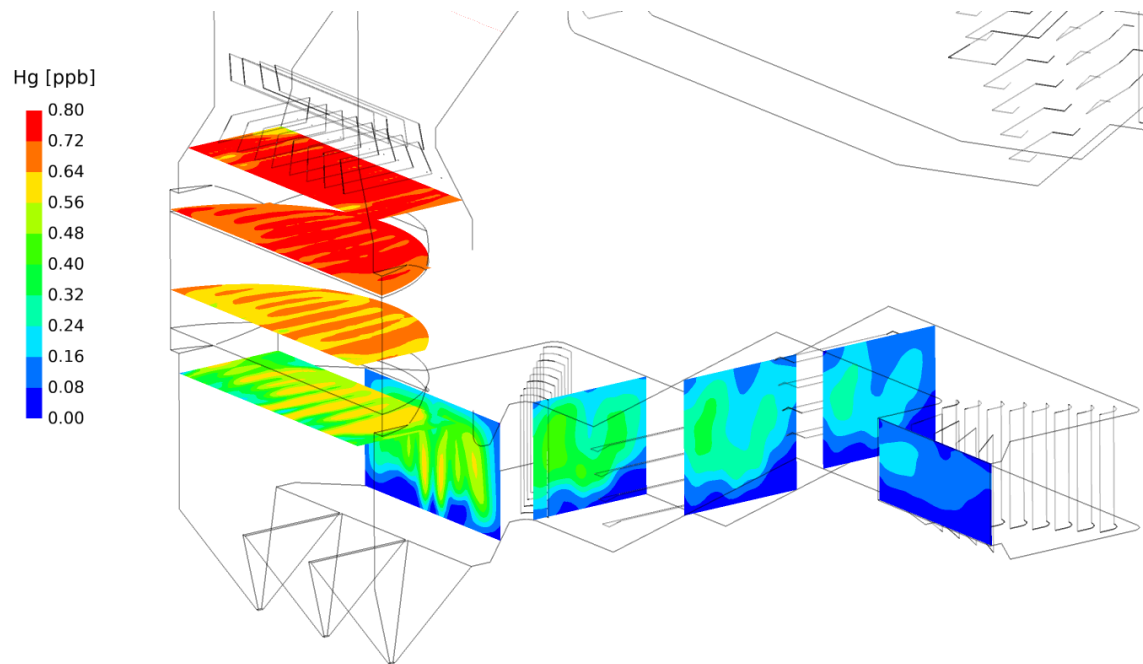
Carbon Concentration



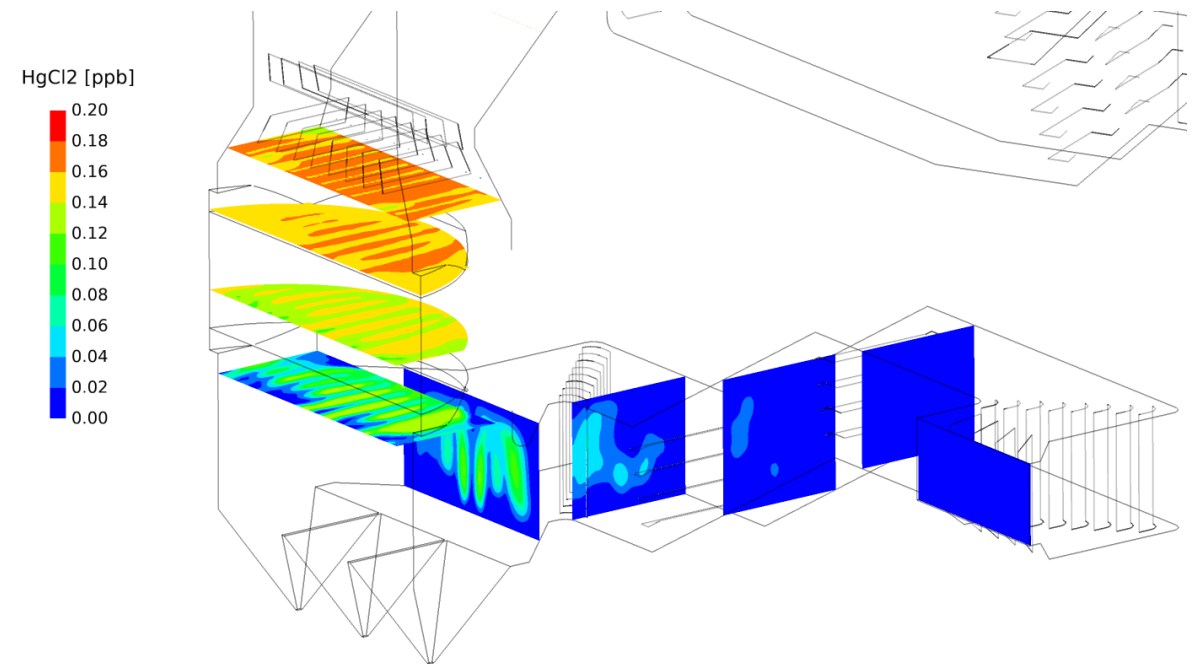
Good mixing however,
Gaps Still Present
Carbon Biased to the Bottom

