

# Impact of CFD Enhancements for Modeling Coal-fired Boiler Oxy-Combustion Retrofits

Bradley Adams, Brydger Van Otten

---



# Overview

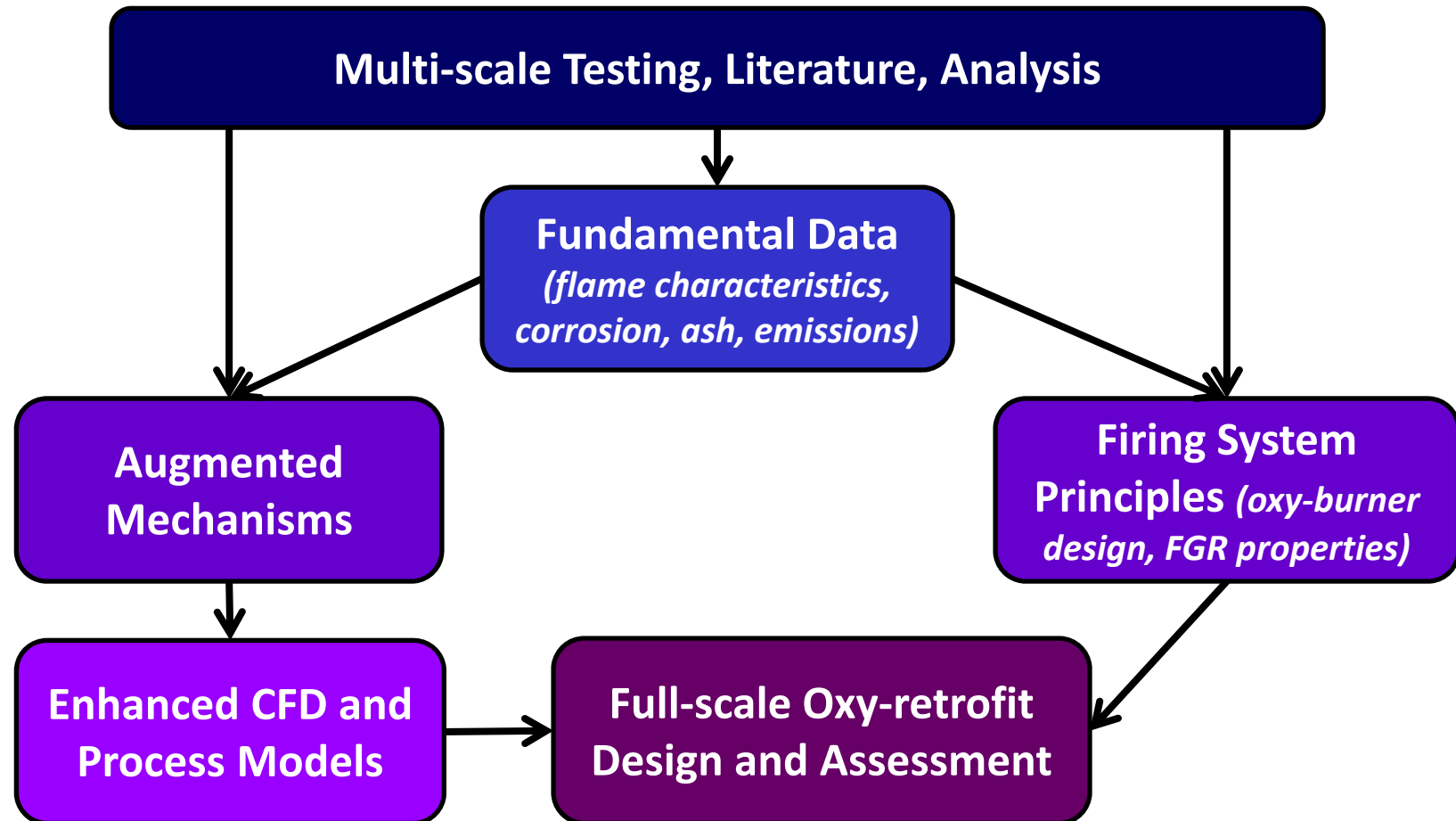
---

- ☐ Retrofit Assessment Approach
- ☐ Boiler Retrofit Design
- ☐ *Glacier* CFD Software
- ☐ CFD Enhancements and Results
- ☐ Conclusions



