CFD Modeling of Multi-scale Air- and Oxy- coal Combustion Experiments

For Energy and Environmental Solutions

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NETL Workshop on Multi-phase Flow Science

Pittsburgh, PA

August 16-18, 2011

Program Overview

- **<u>Objective:</u>** ***Characterize* and *predict* performance and operational impacts of oxy-combustion retrofit designs on existing coal-fired boilers**
- **<u>Approach:</u> Utilize multi-scale testing and theoretical investigations to develop:**
  - **Fundamental data that describe combustion characteristics, corrosion rates, and ash properties during oxy-coal firing**
  - **Validated mechanisms that describe oxy-combustion processes**
  - **Firing system principles that guide oxy-burner design and flue-gas recycle implementation**
- **Incorporate validated mechanisms into CFD software to evaluate full-scale oxy-combustion retrofit designs**

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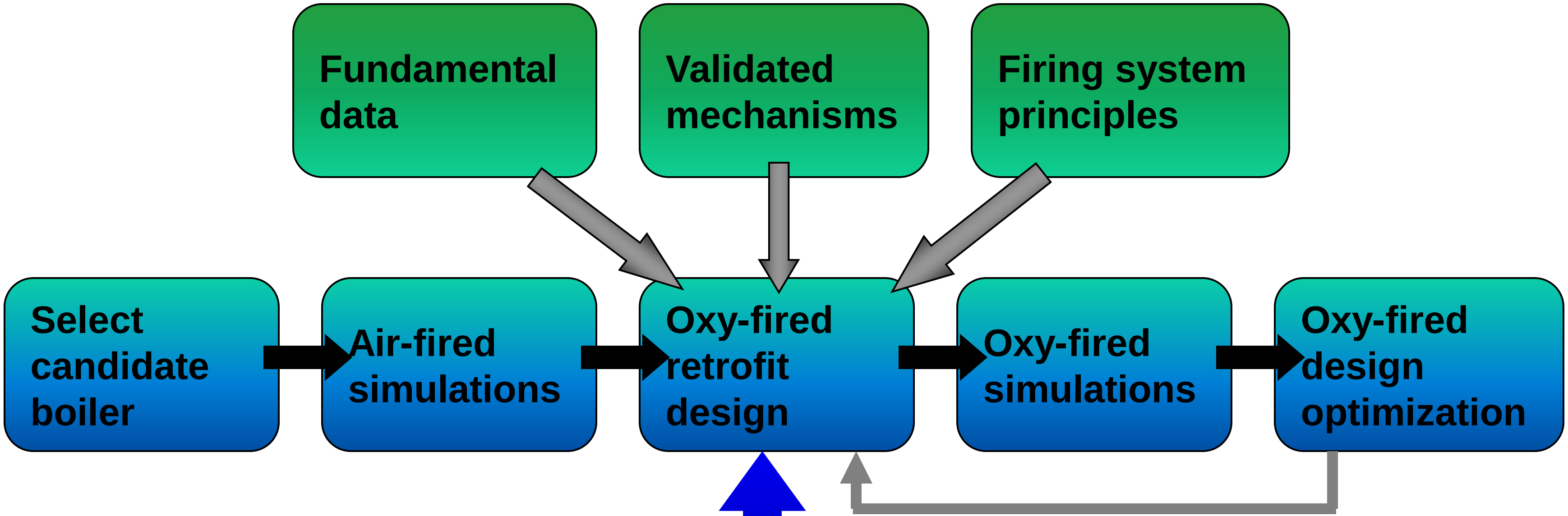
Program Overview

Team Member	Project Role
REI	*program management, testing oversight, mechanism development, simulations*
University of Utah	*laboratory and pilot-scale testing, mechanism development*
Siemens/ABT	*burner technology*
Praxair	*oxygen supply*
Brigham Young Univ.	*soot measurements*
Corrosion Management	*corrosion tests, mechanism development*
Sandia National Labs	*bench-scale testing, mechanism development*
Vattenfall AB	*mechanism development, validation data*
PacifiCorp, Praxair, Southern Company, Vattenfall, DTE Energy	*Advisory Panel provides industrial perspective on R&D needs, retrofit requirements and constraints, suggested assessment studies*

Program Overview



Design and optimization criteria:

- Match air-fired heat duties
- Maximize combustion efficiency
- Minimize surface impacts (corrosion, slagging, fouling)
- Minimize trace pollutant emissions

Program Schedule

- **Year 1 Key Tasks (ending 9/30/09)**
  - **Initiate char oxidation and OFC experiments**
  - **Design and fabricate pilot-scale oxy-burner**
  - **Complete initial slagging and fouling mechanism development**
- **Year 2 Key Tasks (ending 9/30/10)**
  - **Complete OFC ash characterization measurements without FGR**
  - **Continue char oxidation experiments and mechanism development**
  - **Complete pilot-scale burner, slagging, fouling, corrosion testing**
- **Year 3 Key Tasks (ending 3/31/12)**
  - **Finish char oxidation experiments and validate mechanism**
  - **Complete OFC ash characterization measurements with FGR**
  - **Validate slagging, fouling, corrosion, sooting mechanisms**
  - **Implement validated mechanisms into CFD code**
  - **Complete boiler retrofit assessment**

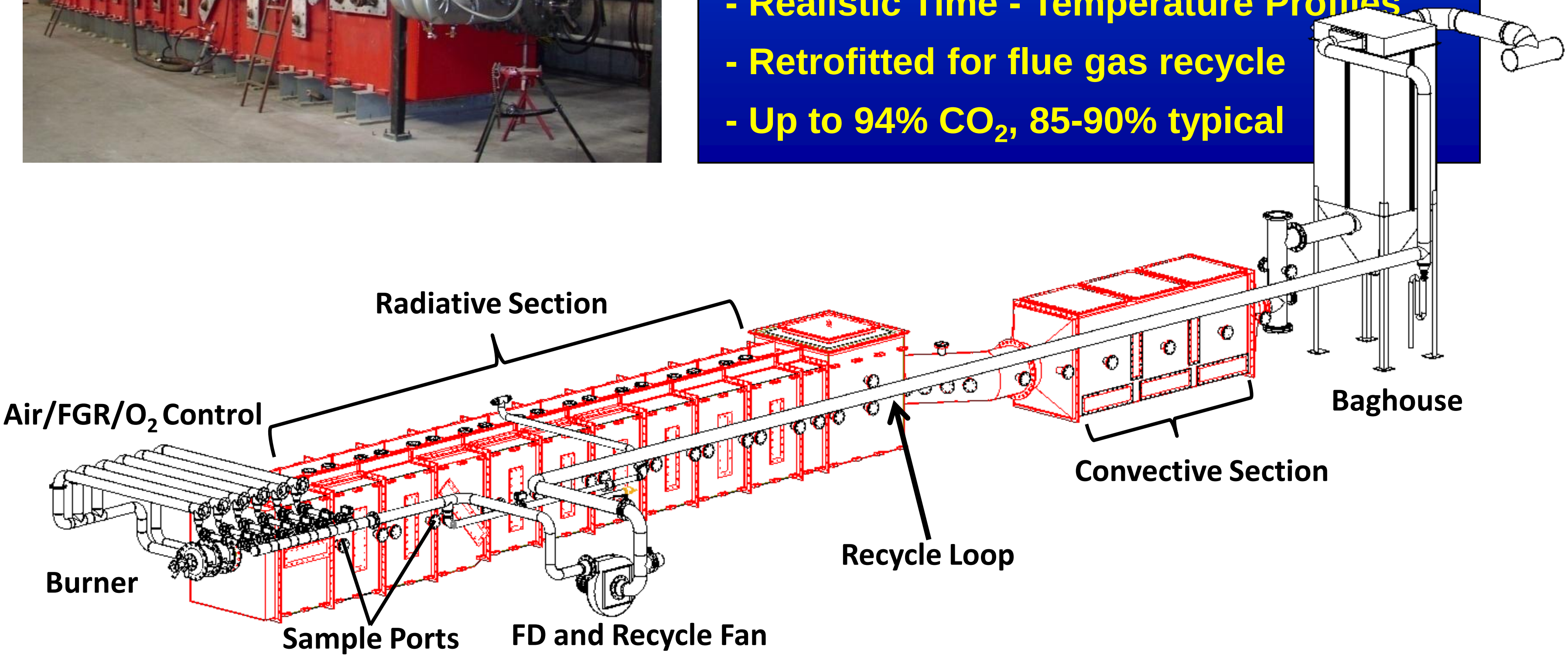
Multi-scale Experiments

- **Bench-Scale Optical Entrained Flow Reactor**
  - **Char Oxidation Kinetics**
- **100 kW Oxy-Fuel Combustor (OFC) Tests**
  - **Ash Deposition and Characterization**
  - **Soot Evolution**
- **1.2 MW Pilot-Scale Furnace (L1500) Tests**
  - **Impacts of Burner Configuration**
  - **Heat Flux, Corrosion and Particle Deposition**
  - **Flue Gas Chemistry, Sooting**

3.5 MBtu/hr Pilot-Scale Furnace (L1500)

L1500 Capabilities:

