Application of Soot Model to a Pulverized Coal-Fired Boiler : *Pilot-scale Study*

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17th Annual ACERC Technical Conference
Salt Lake City, Utah
February 20 - 21, 2003

Outline

- Background
- Soot Model
- Experimental
- Pilot-scale Study
  - Model verification
  - Impact of burner and OFA operation
- Conclusions
- Future Options

Background

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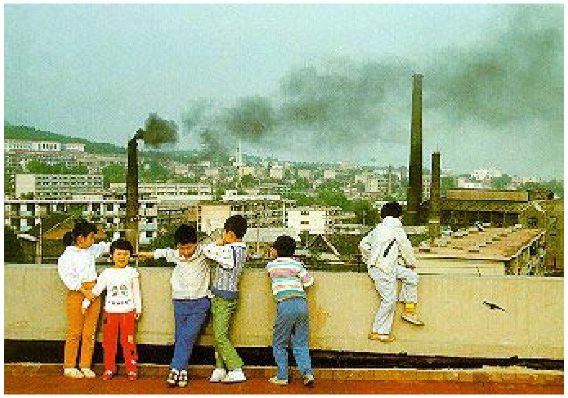
- Low NOx combustion can result in significant concentrations of submicron soot particles.
- Potential Impacts:
  - Increase in fine particulate emissions and opacity
  - Boiler heat imbalances due to enhanced lower furnace radiation
  - Potential decrease in effectiveness of air staging for NOx control
  - Ash salability
- Computational Fluid Dynamics



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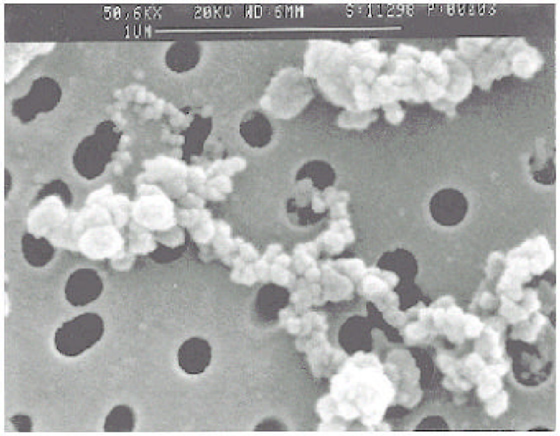
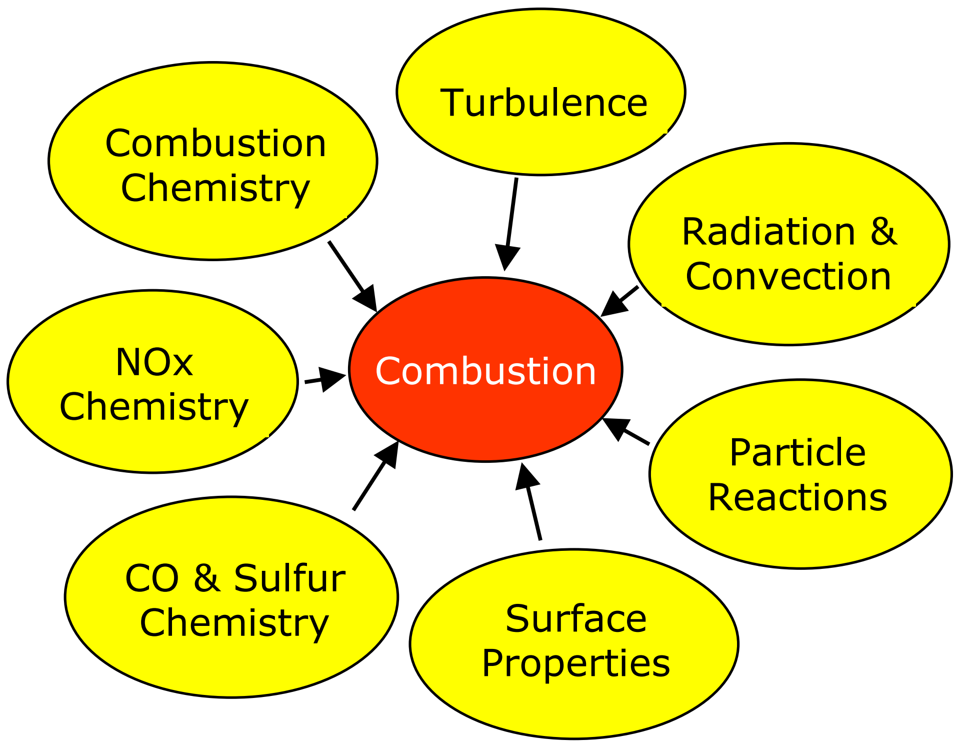


Veranth, J.M.; Fletcher, T.H.; Pershing, D.W. and Sarofim, A.F. Fuel, 79(9), 1067-1075 (2000).

GLACIER Overview

- Advanced CFD Code
- Over 100 combustion system modeled
- Over 8 years of industrial application
- Designed to handle "real-world" applications
  - Judicious use of sub-models & numerics
  - Qualified modelers