# Retrofit Assessment Approach

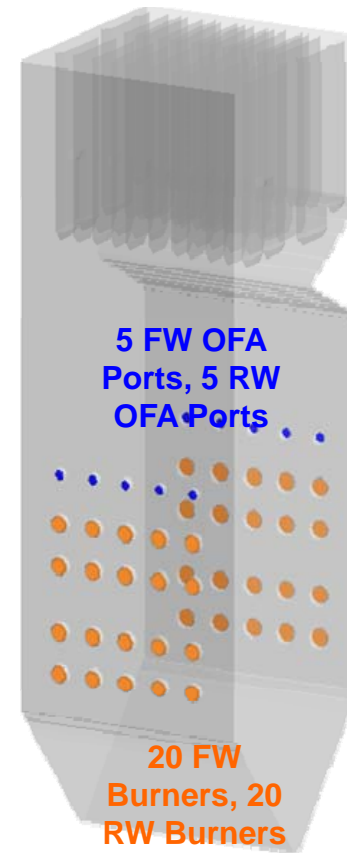
---



# PacifiCorp Hunter Unit 3 Retrofit

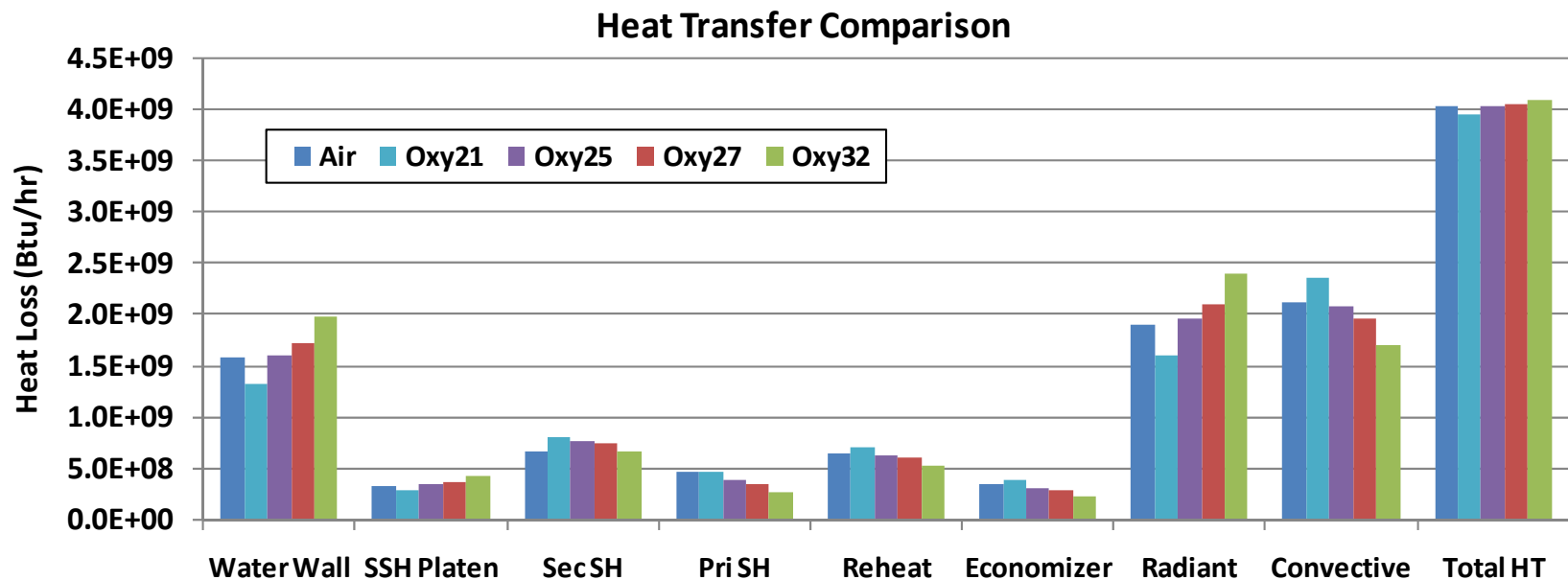
---

- ❑ 480 MW opposed-wall, staged firing, Utah bituminous coal
  - Focus on radiant furnace results
- ❑ Main retrofit tasks:
  - Determine firing conditions (REI)
  - Design oxy-burner (Siemens)
  - Match air-fired heat transfer
- ❑ Oxy-coal firing potential impacts:
  - Char oxidation / LOI
  - Sooting
  - Radiative heat transfer
  - Slagging
  - Corrosion
  - Emissions



# Retrofit – Firing Conditions

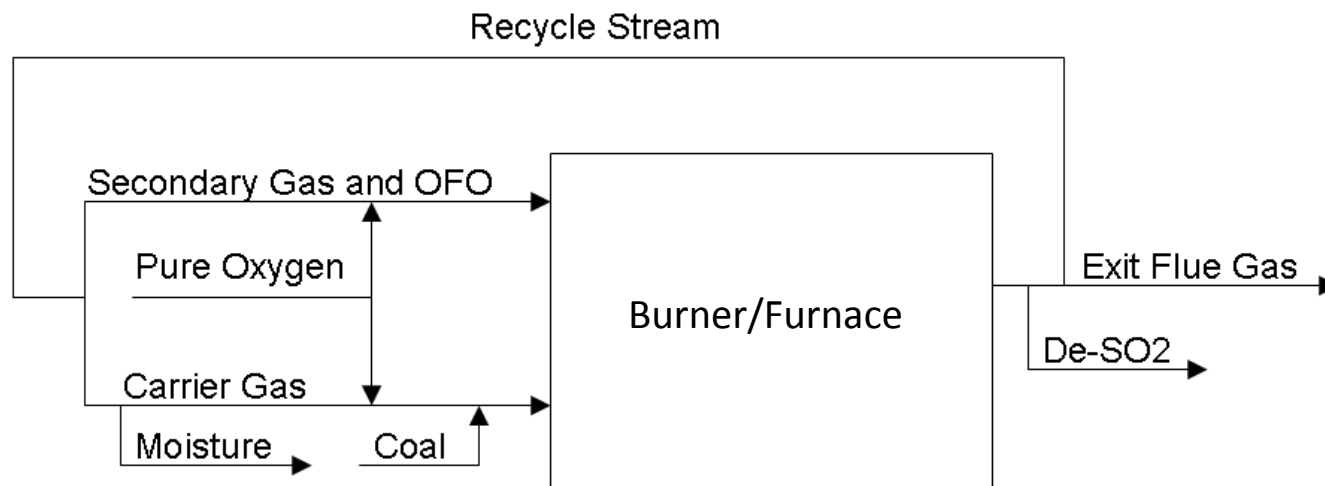
- ❑ Retrofit Task 1 – determine firing conditions (REI):
  - Based on SteamGen Expert process model (combustion + steam circuit)
  - Suggests 25-27% O<sub>2</sub> in O<sub>2</sub>/FGR mixture would best match air-fired heat transfer (O<sub>2</sub> and FGR mixed at burner)