- Realistic Burner Turbulent Mixing Scale
- Realistic Radiative Heat Flux Conditions
- Realistic Time - Temperature Profiles
- Retrofitted for flue gas recycle
- Up to 94% CO_2, 85-90% typical

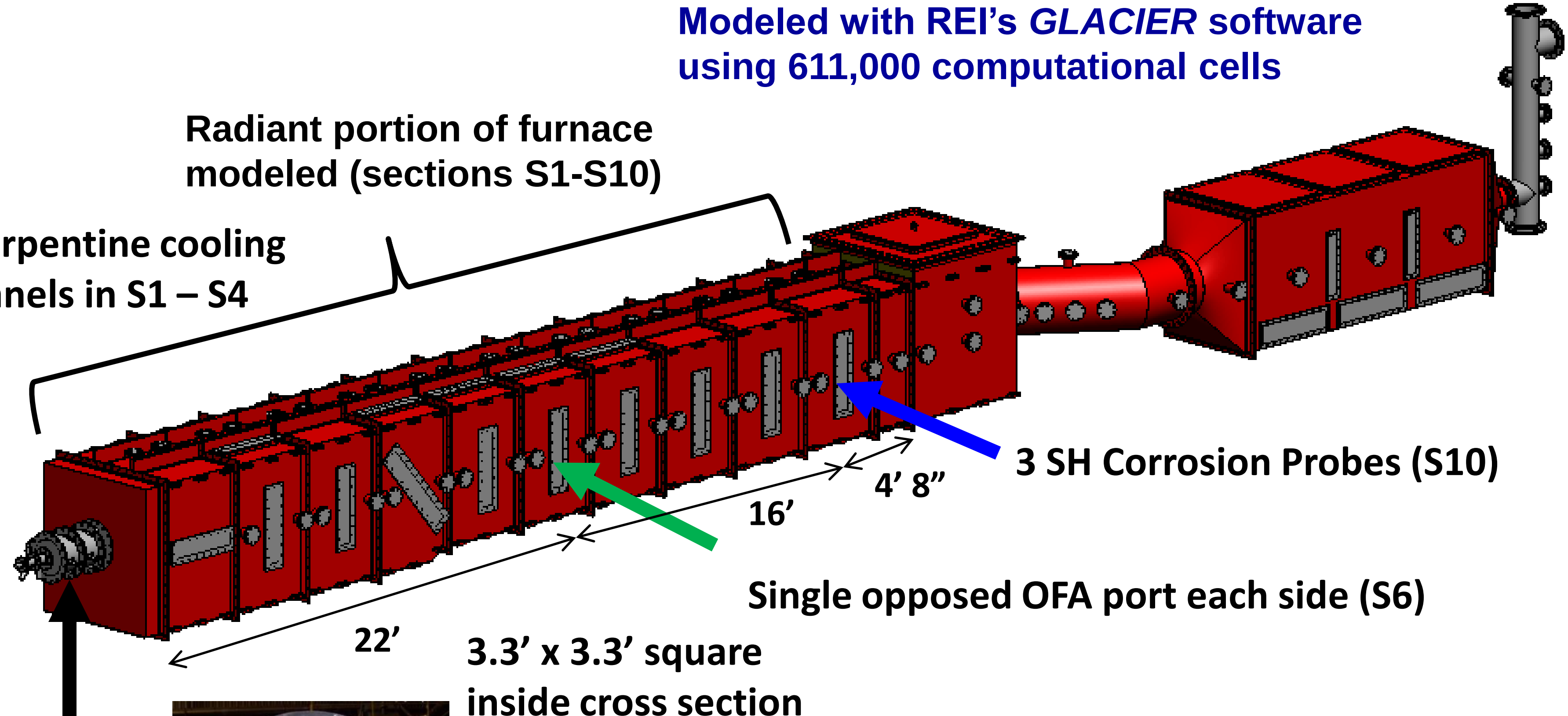


Furnace Model Geometry

Modeled with REI's *GLACIER* software using 611,000 computational cells

Radiant portion of furnace modeled (sections S1-S10)

Serpentine cooling panels in S1 – S4



3 SH Corrosion Probes (S10)

Single opposed OFA port each side (S6)

3.3' x 3.3' square inside cross section

Burner

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Operating Conditions

Coal Property	Utah Skyline
Moisture (%)	3.18
Ash (%)	8.83
C (%)	70.60
H (%)	5.06
N (%)	1.42
S (%)	0.53
O (%)	10.38
Volatile (%)	38.60
Fixed C (%)	49.39
HHV (Btu/lb)	12,606

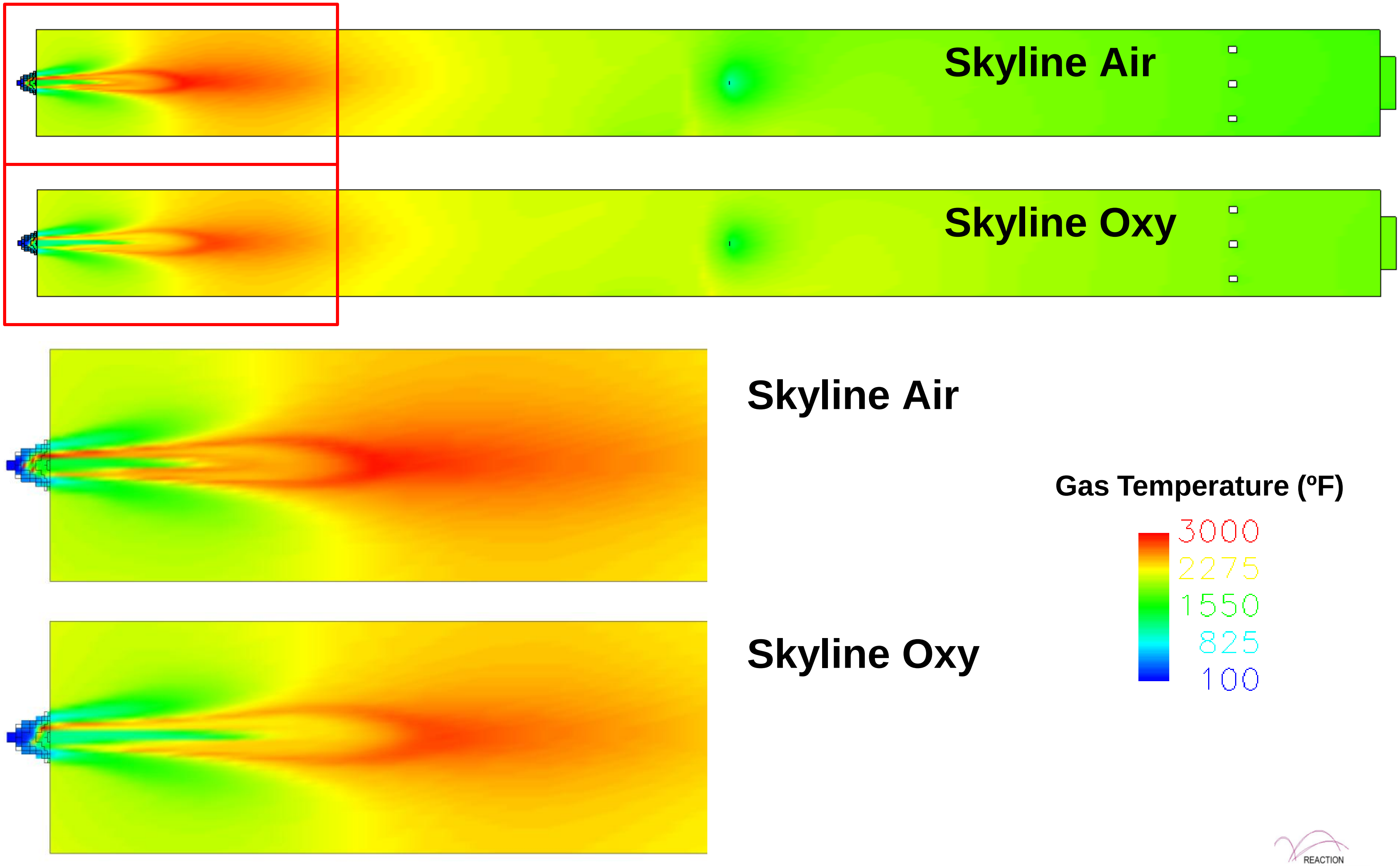
Parameter	Units	Air	Oxy
Firing Rate	MBtu/hr	3.5	3.5
Excess O_2	%, dry	3.14	3.07
BSR		0.9	0.9
Primary Gas/Fuel		1.8	1.8
Burner IS / OS		20/80	20/80
Overall O_2	%, wet	21	27
Burner O_2	%, wet	21	27
Primary O_2	%, wet	21	21
IS O_2	%, wet	21	28.7
OS O_2	%, wet	21	28.7

Baseline CFD Model Results

(without newly developed sub-models)