Elemental and Oxidized Hg

Elemental Hg



Oxidized Hg

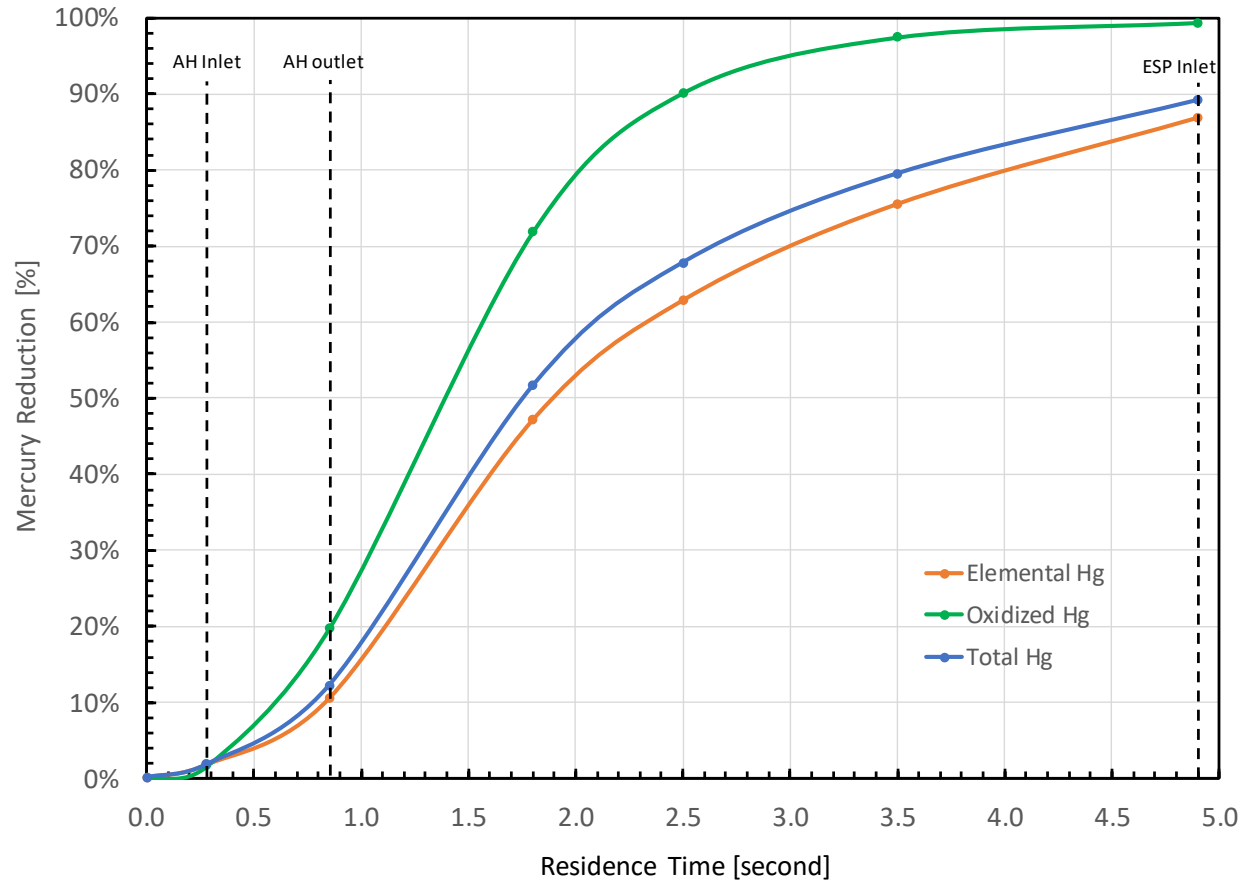


Hg Reduction Performance: Testing vs. Prediction

	Unit	Field Data	CFD Prediction
Hg Reduction – elemental	[%]	-	86.9%
Hg Reduction – oxidized	[%]	-	99.4%
Hg Reduction - total	[%]	88.4%	89.2%