# Retrofit – Oxy-Burner Design

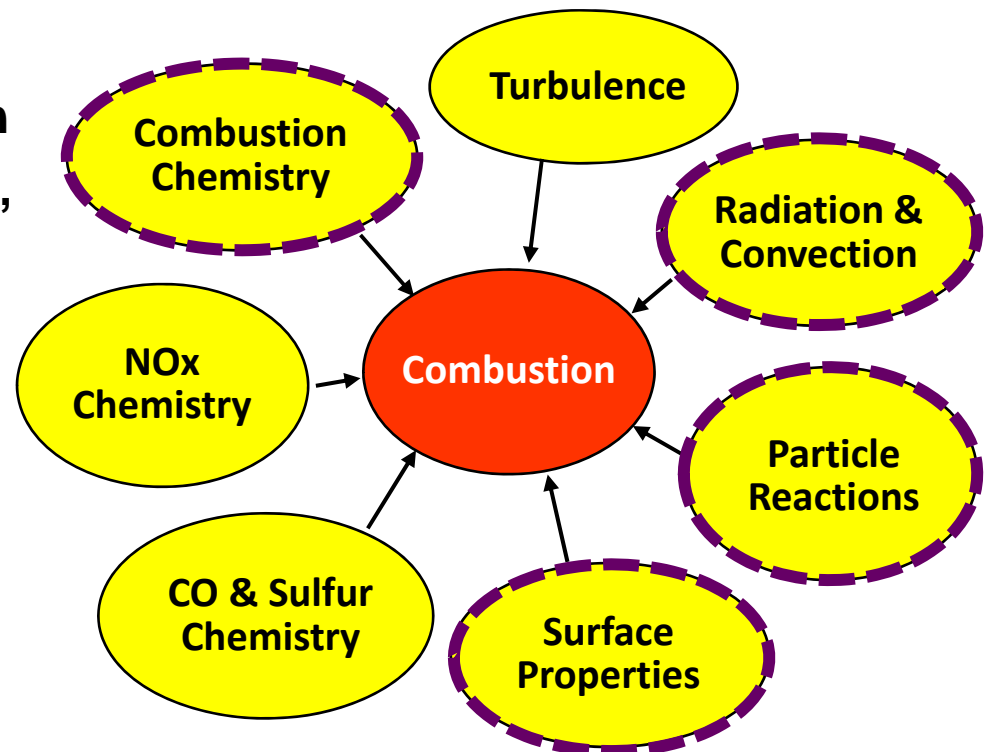
## □ Retrofit Task 2 – oxy-burner design (Siemens):

- 1) Estimate  $O_2$  and flue gas flows (SR, excess  $O_2$ )
- 2) Determine scaling factors to produce aerodynamic similitude
- 3) Account for heterogeneous  $O_2$ /FGR mixtures
- 4) Allocate flows to burner sections and overfire gas ports
- 5) Size burner sections and OFG ports (fit in existing boiler cut-outs)



# REI's *Glacier* CFD Software

- ❑ 20+ years of development and application to coal combustion
- ❑ Advanced chemistry (NO<sub>x</sub>, CO, sulfur, soot, ash)
- ❑ Two-phase flow
  - Heterogeneous reactions (volatiles, char, soot)
  - Burnout / LOI
  - Deposition, slagging, sintering
  - Multiple fuels
- ❑ Radiative heat transfer
- ❑ Corrosion (H<sub>2</sub>S, pyrite, sulfur)
- ❑ Erosion
- ❑ Variable surface conditions, coupling to steam circuit

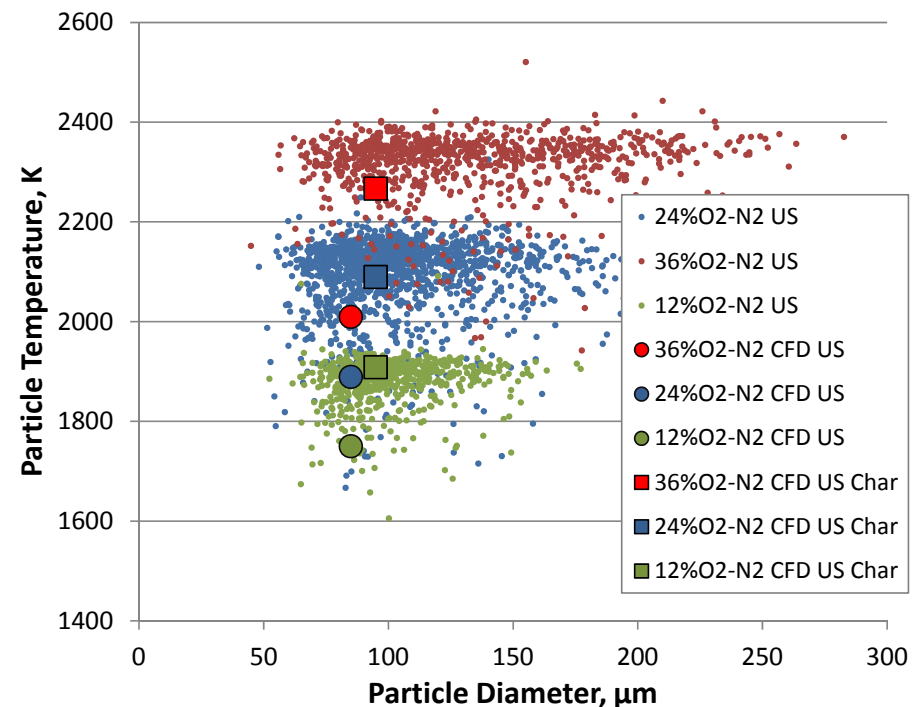


Compare air-fired and oxy-fired results,  
with and without upgraded sub-models



# Extended Char Oxidation Sub-Model

- Based on work by Shaddix and Geier<sup>1</sup> at Sandia using measurements in Sandia's Entrained Flow Reactor and SKIPPY modeling
- Started with heterogeneous surface reactions
- Added Extended Single Film model including:
  - Steam gasification
  - CO<sub>2</sub> gasification



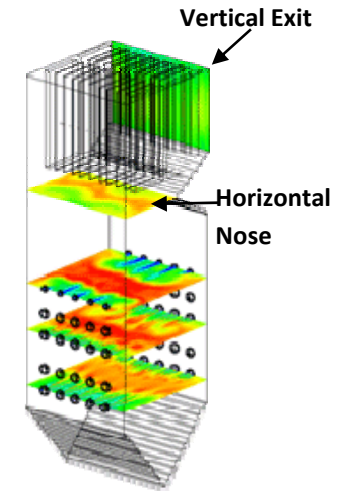
<sup>1</sup> M. Geier, C. Shaddix, K. Davis, H. Shim, "On the Use of Single-Film Models to Describe the Oxy-fuel Combustion of Pulverized Coal Char", 2011 Clearwater Clean Coal Conference