	Skyline Air Model	Skyline Air Ave Measured	Skyline Oxy Model	Skyline Oxy Ave Measured
Exit Temp (°F)	1743		1872	
Exit O_2 (%, dry)	3.14	3.18	3.03	3.07
Exit CO (ppmv, dry)	<1	16	126	90
Exit SO_2 (ppmv, dry)	444	425	1,788	1754
Exit CO_2 (%, dry)	15.9	15.9	89.9	89.9
Exit H_2O (%)	6.7		25.6	
Gas Sensible Heat (%)	39.7		41.1	
Wall Heat Loss (%)	59.6		58.5	
Rad. / Conv. (%)	41.4 / 18.2		46.5 / 12.0	

Predicted Gas Temperature



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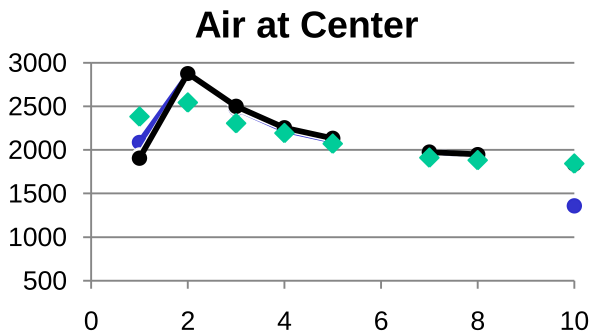
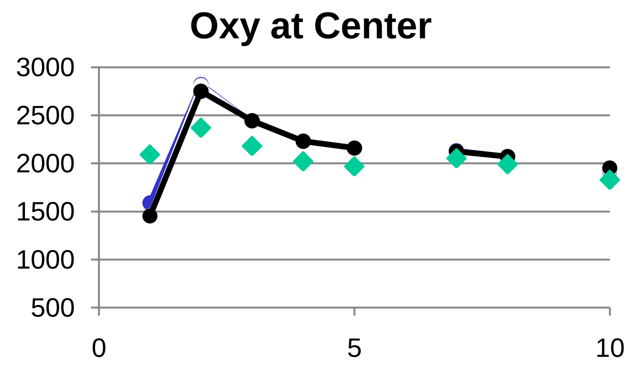
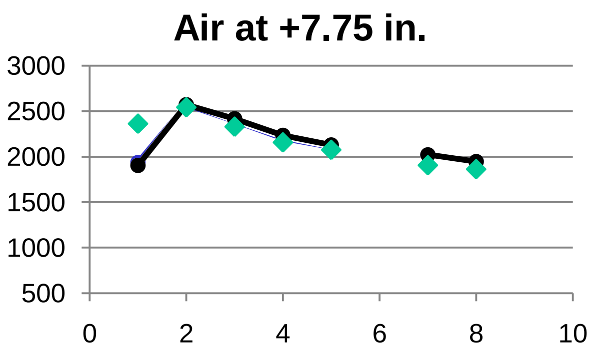
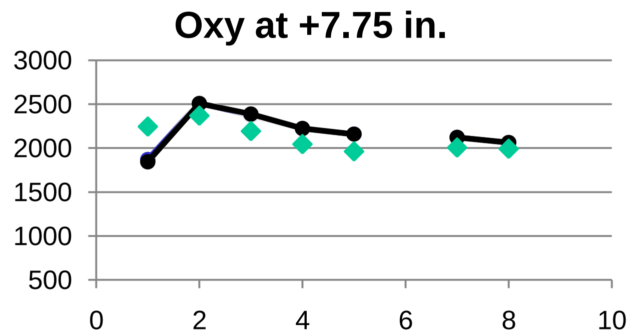
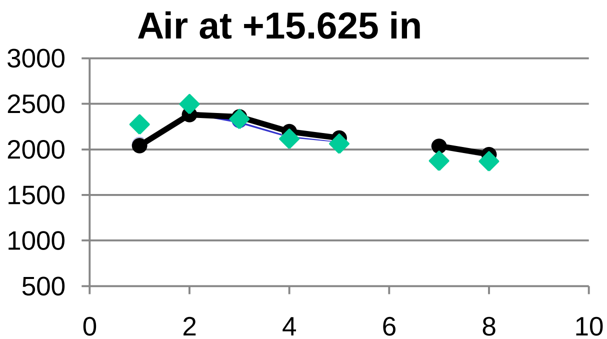
Radial Gas Temperature Comparison

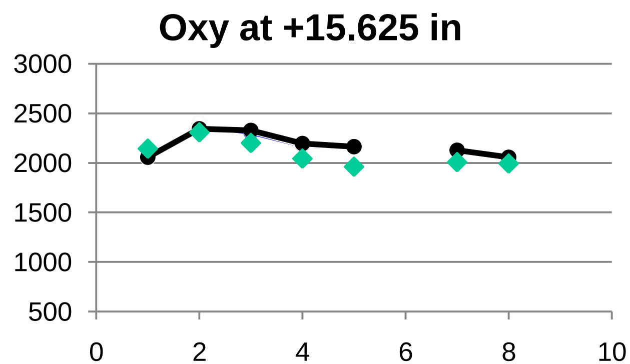












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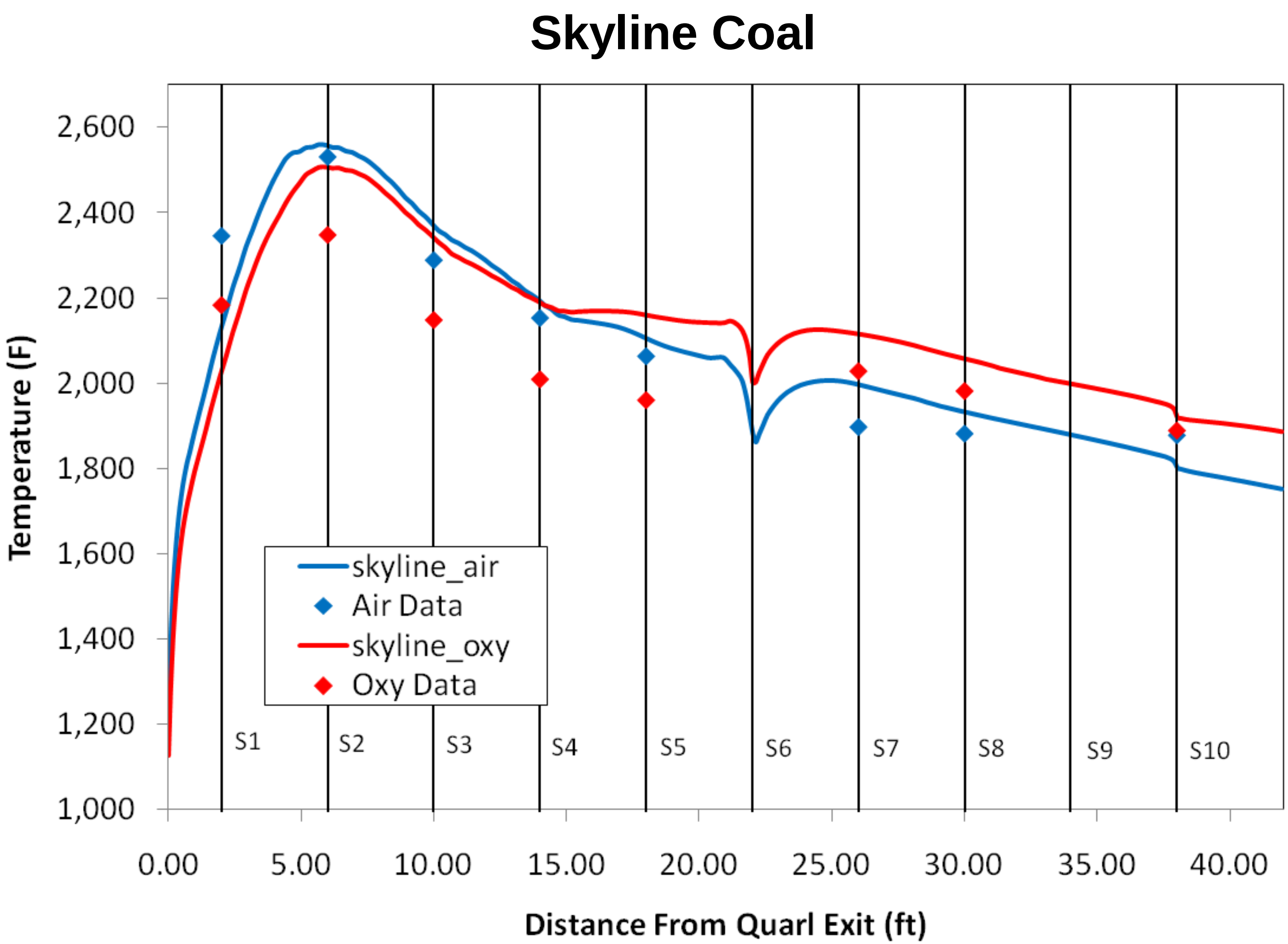
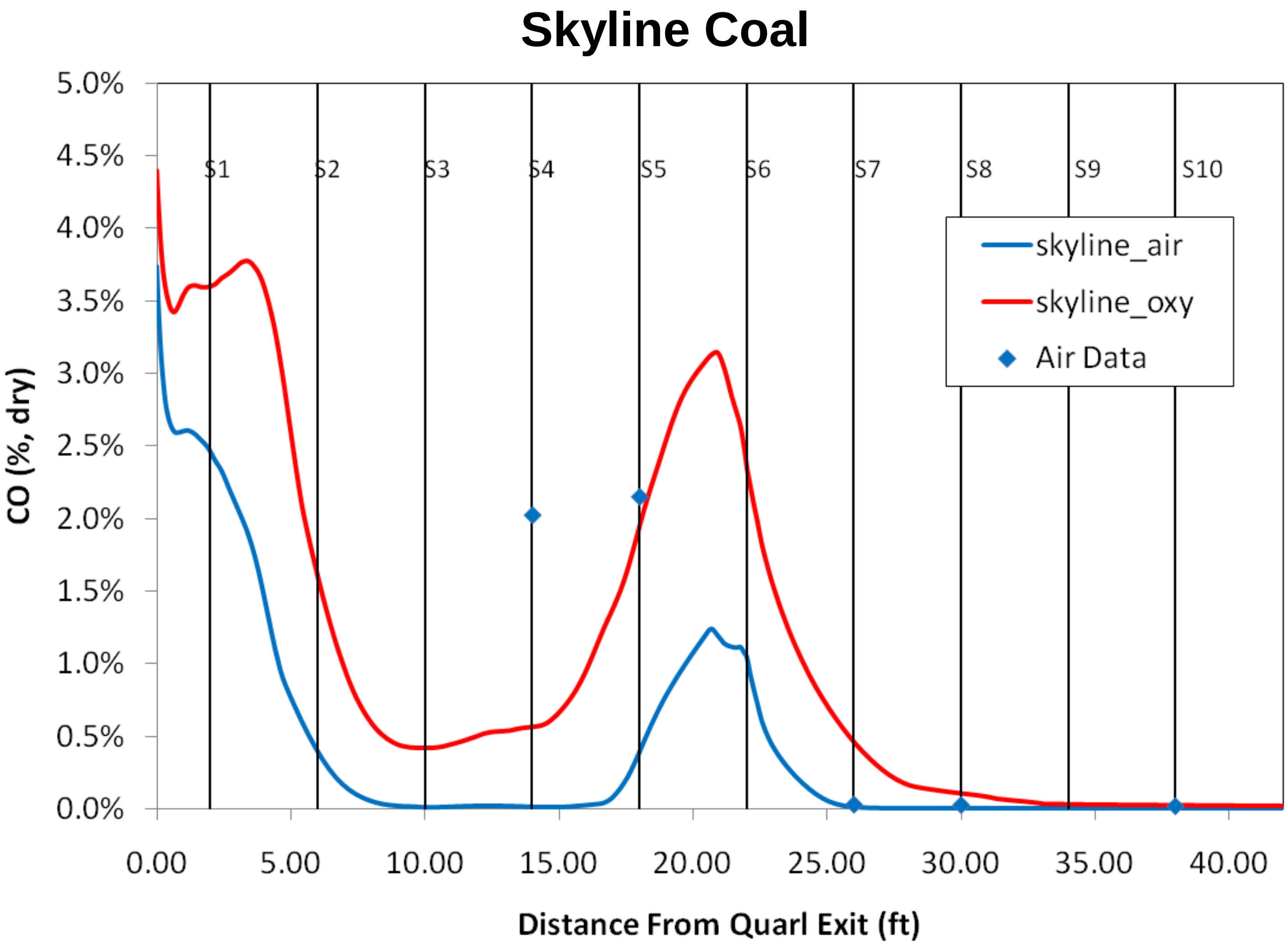
Average Gas Temperature Comparison