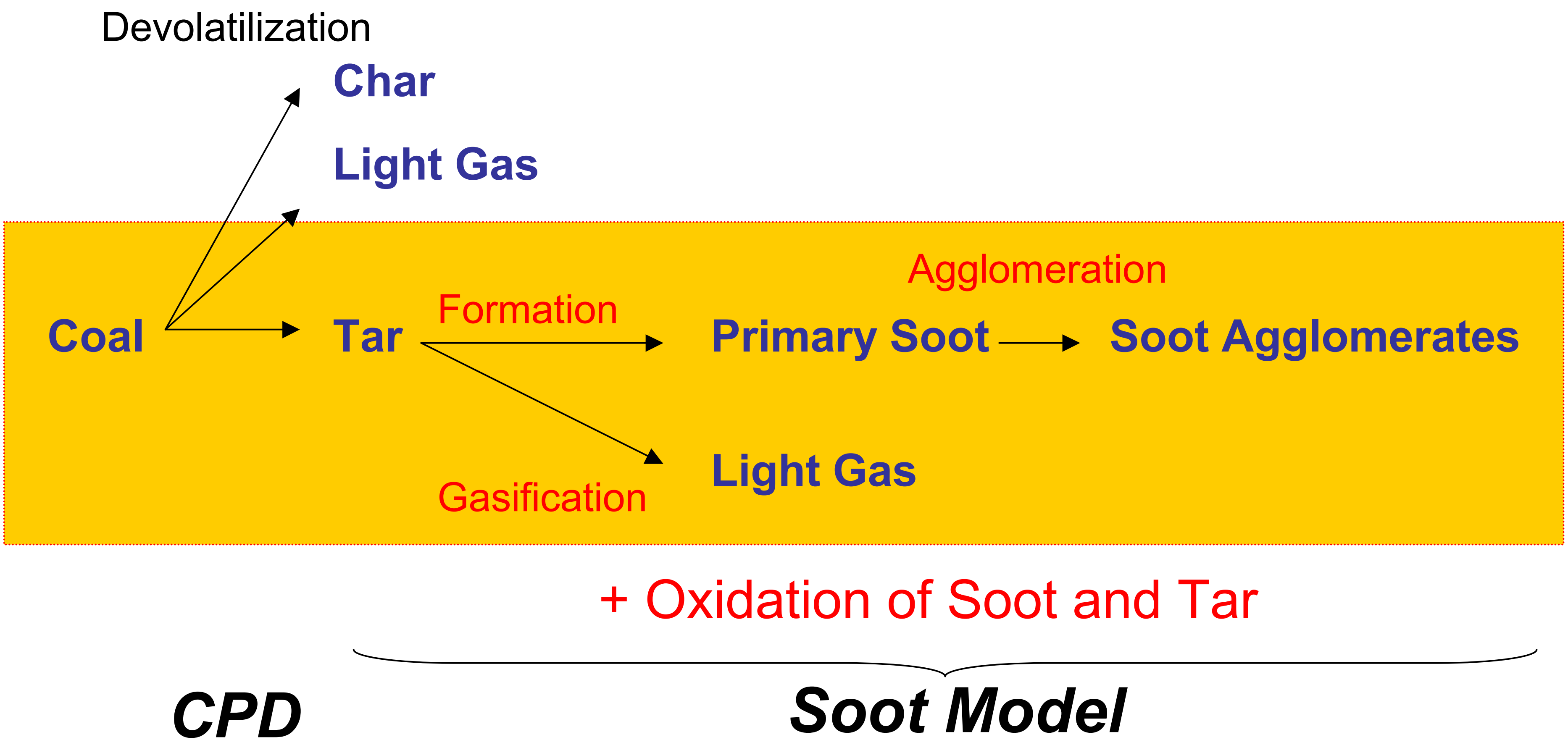


Soot Model

- Semiempirical model*
  - Soot is assumed to form from only tar.
  - Tar yields is calculated by CPD model† based on measured coal characteristics.
  - Three equations for conservation of the mass of soot and tar, and the 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.*

Assumed Mechanism



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

Conservation Equations

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$$\vec{\nabla}\cdot\left(\rho_g \vec{u} X\right) = \vec{\nabla}\cdot\left(\frac{\mu}{\sigma}\vec{\nabla}X\right) + \rho_g S$$

	X	S
Mass of Soot	Y_C	$S_{Yc} = \dot{r}_{FC} - \dot{r}_{OC}$
Mass of Tar	Y_T	$S_{Y_T} = \dot{r}_{FT} - \dot{r}_{FC} - \dot{r}_{GT} - \dot{r}_{OT}$
Number of Soot Particles	N_C	$S_{Nc} = \left(\frac{N_a}{M_C C_{\min}}\right)\dot{r}_{FC} - \dot{r}_{AN}$

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

Reaction Rates

	Reaction Rate
Formation of Tar	$\dot{r}_{FT} = SP_{tar}$
Oxidation of Tar	$\dot{r}_{OT} = \rho_g [c_T][c_{O2}] A_{OT} e^{-E_{OT}/RT}$
Gasification of Tar	$\dot{r}_{GT} = [c_T] A_{GT} e^{-E_{GT}/RT}$
Formation of Soot	$\dot{r}_{FC} = [c_T] A_{FC} e^{-E_{FC}/RT}$
Oxidation of Soot	$\dot{r}_{OC} = SA_{v,C} \frac{p_{O2}}{T^{1/2}} A_{OC} e^{-E_{OC}/RT}$ $\quad SA_{v,C} = \rho_g (\pi N_C)^{\frac{1}{3}} \left(\frac{6Y_C}{\rho_C}\right)^{\frac{2}{3}}$
Agglomeration of the particles per unit mass	$\dot{r}_{AN} = 2C_a \left(\frac{6M_C}{\pi\rho_C}\right)^{\frac{1}{6}} \left(\frac{6kT}{\rho_C}\right)^{\frac{1}{2}} \left(\frac{\rho_g Y_C}{M_C}\right)^{\frac{1}{6}} (\rho_g N_C)^{\frac{11}{6}}$

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

Arrhenius Constants

Term	A	E (kJ/gmol)
Tar Oxidation	6.77×10^{5} (1/s)	52.3
Tar Gasification	9.77×10^{10} (1/s)	286.9
Soot Formation	5.02×10^{8} (1/s)	198.9
Soot Oxidation	1.09×10^{4} ($K^{1/2}$/s)	164.5

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

Carbonization Rate

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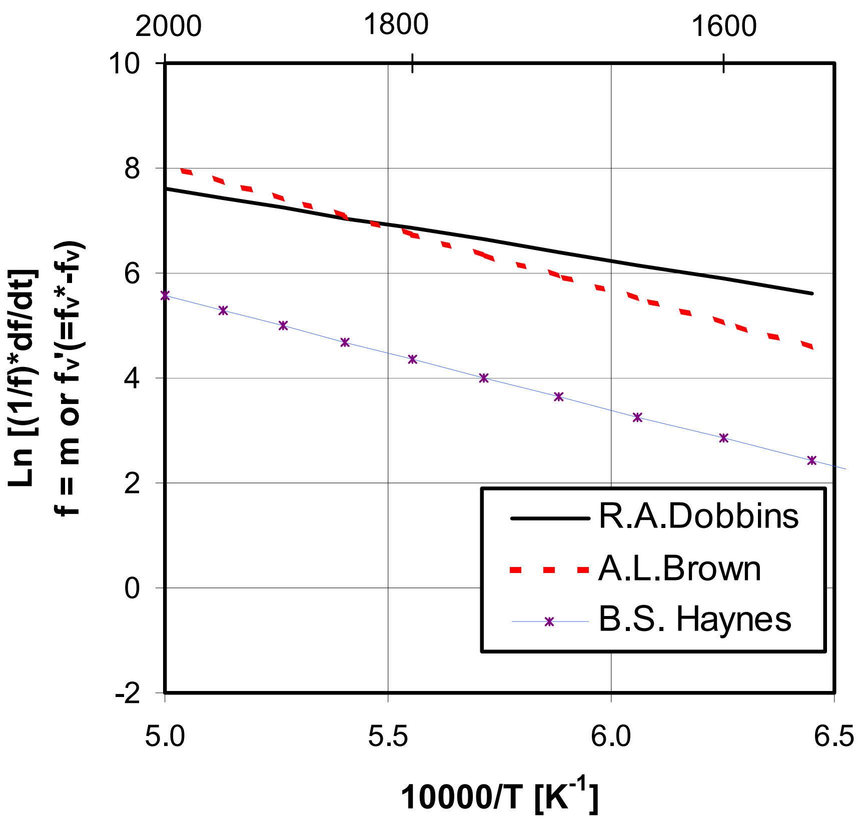