# Char Oxidation Results

	Air	Air w/ Char	Oxy27	Oxy27 w/ Char
<b>Horizontal Nose Plane</b>				
Temperature (°F)	2418	2417	2461	2473
CO Concentration, wet (ppm)	4,414	6,168	9,886	15,123
<b>Vertical Exit Plane</b>				
Temperature (°F)	1649	1644	1622	1641
CO Concentration, wet (ppm)	1,032	1,436	2,429	3,815
Unburned Carbon in Fly Ash	7.4%	3.8%	8.6%	2.2%

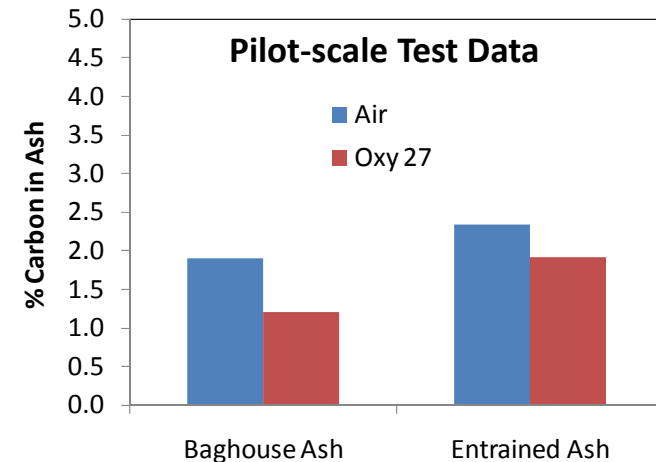


## ❑ Original char oxidation model predicts:

- Very high unburned carbon in ash
- Increased UBC for oxy-combustion

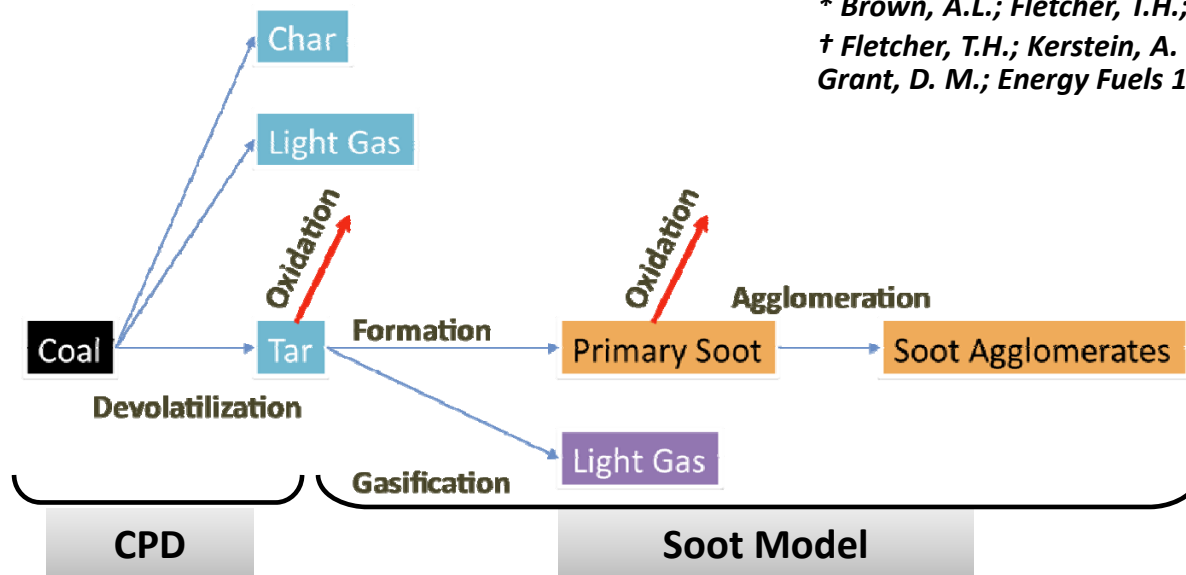
## ❑ New char oxidation model predicts:

- Reasonable UBC concentrations  
(2 - 3% UBC observed at the plant)
- Decreased UBC for oxy-combustion
- Increased CO concentrations



# Soot Sub-Model

- ❑ Coal-derived soot is assumed to form from only tar\*
  - Relatively constant mass of soot plus tar after devolatilization
  - Acetylene and benzene are not found in significant quantities
- ❑ Tar yields calculated by CPD model<sup>†</sup> based on measured coal properties
- ❑ CFD code tracks three equations for conservation of mass of soot, tar, and number of soot particles



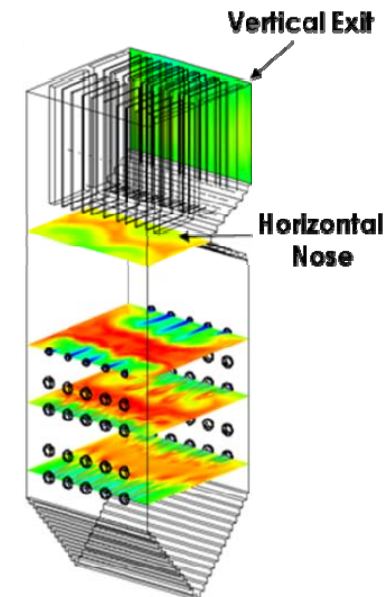
\* Brown, A.L.; Fletcher, T.H.; *Energy Fuels* 1998, 12, 745-757.

† Fletcher, T.H.; Kerstein, A. R.; Pugmire, R. J.; Solum, M. S.; Grant, D. M.; *Energy Fuels* 1992, 6, 414-431.