Average CO Concentration Comparison



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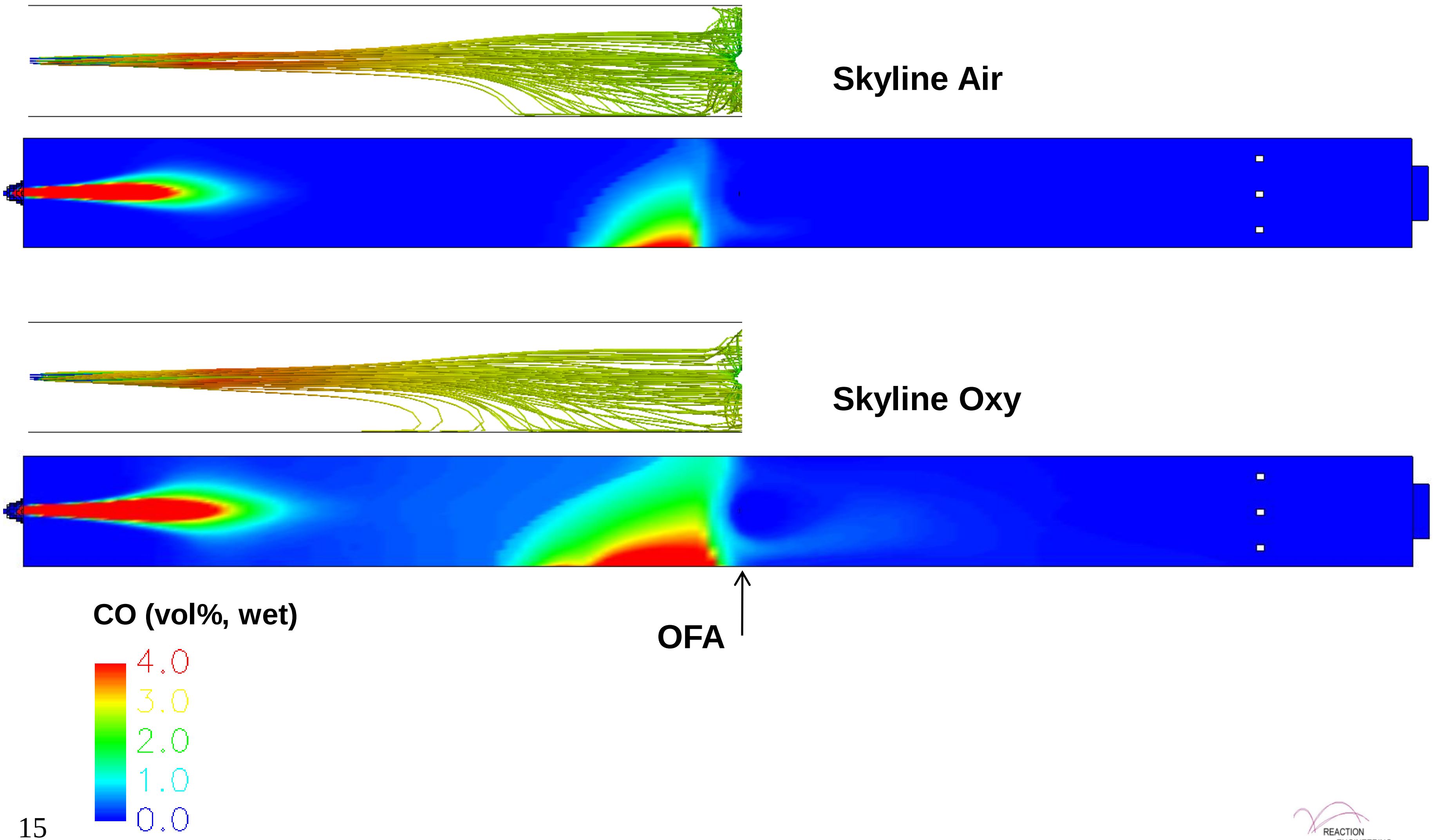
Particle Trajectories and CO Profiles



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Extended Char Oxidation Model

- **Model development previously presented** *(Geier, Shaddix, Davis, Shim, "On the Use of Single-Film Models to Describe the Oxy-fuel Combustion of Pulverized Coal Char", 2011 Clearwater Clean Coal Conference)*
- **Based on work by Shaddix and Geier at Sandia using measurements in EFR and SKIPPY modeling**
- **Start with heterogeneous surface reactions**
- **Add Extended Single Film model including:**
  - **Steam gasification**
  - **CO_2 gasification**