	A [sec^{-1}]	E [kJ/mol]
R. A. Dobbins et al. [1996]	1.78×10^6	113
A. L. Brown et al. [1998]*	5.02×10^8	198.9
B. S. Haynes et al. [1983]	1.3×10^7	180

* Reference can be found in 'Brown, A. L.;Fletcher, T.H. *Energy & Fuels* **1998**, 12, 745-757.'
Haynes, B. S.;Wagner, H.G. *Z. Phys. Chem.* [N.S.] **1983**, 133, 201-213

Pilot-scale Test Furnace

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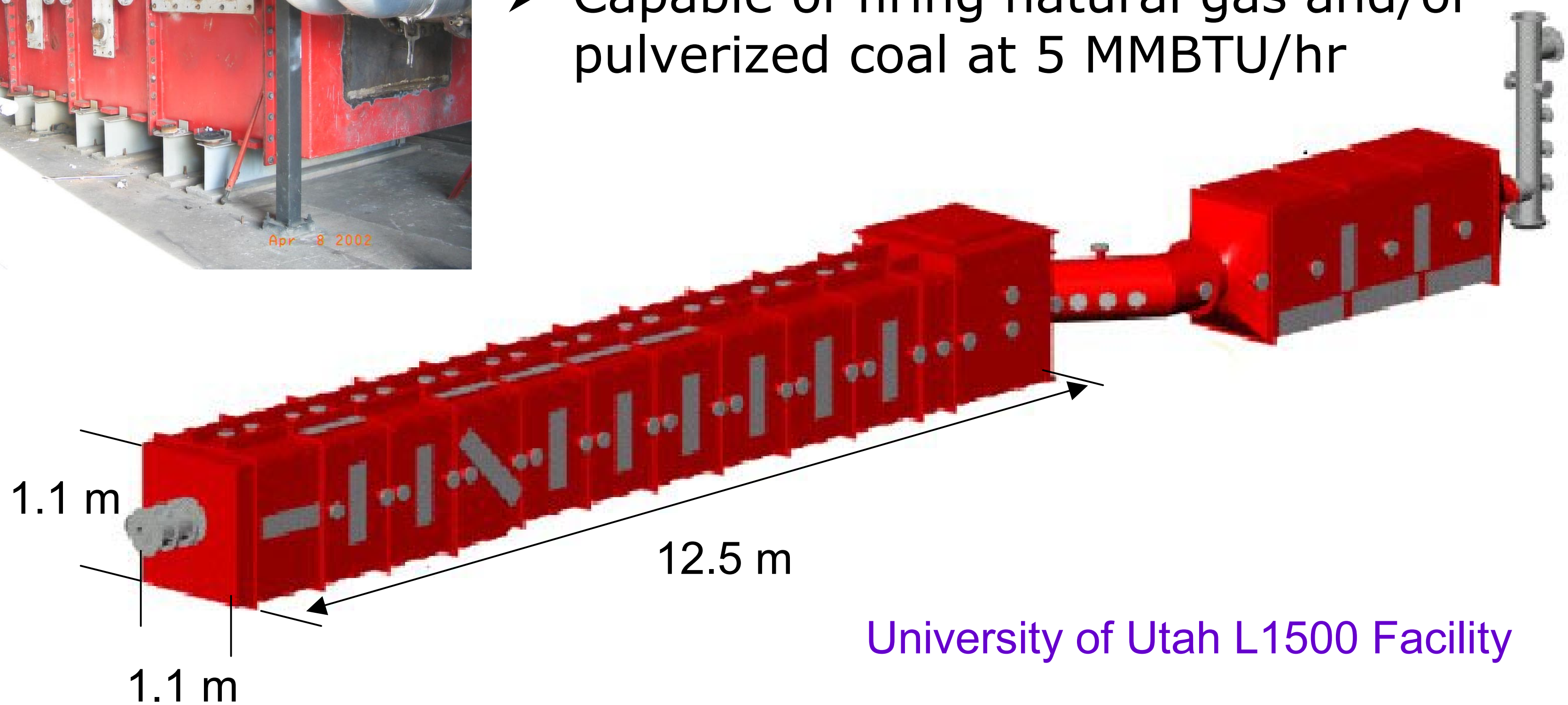
- The horizontal-fired combustor is 1.1 m x 1.1 m square and 12.5 meters long
- Capable of firing natural gas and/or pulverized coal at 5 MMBTU/hr



University of Utah L1500 Facility

5 MMBtu/hr Low NOx Burner

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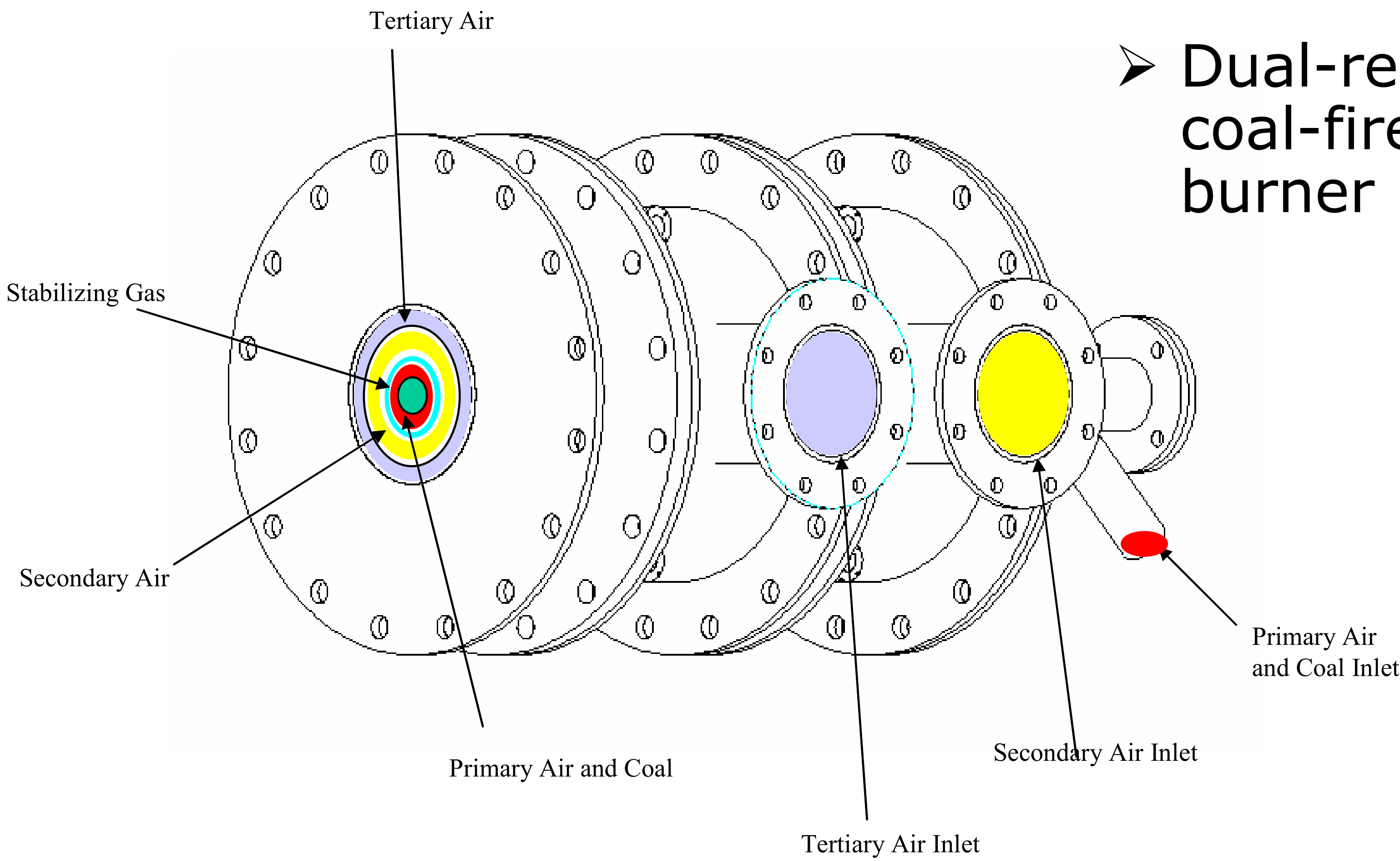