# Soot Results

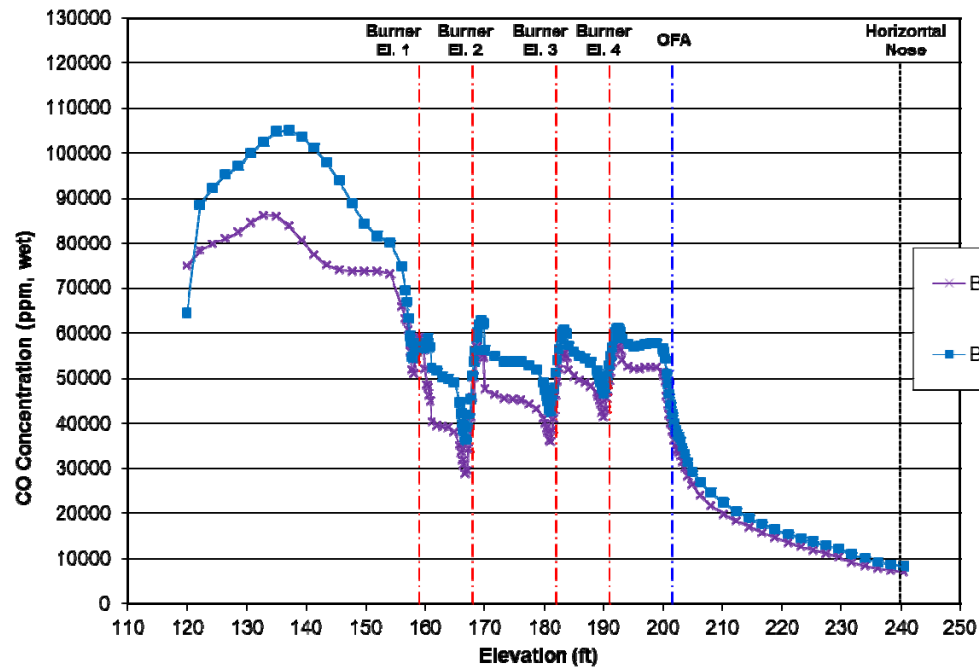
	Skyline Bituminous Coal		
	Baseline	Baseline w/ soot	Oxy26 w/ soot
<b>Horizontal Nose Plane</b>			
Temperature (°F)	2502	2518	2582
CO Concentration, wet (ppm)	7,038	8,454	16,451
<b>Vertical Exit Plane</b>			
Temperature (°F)	1785	1787	1765
CO Concentration, wet (ppm)	1,745	3,060	5,663
O <sub>2</sub> Concentration, wet (%)	3.2%	3.3%	2.9%
Unburned Carbon in Fly Ash	3.3%	3.6%	2.1%



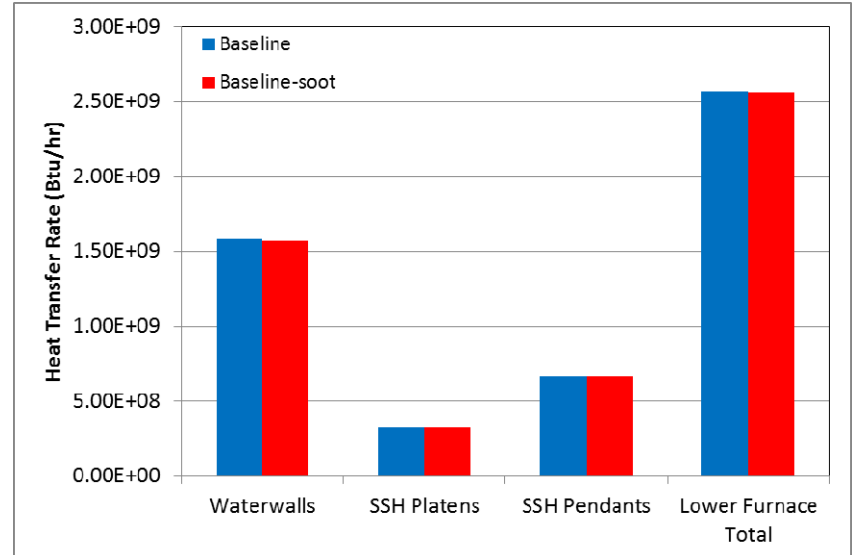
- ❑ Including soot sub-model had only minor impact on results, largest impact was on CO concentration
- ❑ Soot formation/destruction depends on oxidant availability and the fuel-oxidizer mixing under given operating conditions



# Soot Results



Lower furnace heat transfer (air-firing)