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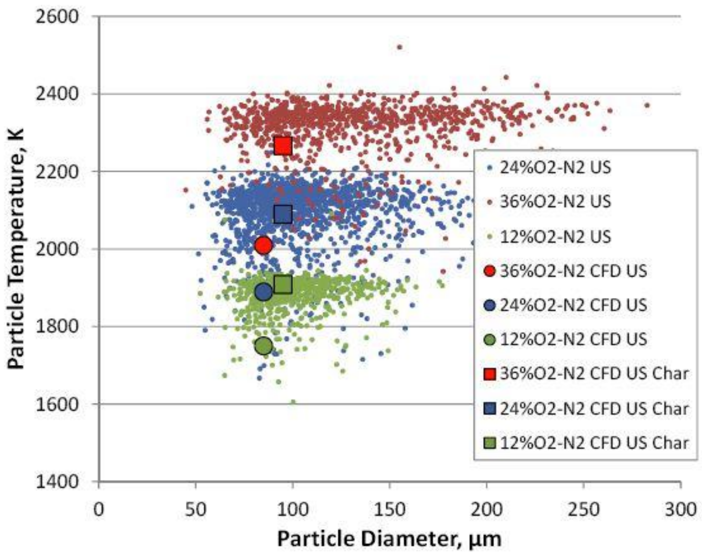
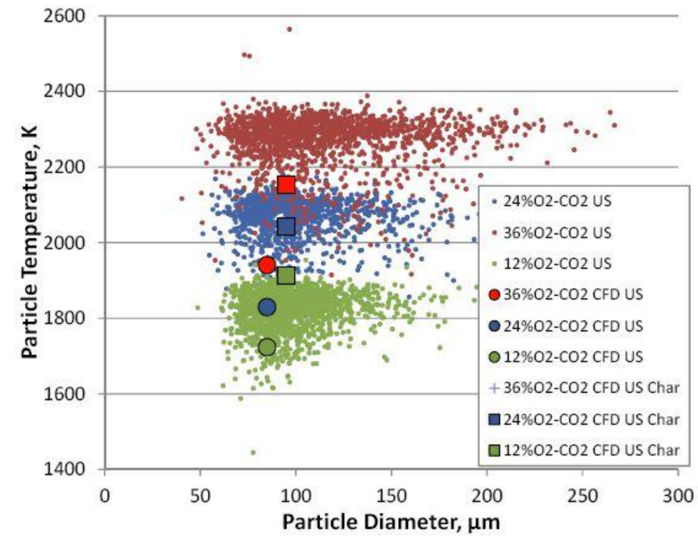
Comparisons with Lab-scale Data