- Dual-register coal-fired burner

Photoacoustic Analyzer

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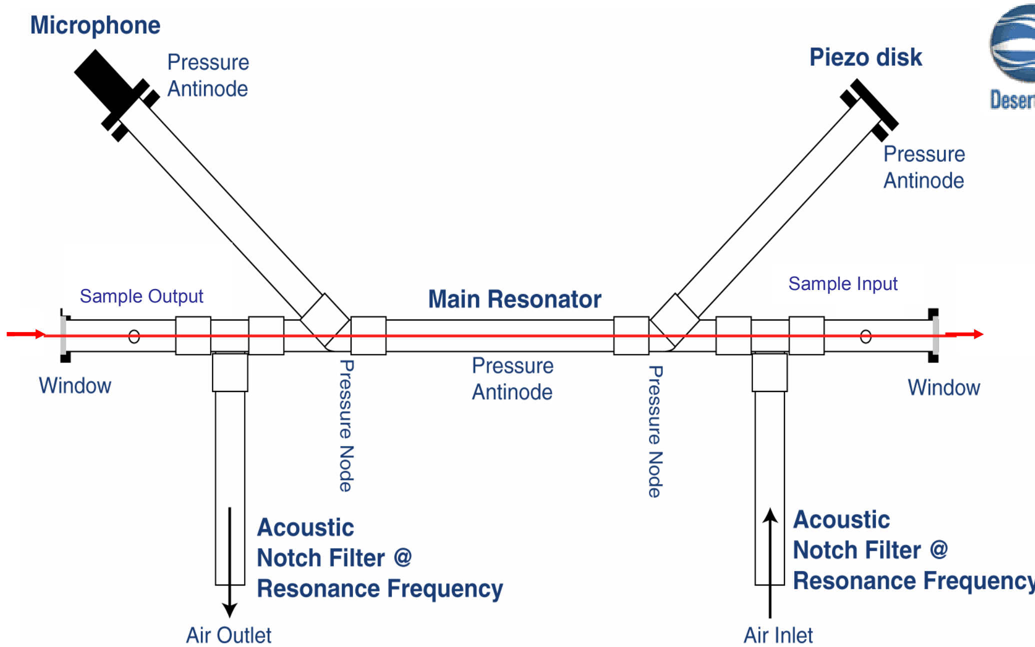

Desert Research Institute

- **<u>Principle</u>**
  - Detection of acoustic pressure wave resulting from surrounding air expansion by light absorbed aerosols

- **<u>Advantages</u>**
  - Direct method to measure in-situ light absorption by aerosol
  - Elimination of possible sample contamination and/or loss when in-direct method is used

Sampling Set-up

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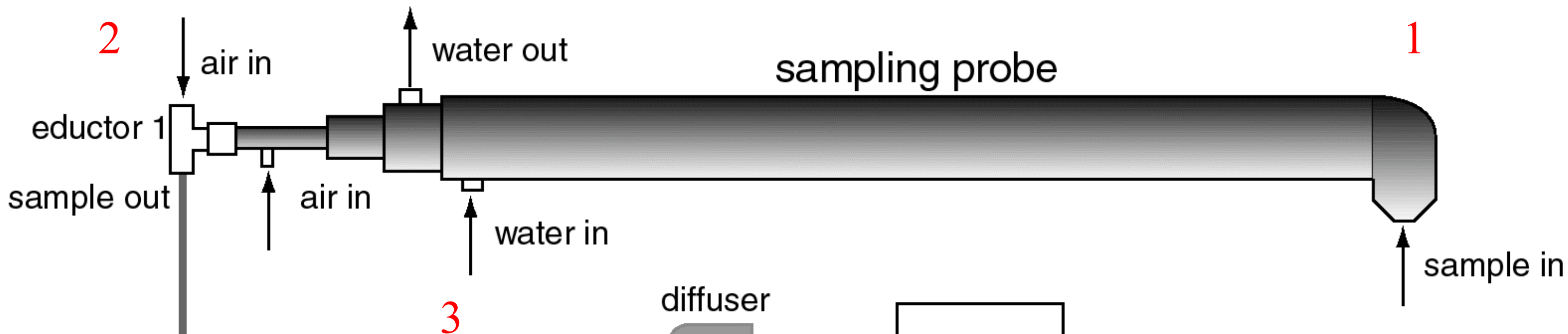
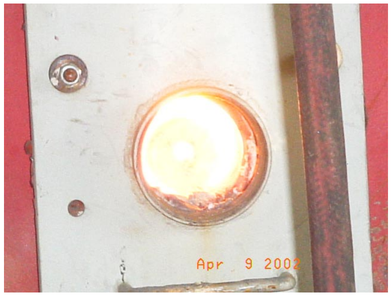
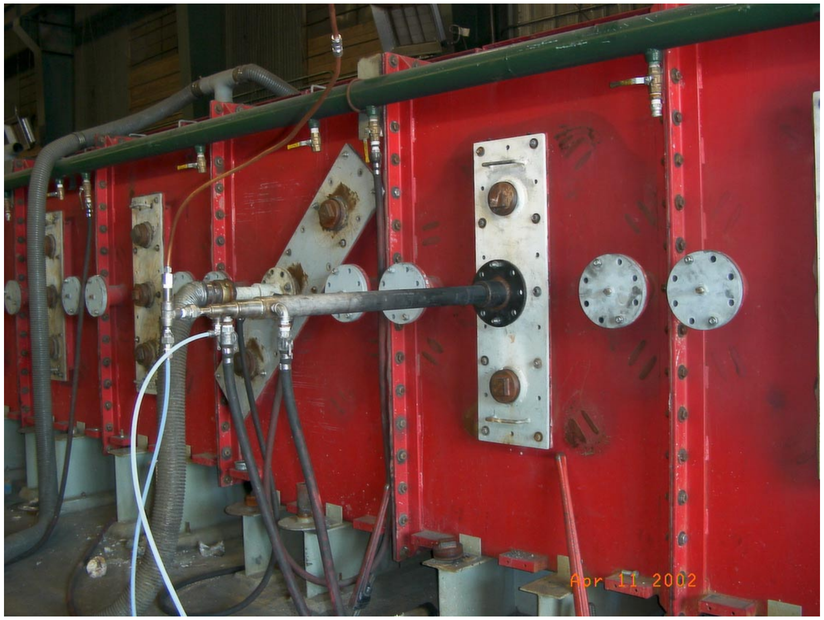