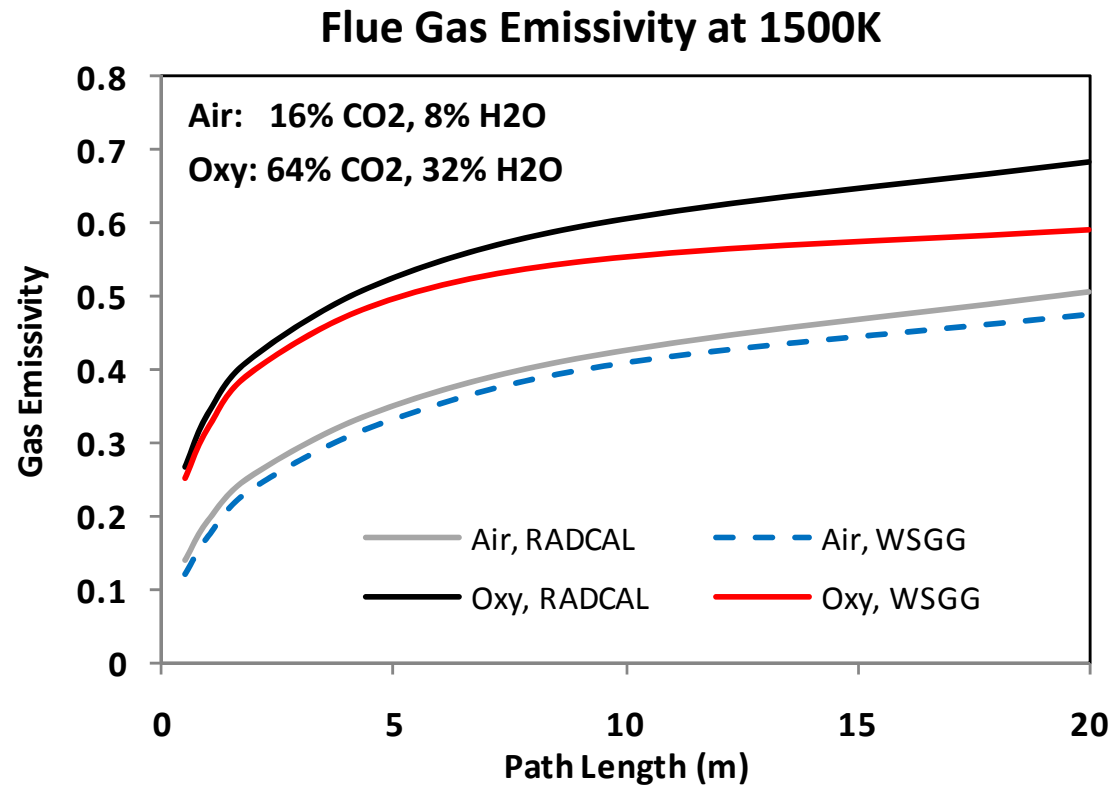
# Radiation Property Sub-Model

---

- ☐ Flame emission =  $f(\epsilon, T_g^4, k_p, T_p^4)$
- ☐ Gas emissivity =  $f(T_g, \text{CO}_2 \text{ \& H}_2\text{O conc., path length})$
- ☐ Compare impact of two gas emissivity sub-models:
  - Modified weighted-sum-of-gray-gas model (WSGG)
    - ☐ Based on curve-fits of measured data (Hottel charts) and high temperature correlations
    - ☐ Potentially limited in oxy-combustion because original measurements done at shorter path lengths and lower  $\text{CO}_2$ ,  $\text{H}_2\text{O}$  concentrations (typical of air-fired combustion)
  - Statistical Narrow Band model (RADCAL)
    - ☐ Based on statistical representation of full radiation spectrum
    - ☐ Extends emissivity calculations beyond original data range
    - ☐ More accurate but more computationally expensive



# Emissivity Sub-model Comparison

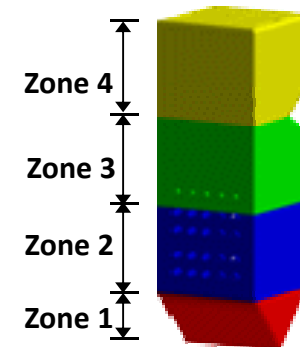
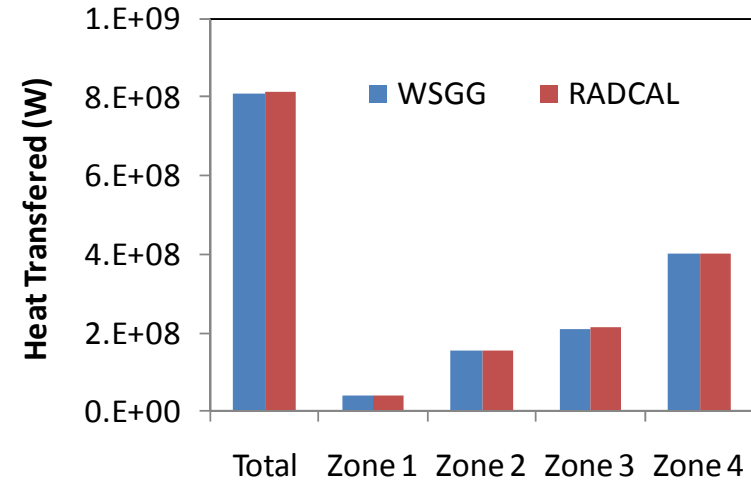
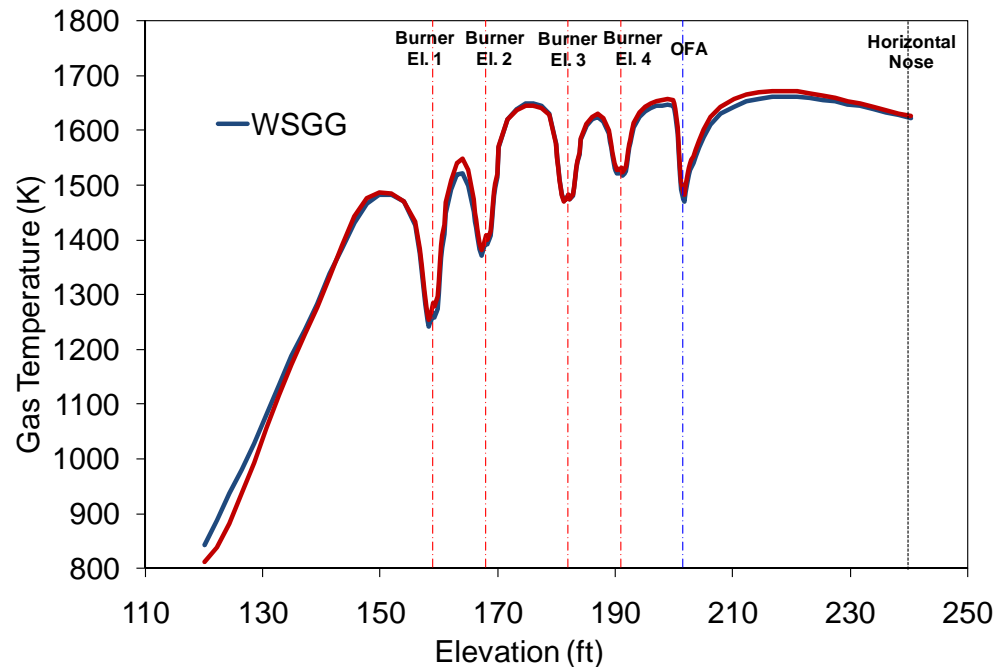