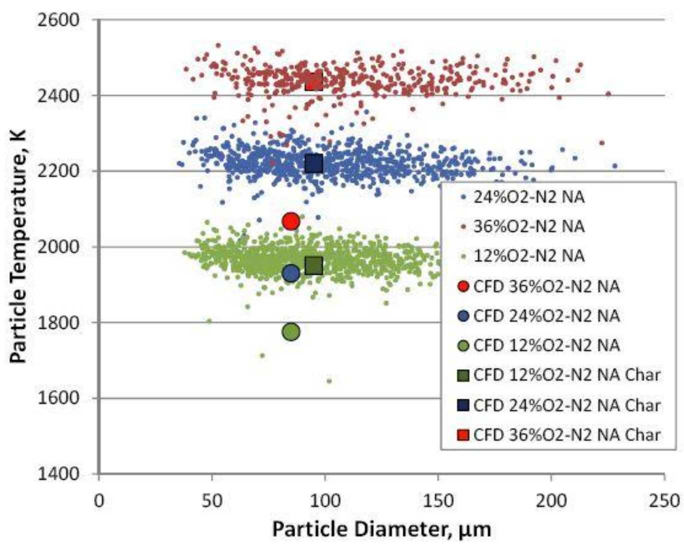
N_2 Balance | **CO_2 Balance**

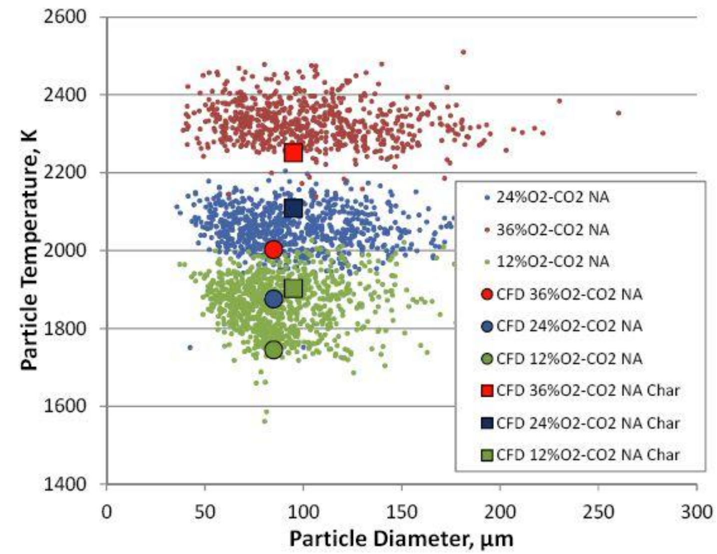
Skyline





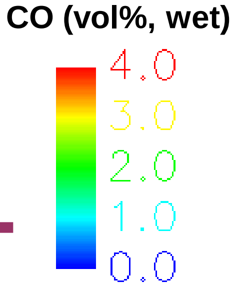
PRB



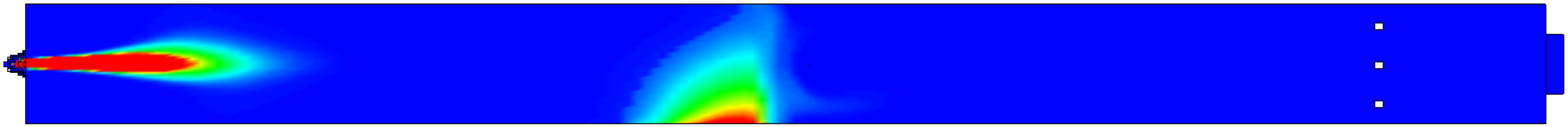


CO Concentration Profiles

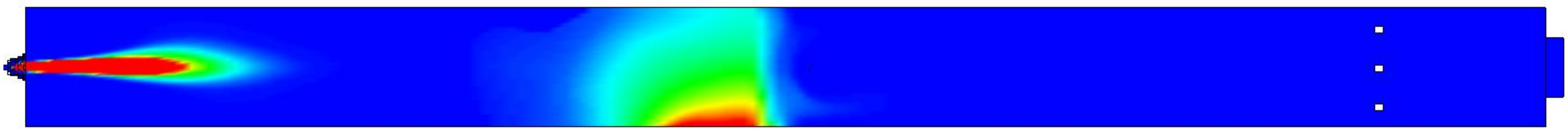
Skyline Coal



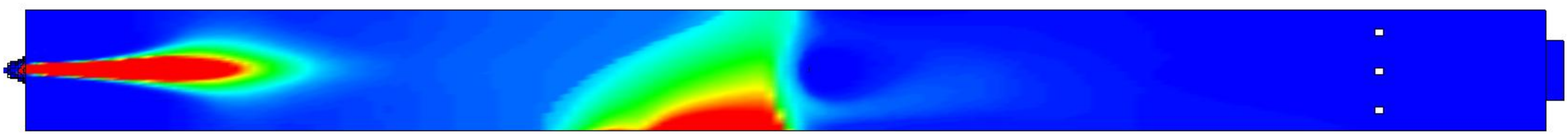
Air With Original Char Oxidation



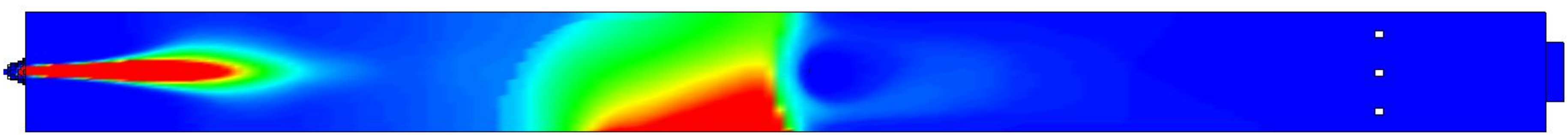
Air With Extended Char Oxidation



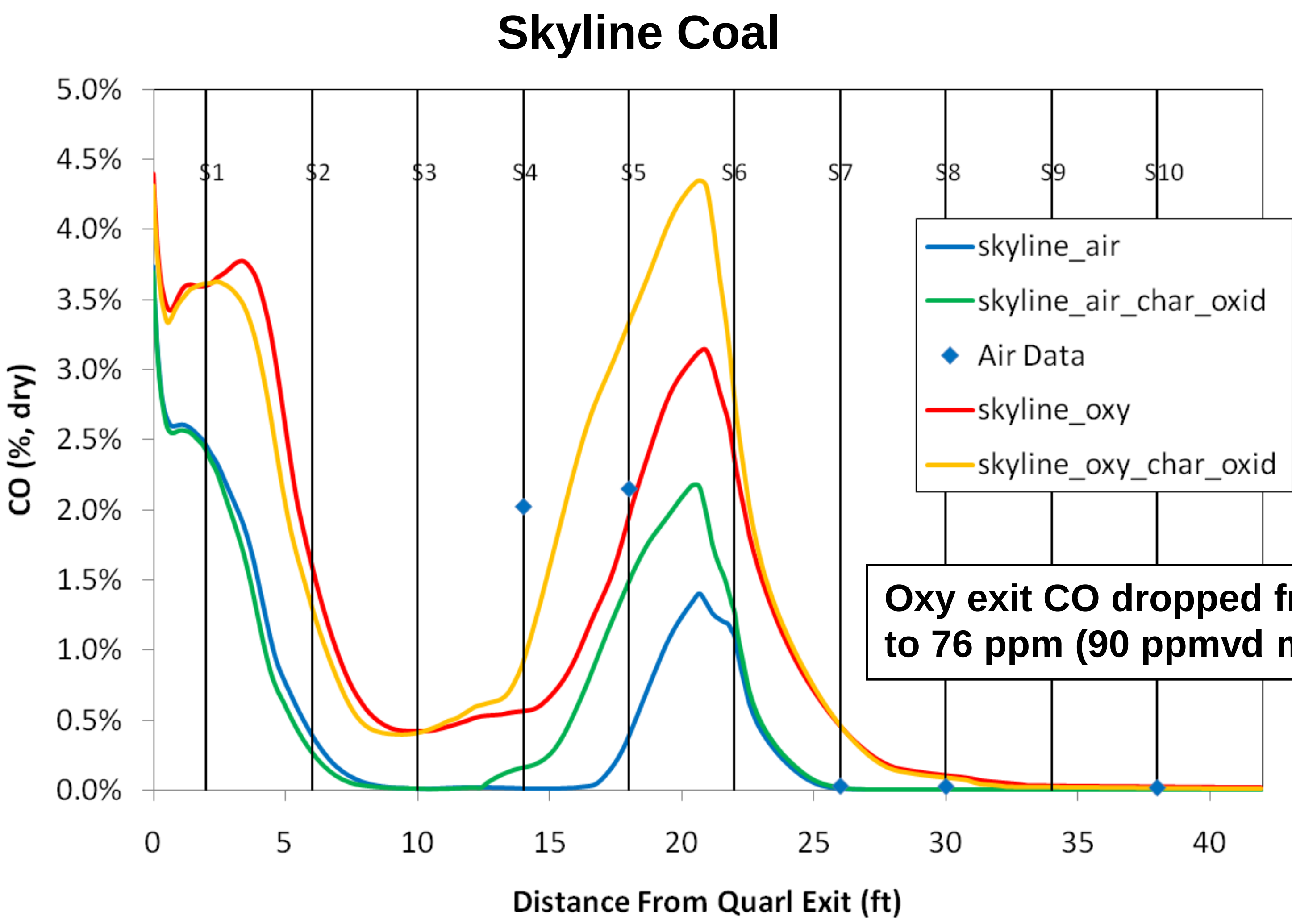
Oxy With Original Char Oxidation



Oxy With Extended Char Oxidation



CO Concentration Comparison



Oxy exit CO dropped from 126 to 76 ppm (90 ppmvd measured)

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Radiative Emissivity Model Impacts

- **Evaluate impact of narrow band gas emissivity model**
  - **Original model is hybrid Hottel Chart - weighted sum of gray gases model**
  - **Advanced model is narrow band model based on RADCAL code by NIST**
  - **Previous work has suggested:**
    - **Minimal emissivity impacts for short path lengths**
    - **Particle radiation dominates gas radiation in flame zone**

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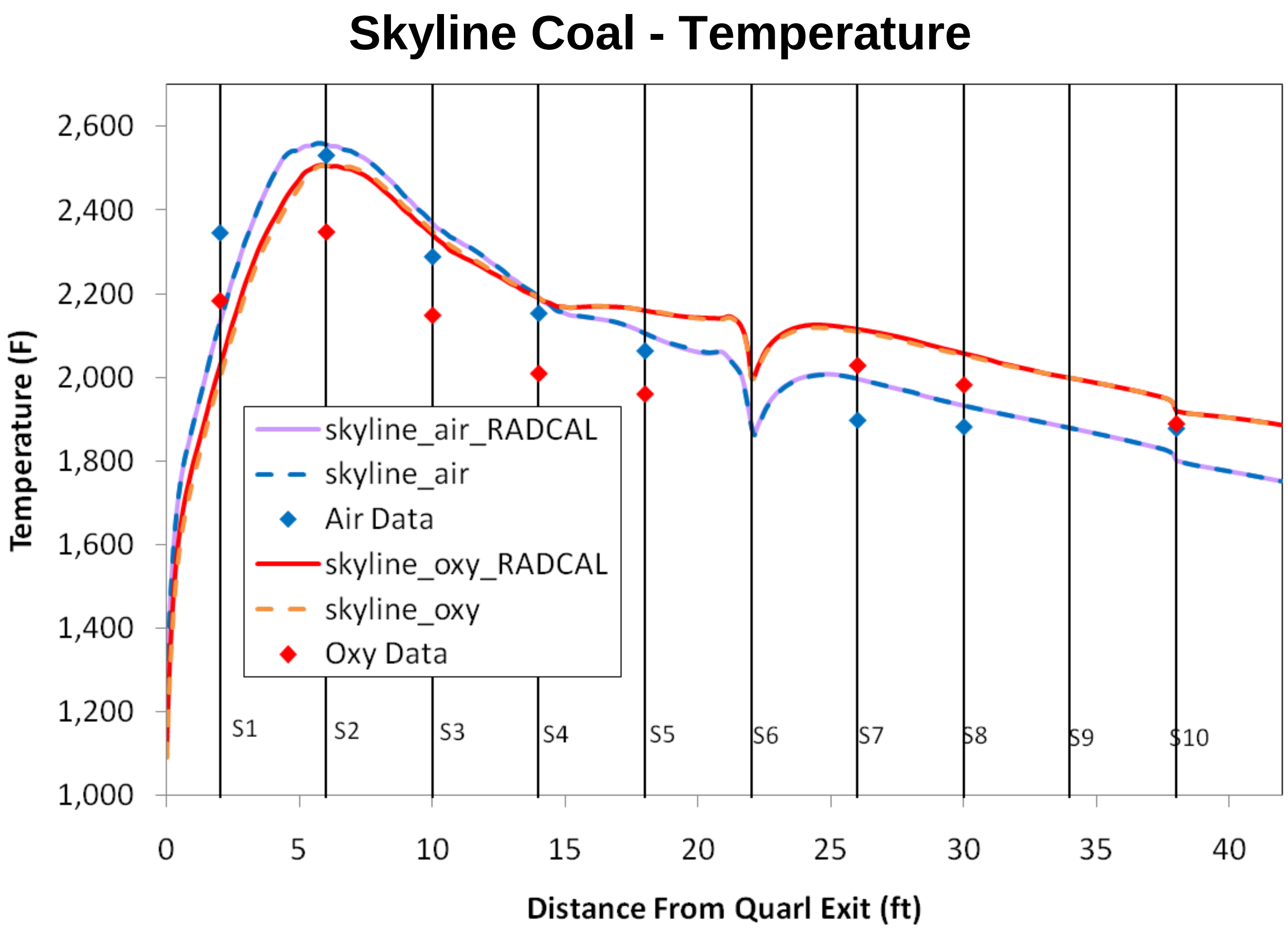
Radiative Emissivity Model Comparison



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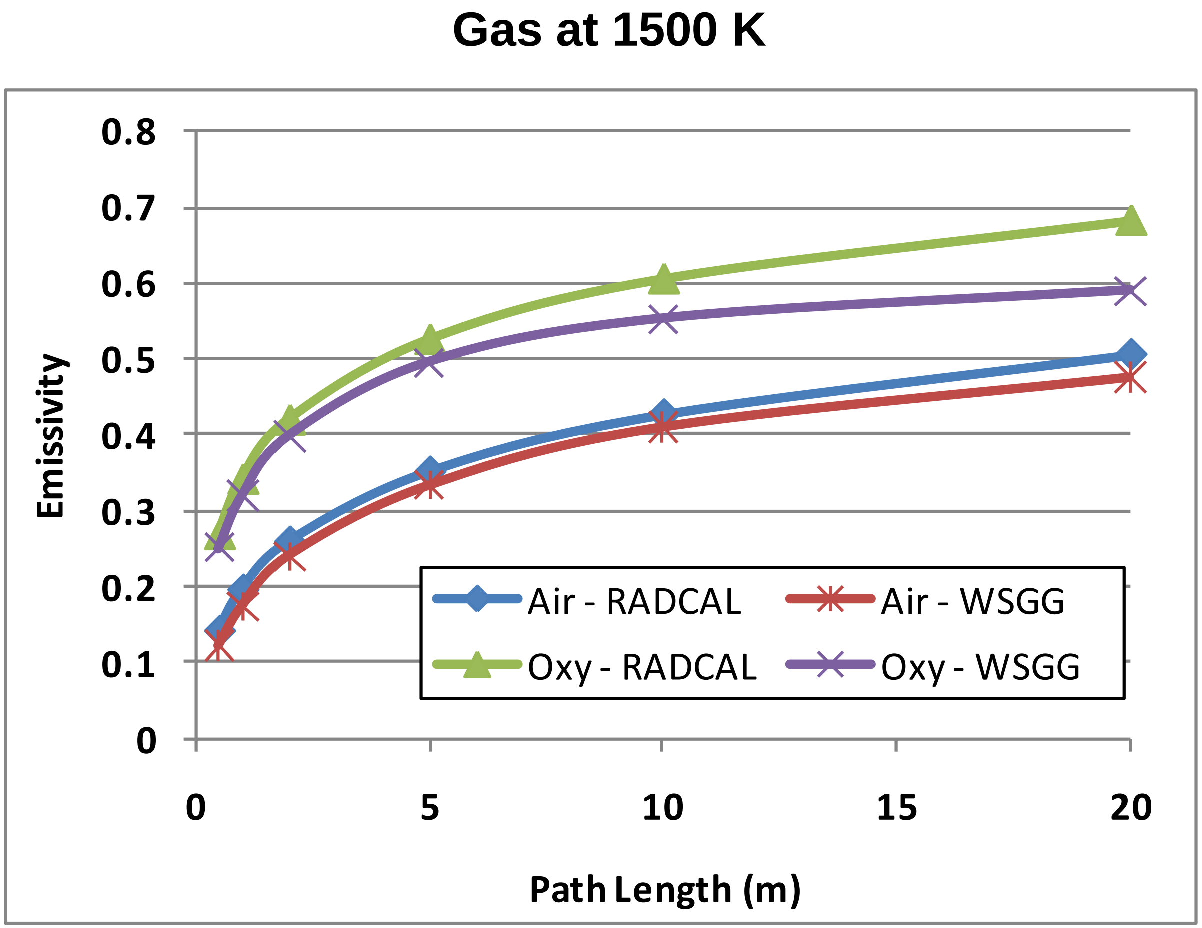
Emissivity Model Comparison