- Water-cooled, air-quenched transpiration sampling probe
- Four stage dilutions: At the transpiration probe tip (1) and three eductors (2, 3, and 4)
- Various dilution ratios, ranged from 400 to 3800 (at ambient temperature)

Soot Measurements



Sampling probe at the 3rd section

PA with flow control and data acquisition system

Operating Conditions

	Case 1	Case 2	Case 3	Case 4
Burner Stoichiometry	0.75	0.85	0.95	1.05
Overall Stoichiometry	1.15	1.15	1.15	1.15
Coal Feeding Rate [lb/hr]	320	323	323	325
Air Flow Rate [lb/hr]				
primary	448	449	450	449
secondary	607	693	796	900
tertiary	1,211	1,382	1,592	1,805
staging	1,197	896	597	383
Exit O_2, dry	3.0	3.0	3.0	3.0

- Staging air port (OFA) was located at 4.5 meter from the burner inlet for all cases

Coal Properties

- Proximate analysis

	As Received
Fixed Carbon	45.46
Volatile Matter	39.42
Moisture	4.68
Ash	10.44
Total	**100.0**

- Ultimate analysis

	As Received
Carbon	69.65
Hydrogen	4.42
Nitrogen	1.25
Sulfur	0.40
Oxygen	9.16
Moisture	4.68
Ash	10.44
Total	**100.0**

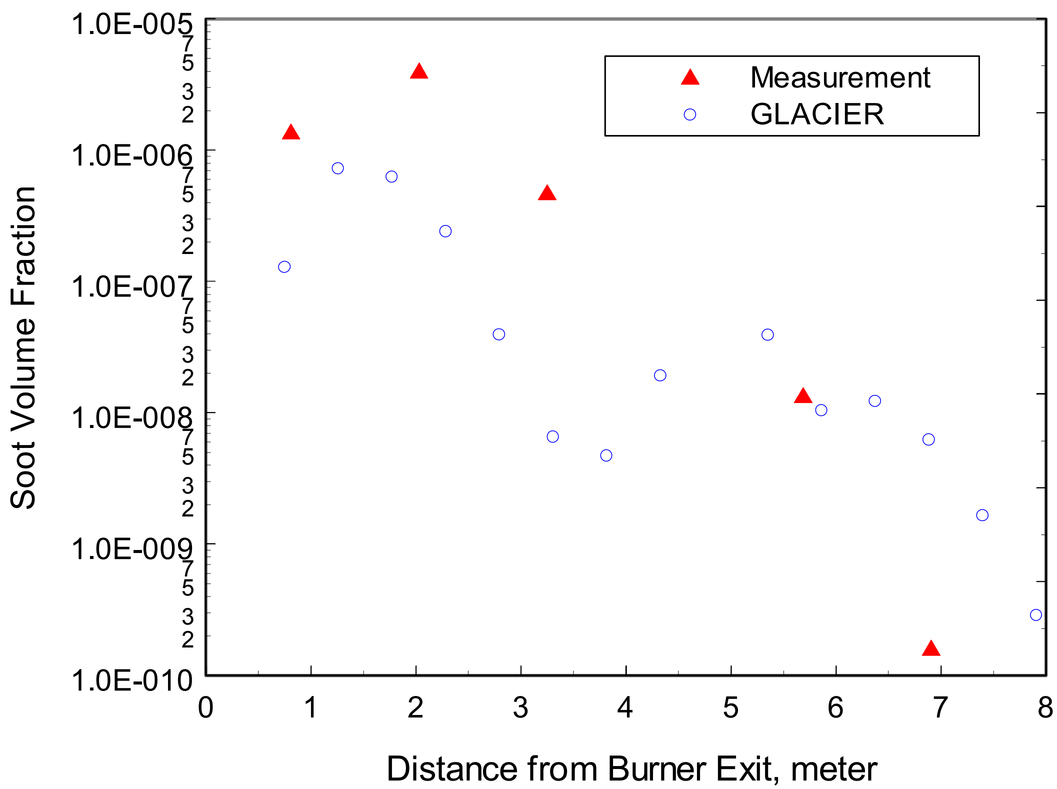
- Coal Particle Size

Size (μm)	Mass Fraction
16.5	0.017
26.4	0.063
40.4	0.283
59.4	0.284
86.8	0.233
122.6	0.072
169.6	0.043
278.5	0.005