□ H<sub>2</sub>O has greater impact on emissivity than CO<sub>2</sub>



# Radiation Comparison

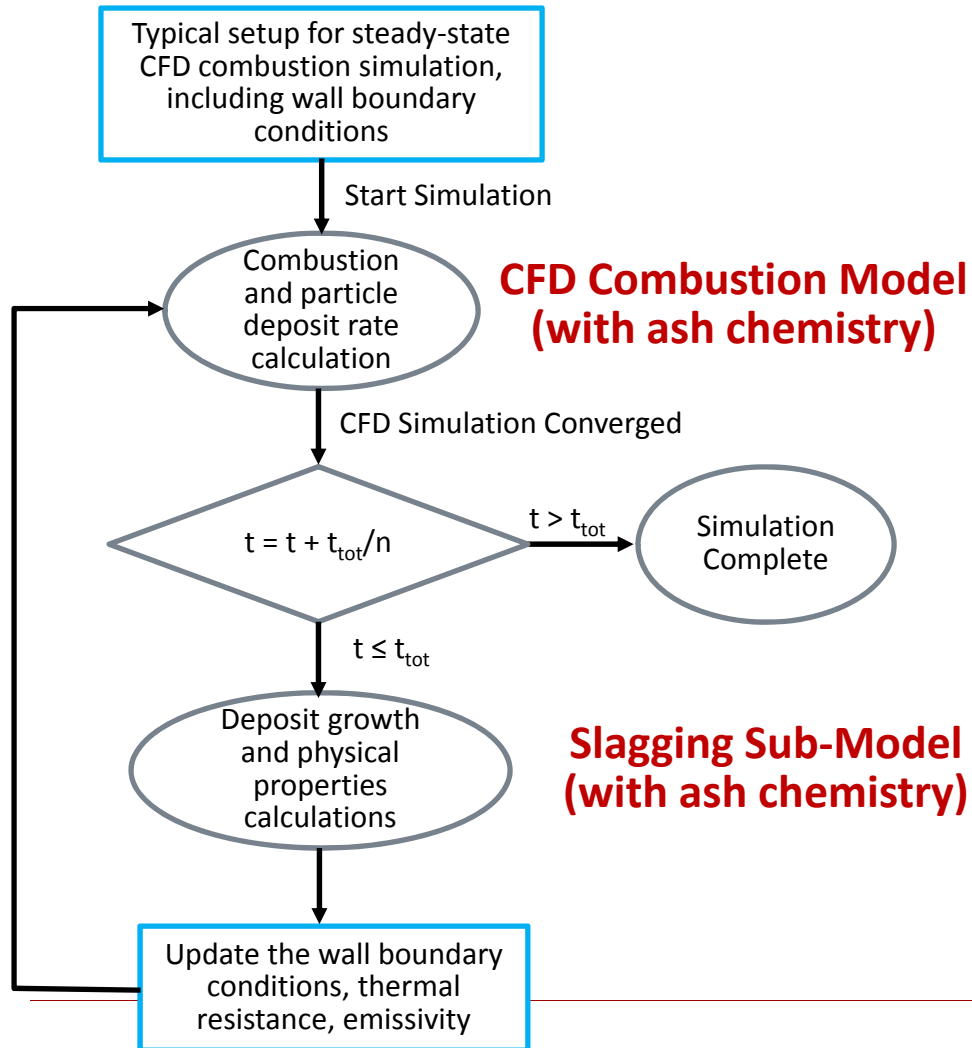
Oxy-coal Firing	WSGG	RADCAL
Horizontal Nose Temp. (°F)	2461	2476
Vertical Exit Temp. (°F)	1621	1626



☐ Flue gas conditions have greater impact than property model calculation



# Ash Chemistry and Slagging Sub-model



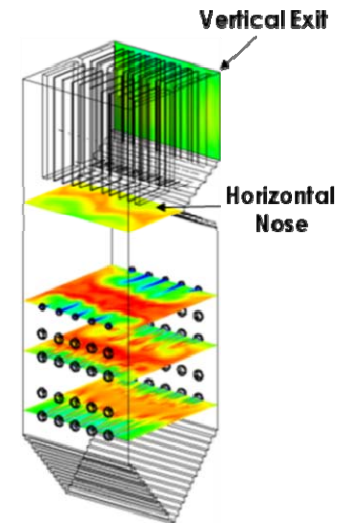
- Mineral matter transformation model used to predict ash size distribution and composition
- Viscosity predicted as a function of ash temperature and composition
- Fraction of particles deposited based on viscosity of impacting particle and surface
- Extent of slagging and sintering calculated as the deposit accumulates





# Slagging Results

	Baseline	Baseline slag	Oxy26	Oxy26 slag
<b>Horizontal Nose Plane</b>				
Temperature (°F)	2518	2554	2582	2566
CO Concentration, wet (ppm)	8,454	9,415	16,451	15,765
<b>Vertical Exit Plane</b>				
Temperature (°F)	1787	1808	1765	1781
CO Concentration, wet (ppm)	3,060	3,404	5,663	5,685
O <sub>2</sub> Concentration, wet (%)	3.3%	3.3%	2.9%	2.7%
Unburned Carbon in Fly Ash	3.6%	1.7%	2.1%	1.1%

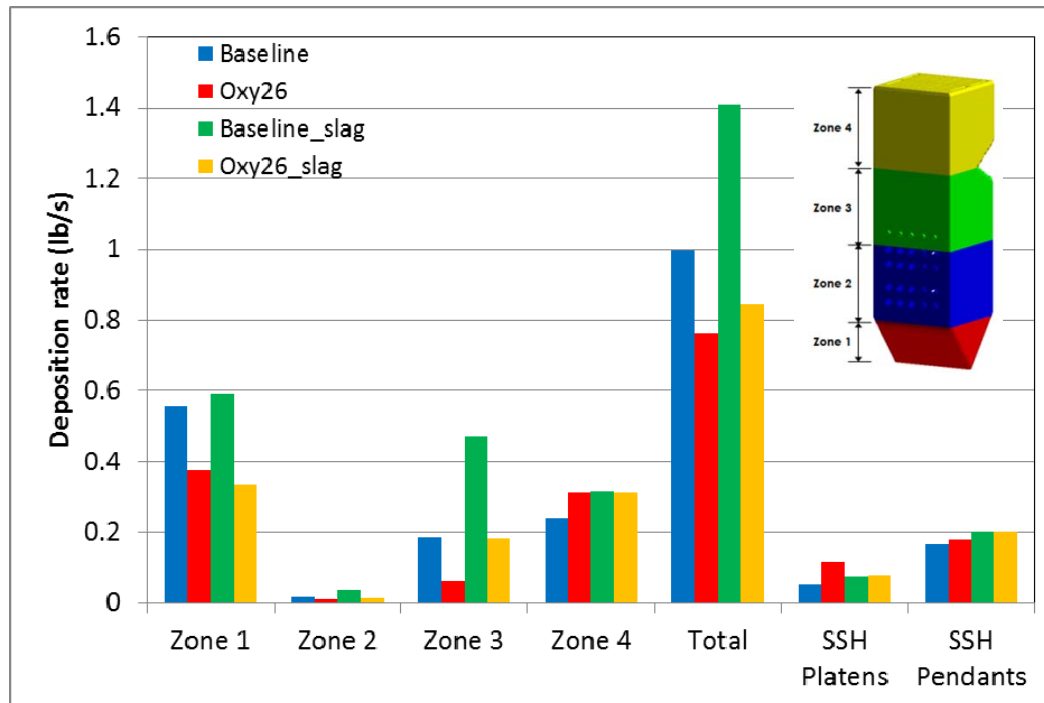


- Minimal overall impacts; air-fired UBC decreased
- Some local differences in heat flux caused by differences in local deposition rates and slag properties