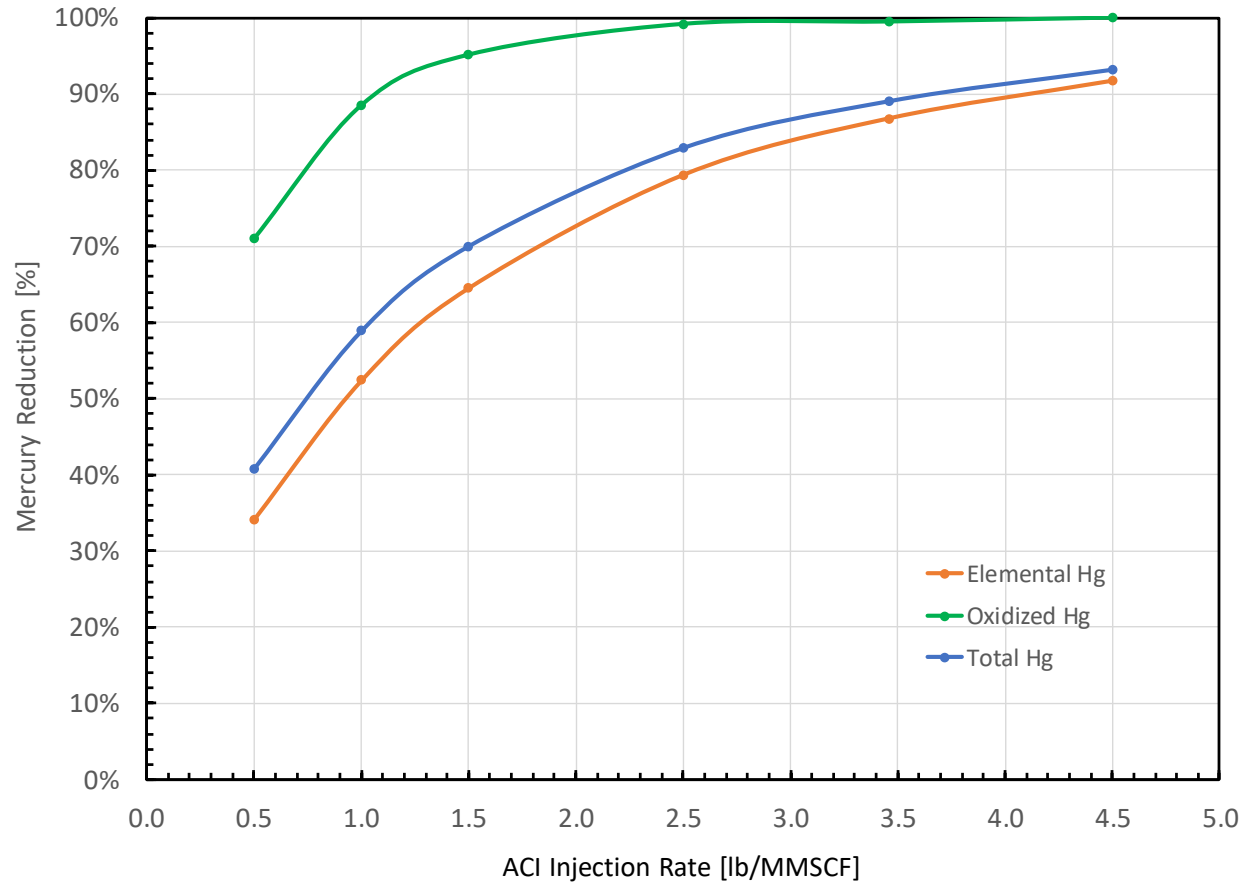
Note: the elemental and oxidized Hg split ratio is 82:18 from reference.

Predicted Performance: Hg Reduction vs. Time



- Due to high temperature, essentially no mercury reduction occurred before AH. Carbon starts absorbing both elemental and oxidized mercury during air preheater and continued throughout the duct till ESP.
- Carbon reacts with oxidized mercury at a faster rate than elemental mercury.

Predicted Performance: Hg Reduction vs. Injection Rate



- The performance curve of **Hg** reduction vs. ACI injection rates was created by simulating cases with different carbon injection rate.

Advantages of Chemistry-Based CFD Model

- Simultaneously evaluate the combined impact of **time**, **temperature** and **mixing**, and their impact on each other and the ultimate results
- Help utility operators, Engineering designers & Equipment suppliers
 - Troubleshoot, optimize duct and injection, retrofit recommendations
 - Develop performance curve for unit operation
 - Understand flow and mixing, internal device impact, injection optimization to maximizing mixing and performance
 - Optimize equipment size, performance enhancement through mixing
- Help sorbent suppliers
 - Address the impact of sorbent size, surface area, porosity
 - Develop high performance sorbent

Experiences with Evaluation of DSI Mixing Devices

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- Lances with spreader or deflector at exit
- Special designed lances
- Multi-nozzle lances
- Lance-less injectors
- Static mixer (or delta wing)
- Baffle plates
- Proprietary & Novel Designs

Summary

- A suite of chemistry submodels have been developed using a single particle reaction mechanism that include simultaneous chemical reaction and diffusion.
- The submodels have been integrated with CFD code to become a unique and powerful tool that is very valuable to anyone designing or operating a DSI or Activated Carbon Injection System.
- These submodels have been validated and applied to engineering projects to develop and/or optimize DSI and ACI systems to improve performance and/or reduce chemical cost.
- Throughout all projects, we have learned that improvement could be made by addressing time, temperature or mixing. And the improvement strategy is very process-specific. These models can be used to explore the improvements in a more timely and cost-effective manner than previous methods.

Thank You!

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