- Mass Average Diameter

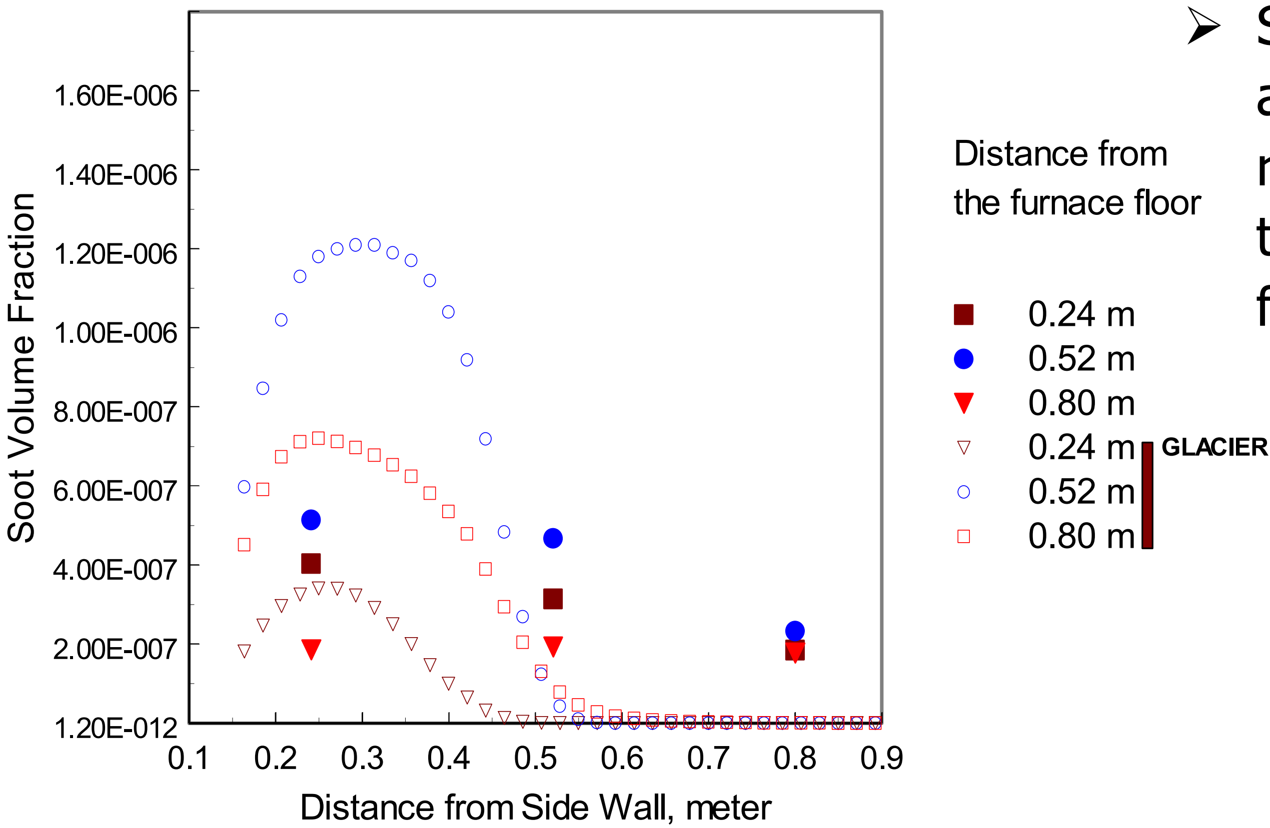
68.0 μm

Soot Volume Fraction



- Soot volume fraction along the centerline of the furnace for Case 1
  - Under-prediction before OFA by a factor of 5
  - Over-prediction after OFA by a factor of 40
  - Swirl and recirculation flow pattern

Soot Volume Fraction



- Soot volume fraction as a function of radial distance from the furnace side wall for Case 1
  - Non-uniform distribution of soot
  - Recirculation and swirl pattern in the furnace

Impact of Burner Stoichiomety

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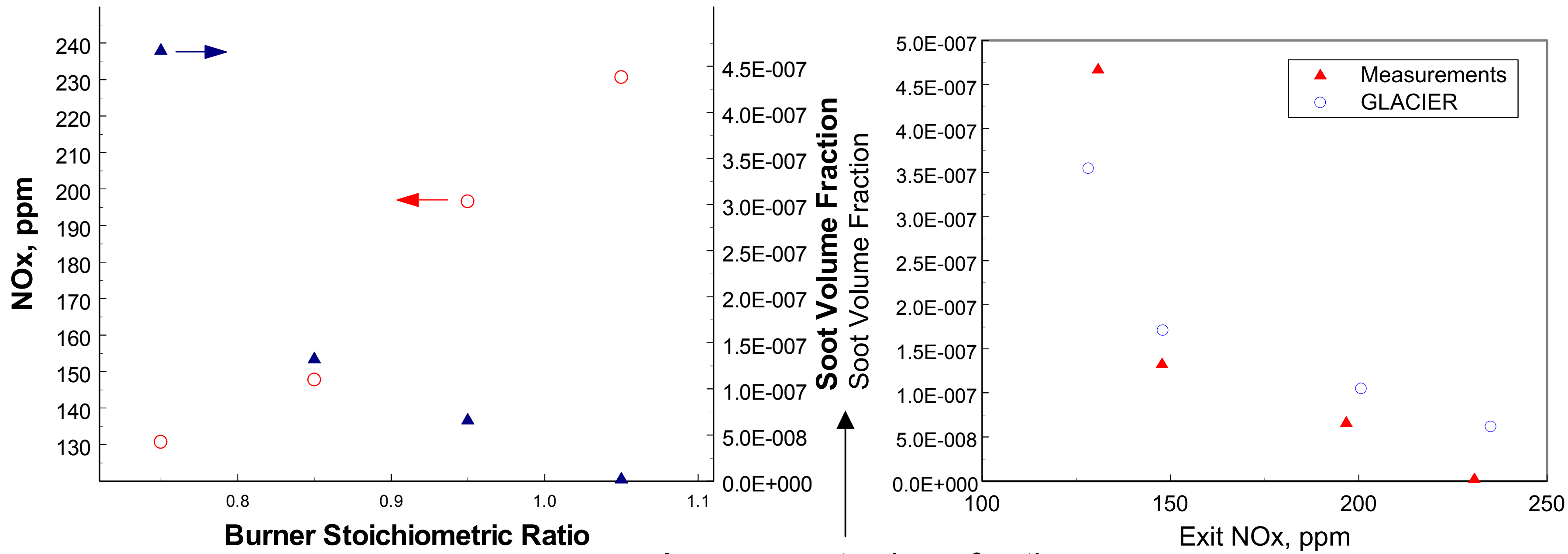

Average soot volume fraction

- With decreasing burner stoichiometry
  - Decrease in NOx
  - Increase in soot volume fraction

- Soot volume fraction vs. NOx
  - Good agreement!

Impact of OFA Location

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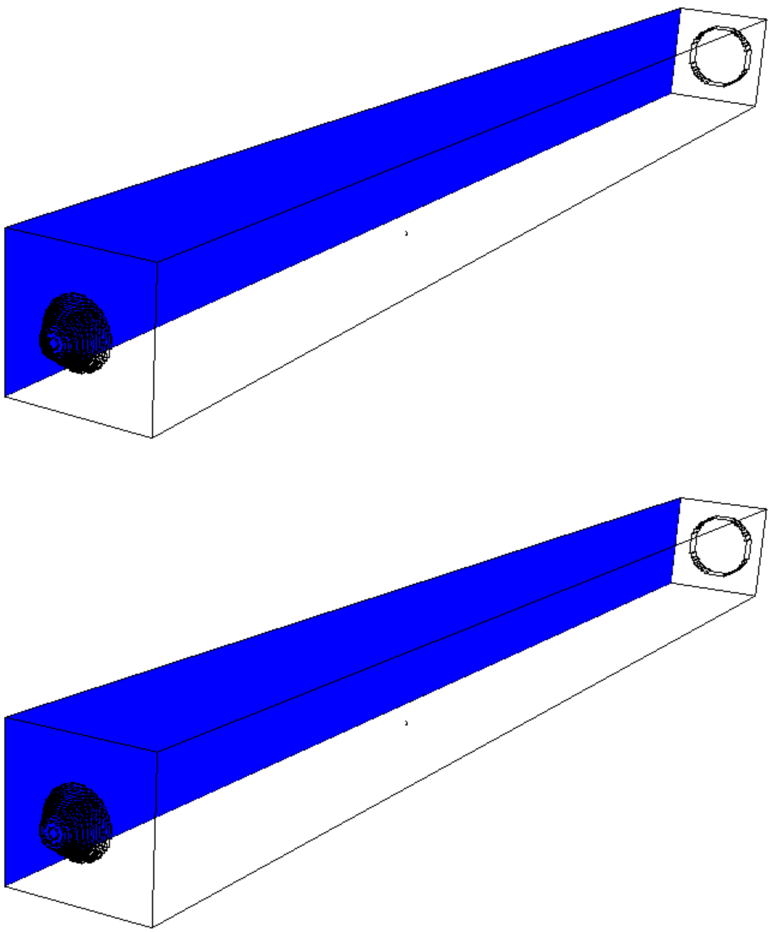
- Hypothesis:
  - Different staging location can be significant in determining soot concentration in flue gas.
- Two cases (OFA 3 and 9)
  - Residence time from fuel injection to OFA port (2 vs 12 sec)
  - Temperature at downstream of the air staging port (1800 vs 1000 K)