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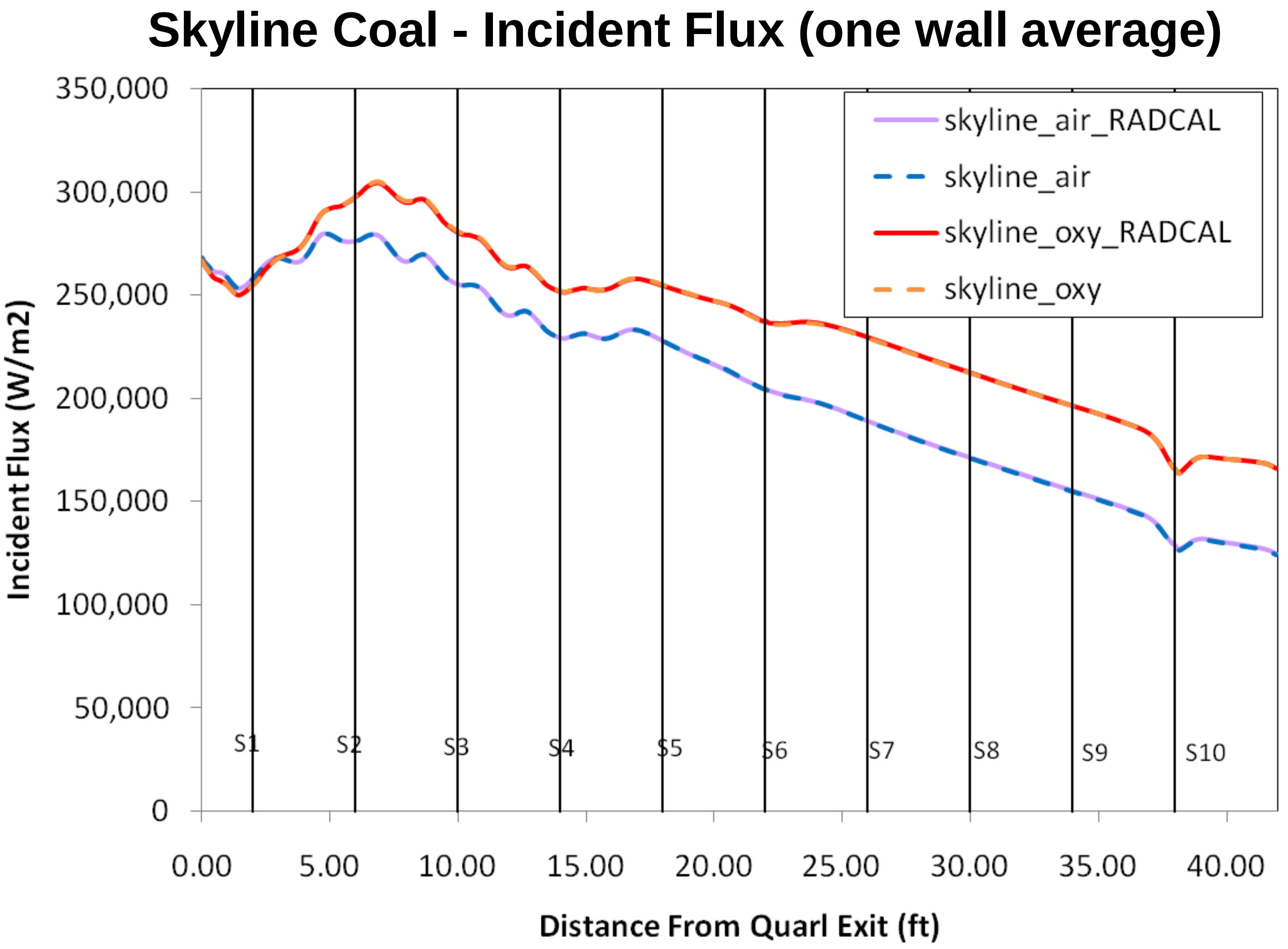
Incident Radiative Heat Flux Comparison



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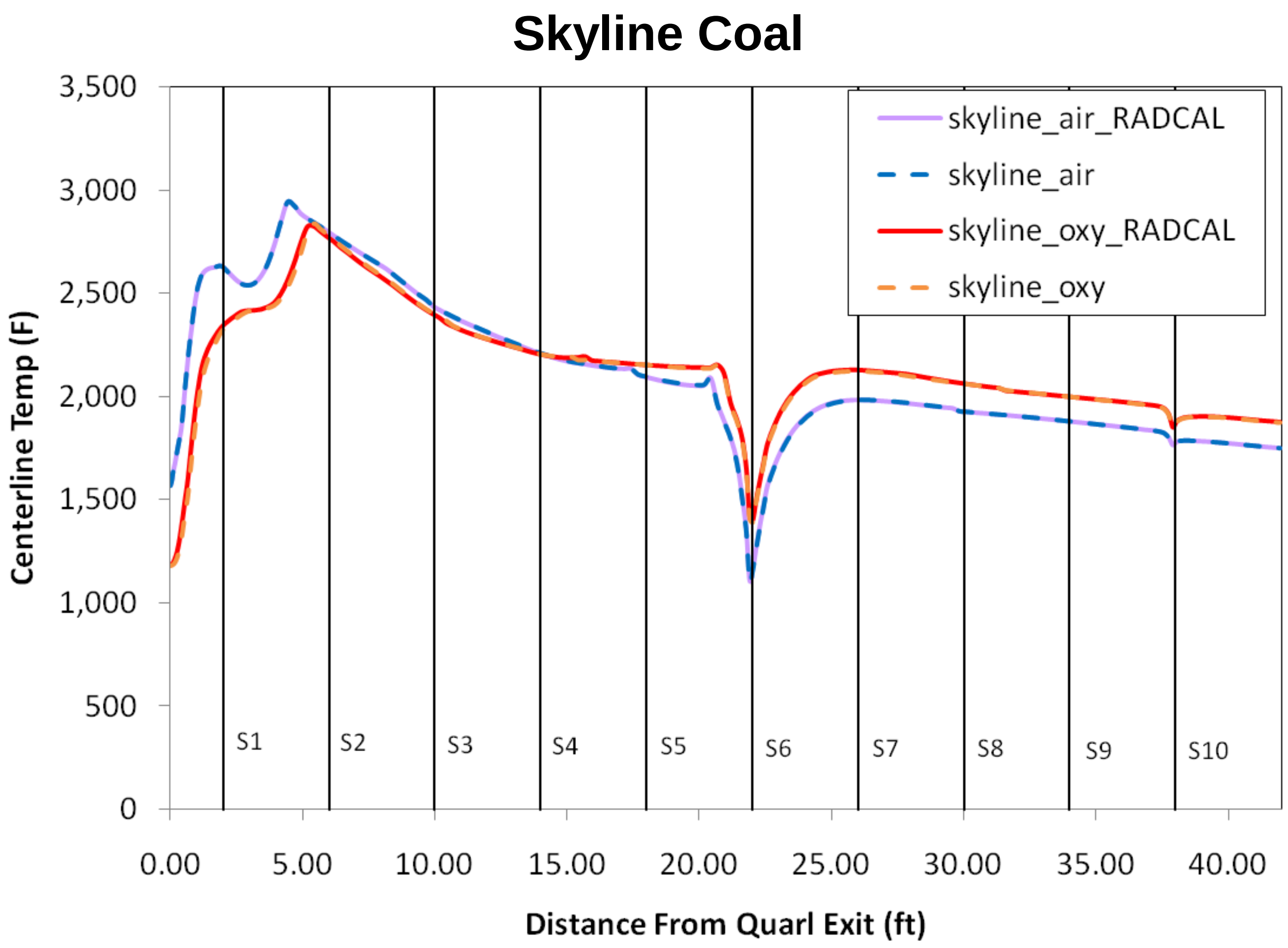
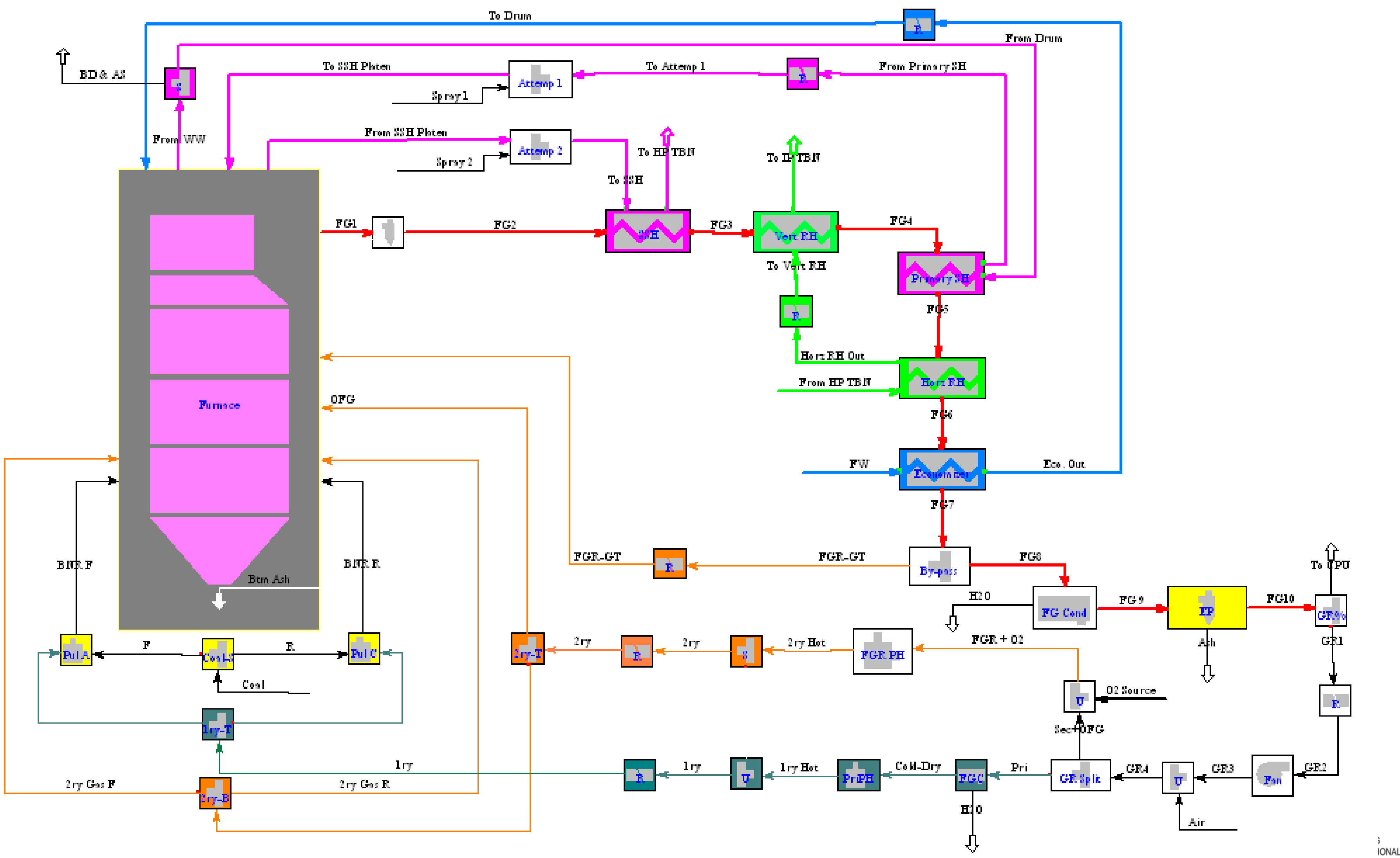
Furnace Centerline Temperature