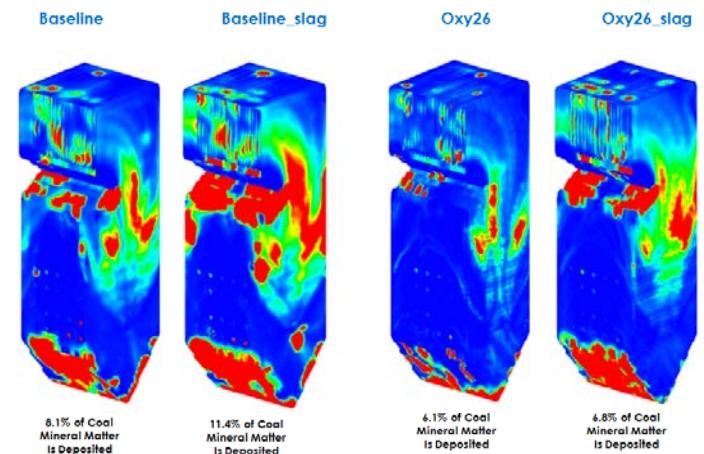


# Slagging Impacts

Deposition Rates



Deposition Flux Profiles

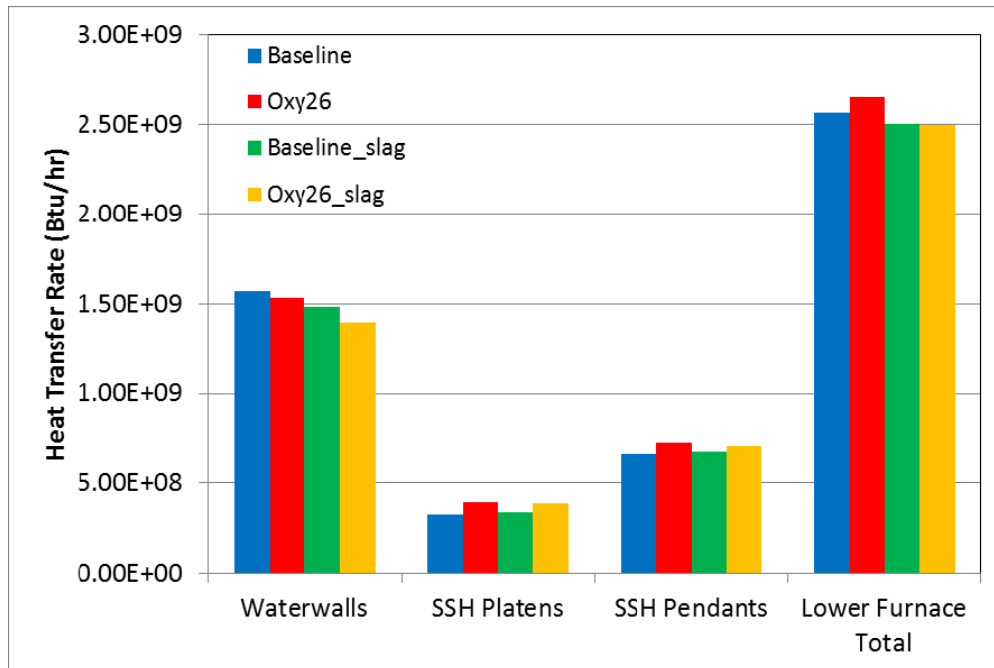


❑ Slagging model increases deposition rates, particularly for air-firing

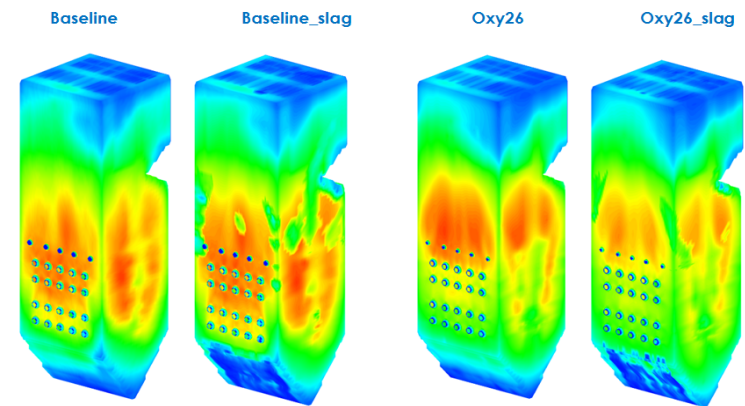


# Slagging Impacts – Heat Transfer

Heat Transfer Rates



Heat Flux Profiles



❑ Slagging model slightly decreases net heat flux to waterwalls



# Conclusions

---

- **Testing and analysis results used to guide retrofit design and upgrade CFD sub-models**
  - Char oxidation was enhanced when steam and CO<sub>2</sub> gasification reactions were included (produced higher CO and lower UBC)
  - Including soot formation had only minor impacts on results, largest impact was increasing CO concentration
  - Improved gas emissivity sub-model had negligible impact
  - Upgraded ash chemistry and slagging sub-model had minimal overall impact; localized changes in deposition rates and surface properties did impact local heat fluxes
- **Upgraded CFD sub-models provide improved predictive capability for oxy-combustion retrofits and new designs**
  - Combustion, heat transfer, slagging, corrosion, emissions

# Acknowledgements

---

CFD results created with *Fieldview* software by Intelligent Light

This material is based upon work supported by the Department of Energy under Award Number DE-NT0005288

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