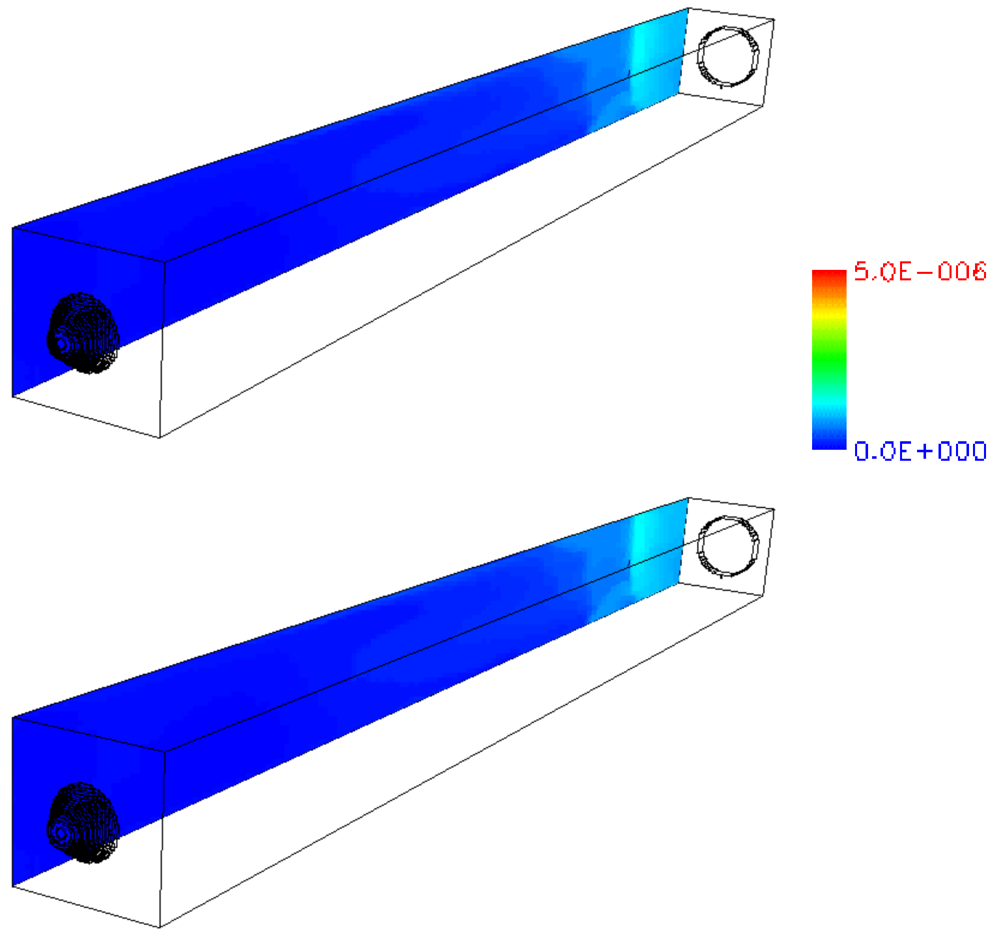
	OFA3 & 9		Illinois #5
Burner Stoichiometric Ratio	0.85		As Received [%]
Overall Stoichiometric Ratio	1.15	C	65.99
Primary air flow rate [lb/hr]	473	H	3.97
Secondary air flow rate [lb/hr]	700	O	8.47
Tertiary air flow rate [lb/hr]	1,392	N	1.29
Staging air flow rate [lb/hr]	929	S	3.49
Coal feeding rate [lb/hr]	345	Ash	9.87
		Moisture	6.92

Movies: Soot Volume Fraction

OFA 3



OFA 9



Soot Volume Fraction

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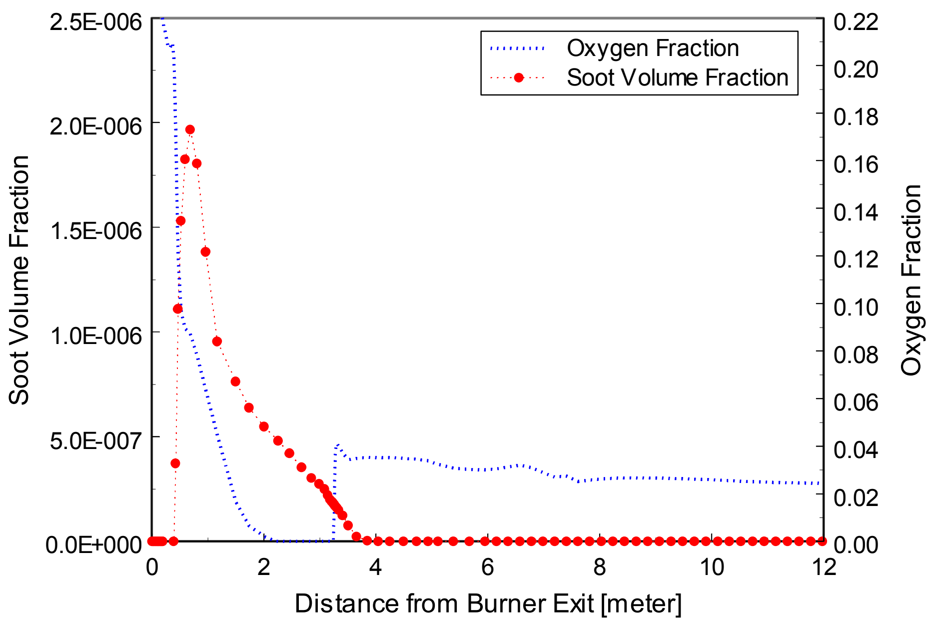
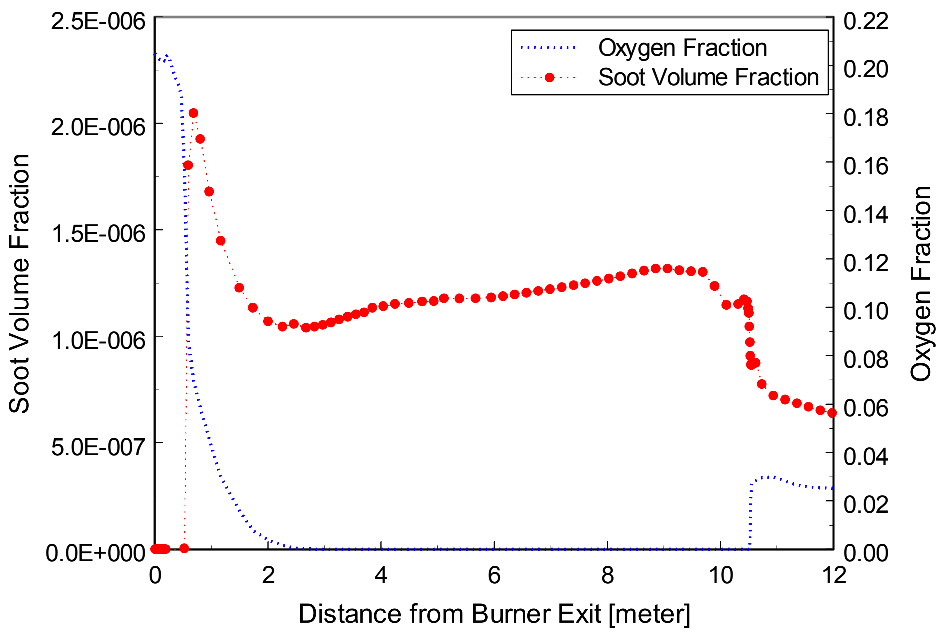
OFA 3