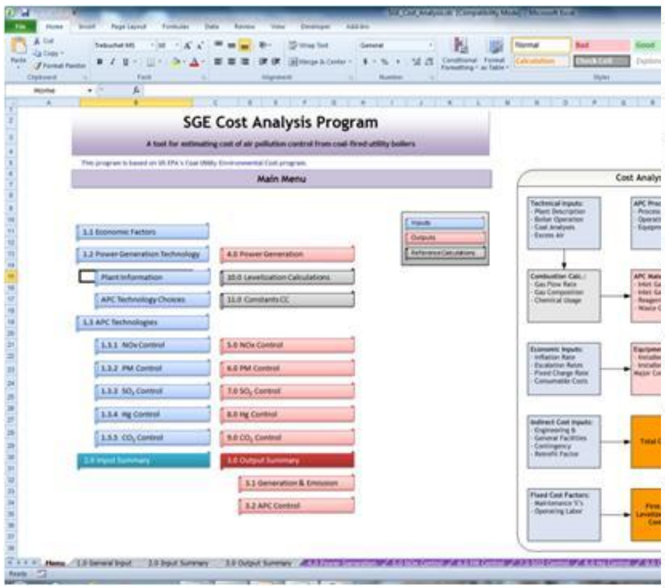
Conclusions

- **Predicted gas temperature trends were correct, including temperature cross-over; oxy-fired predictions higher than measured data in staged zone**
- **Enhanced char oxidation model showed increased CO production in staged zone and better agreement with air data**
- **Refined gas emissivity model had negligible impact on results**
- **Model comparisons are on-going, and will also include soot and corrosion data**
- **Current activity includes oxy-combustion assessment in full-scale boilers (Hunter and River Rouge)**

Steam Gen Expert (SGE) Process Modeling



Oxy-coal Retrofit Cost Analysis



	DOE/NETL*		CUECost	
	Ref	CO_2 Capture	Ref	CO_2 Capture
Gross MW	580	663	580	663
Net MW	550	550	547	555
Heat Rate (Btu/kWh)	8687	12002	8687	12002
Auxiliary power (MW)	30	113	33	108
Base plant load	26	42	26	42
FG Cleanup (SCR, baghouse, FGD, CO_2 capture)	4	26	7	12
CO_2 compression	-	45	-	54
Total plant capital cost ($/kWe)	1647	2913	1729	2904
% increase		77%		68%
Base Plant (including SCR)	1413	1763	1476	1595
PM & SO_x capture	234	297	253	303
CO_2 capture	-	766	-	882
CO_2 compression	-	87	-	124
COE ($/MWh) (levelized)	74.7	135.2	65.3	121.3
Capital	40.2	75.7	31.8	53.2
O&M	34.4	52.4	33.5	61.0
Fuel	18.0	24.9	18.9	29.4
Variable	6.3	11.0	6.4	16.9
Fixed	10.1	16.5	8.2	14.7
CO_2 TS&M	-	7.1	-	7.1
Increase in COE (%)		81		86
$/tonne CO_2 avoided		69		79

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Acknowledgments

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- **University of Utah Industrial Combustion and Gasification Research Facility technical staff**
- **CFD results displayed with Fieldview by Intelligent Light (www.ilight.com)**

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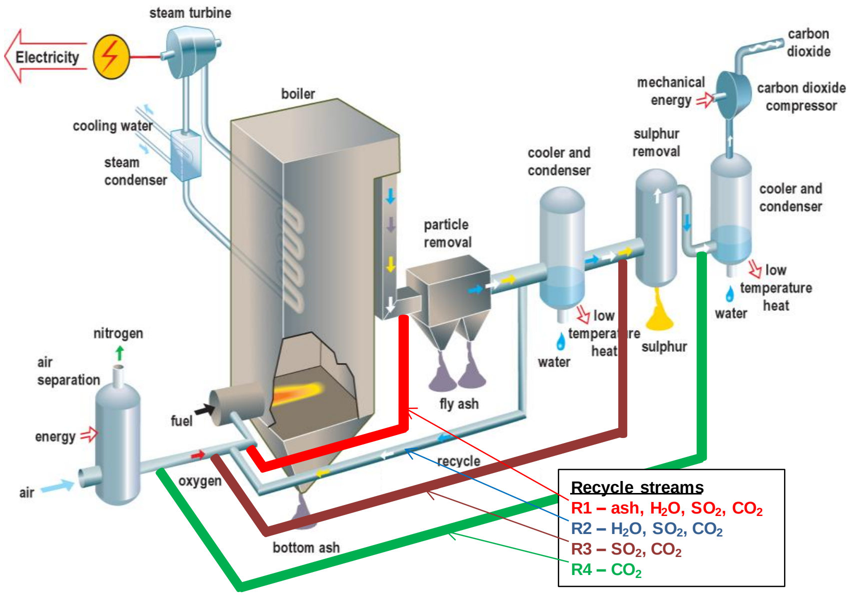
Retrofit Assessment Capability

Evaluate impact of oxy-firing design and flue gas recycle (FGR) ratio and composition on:

- **Combustion Characteristics**
  - **Heat transfer (temperature, emissivity, sooting)**
  - **Particle ignition, char burnout**
  - **NOx, SOx, fine particulates**
- **Surface Characteristics**
  - **Heat flux profiles**
  - **Slagging**
  - **Fouling**
  - **Corrosion**



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