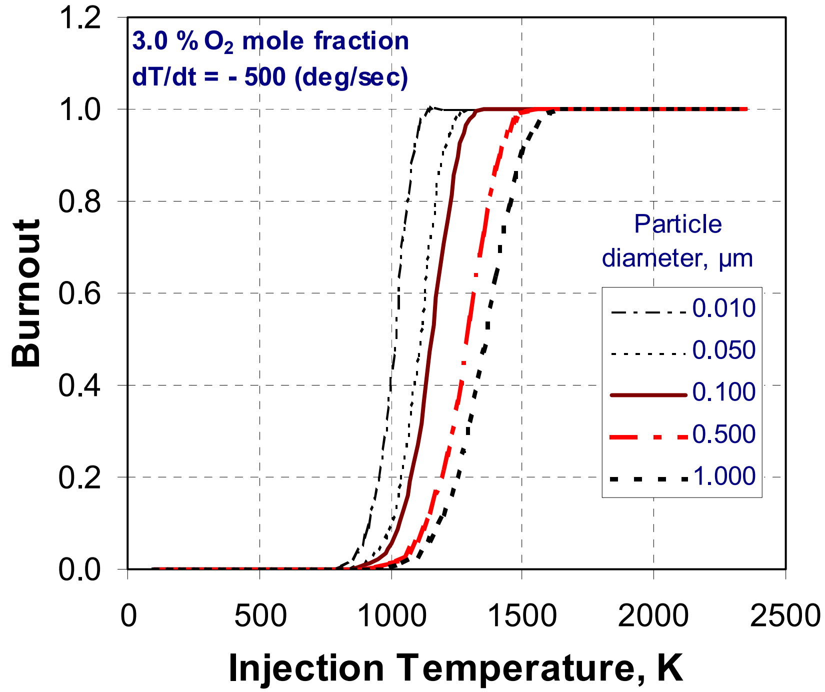


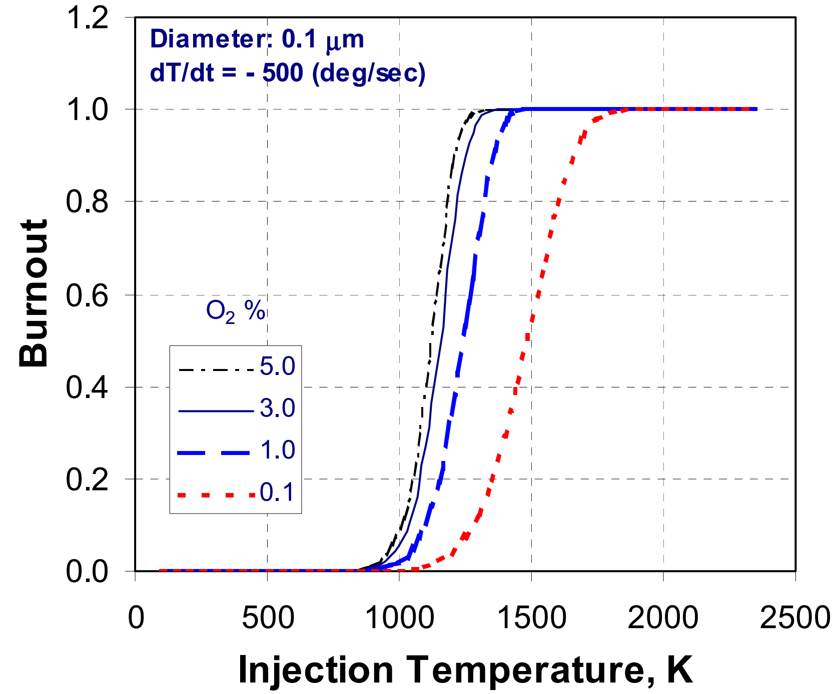
OFA 9



- Complete burnout for OFA 3
- OFA 9 results in high soot concentration in flue gas.
- Increased residence time can cause incomplete burnout resulting in high soot concentration in flue gas.

Soot Burnout Propensity





- Burnout level depends on soot particle size, available O_2, and temperature.

Conclusions

- Predictions showed a good agreement with the measurements.
- Predicted impact of burner operating conditions on soot concentration was in good agreement with the measurements.
- The impact of OFA location can be significant on soot formation/destruction.
- The level of detail provided by the simulations can be a valuable aid in understanding the mechanisms by which combustion modifications affect soot formation/destruction and NOx emissions.

Future Options

- Full-scale simulation (done! Will be presented at the 2003 Clearwater meeting)
- Develop a correlation between soot concentration and visible measurements
- Look at soot impacts on ash properties
- Model improvements:
  - OH oxidation
  - Thermophoresis
  - Deposition
  - Nitrogen chemistry

Acknowledgements

- Funding has been provided by the Department of Energy
- Prof. Fletcher and Dr. Hill @ Brigham Young University
- Ryan Okerlund @ University of Utah
- Jim Valentine and Dave Wang @ REI