WRI 06-R019

FINAL REPORT

REDUCTION OF NOx EMISSION FROM COAL COMBUSTION THROUGH OXYGEN ENRICHMENT

Task 49 Final Report
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For
BOC Process Gas Solutions
Murray Hills, New Jersey

And
U.S. Department of Energy
National Energy Technology Laboratory
Morgantown, West Virginia

By
Western Research Institute
Laramie, Wyoming

DISCLAIMER

ABSTRACT

BOC Process Gas Solutions and Western Research Institute (WRI) conducted a pilot-scale test program to evaluate the impact of oxygen enrichment on the emissions characteristics of pulverized coal. The combustion test facility (CTF) at WRI was used to assess the viability of the technique and determine the quantities of oxygen required for NOx reduction from coal fired boiler. In addition to the experimental work, a series of Computational Fluid Dynamics (CFD) simulations were made of the CTF under comparable conditions.

A series of oxygen enrichment test was performed using the CTF. In these tests, oxygen was injected into one of the following streams: (i) the primary air (PA), (ii) the secondary air (SA), and (iii) the combined primary and secondary air. Emission data were collected from all tests, and compared with the corresponding data from the baseline cases. A key test parameter was the burner stoichiometry ratio.

A series of CFD simulation models were devised to mimic the initial experiments in which secondary air was enriched with oxygen. The results from these models were compared against the experimental data.

Experimental evidence indicated that oxygen enrichment does appear to be able to reduce NOx levels from coal combustion, especially when operated at low over fire air (OFA) levels. The reductions observed however are significantly smaller than that reported by others (7-8% vs. 25-50%), questioning the economic viability of the technique. This technique may find favor with fuels that are difficult to burn or stabilize at high OFA and produce excessive LOI.

While CFD simulation appears to predict NO amounts in the correct order of magnitude and the correct trend with staging, it is sensitive to thermal conditions and an accurate thermal prediction is essential. Furthermore, without development, Fluent's fuel-NO model cannot account for a solution sensitive fuel-N distribution between volatiles and char and thus cannot predict the trends seen in the experiment.

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EXECUTIVE SUMMARY

BOC Process Gas Solutions and Western Research Institute (WRI) conducted a pilot-scale test program to evaluate the impact of oxygen enrichment on the emissions characteristics of pulverized coal.

BOC has a specific interest in how low levels of oxygen enrichment can affect coal combustion with the view to reducing NOx levels. The combustion test facility (CTF) at WRI was used to assess the viability of the technique and determine the quantities of oxygen required for NOx reduction from coal fired boiler. In addition to the experimental work, a series of Computational Fluid Dynamics (CFD) simulations were made of the CTF under comparable conditions.

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Experimental evidence indicated that oxygen enrichment does appear to be able to reduce NOx levels from coal combustion, especially when operated at low over fire air (OFA) levels. The reductions observed however are significantly smaller than that reported by others (7-8% vs. 25-50%), questioning the economic viability of the technique. It is possible that burners with clearly defined fuel-rich flame stabilization zones may exhibit better NOx reductions. It is also possible that this technique may find favor with fuels that are difficult to burn or stabilize at high OFA and produce excessive LOI.

While CFD simulation appears to predict NO amounts in the correct order of magnitude and the correct trend with staging, it is sensitive to thermal conditions and an accurate thermal prediction is essential. Furthermore, without development, Fluent’s fuel-NO model cannot account for a solution sensitive fuel-N distribution between volatiles and char and thus cannot predict the trends seen in the experiment.

BACKGROUND

BOC has a specific interest in how low levels of oxygen enrichment can affect coal combustion with the view to reducing NOx levels. It is well understood that oxygen enrichment at a given stoichiometry (air/fuel ratio) will increase local temperatures, due to a reduction in the local concentration of diluent nitrogen. This leads to increases in heating, reaction rates and flame stability. This raises the potential for reducing NOx emissions through a number of mechanisms:

- Enhancing the pyrolysis of the coal particle through exposure to higher temperatures has the effect of both increasing the rate and driving more nitrogen out as NH_3 and HCN into an oxidant depleted region near the burner, where the reduction to N_2 is likely. This leads to lower fuel bound nitrogen levels left for oxidation further down stream in the combustor, thus reducing the usual emissions of fuel-NOx prevalent from coal combustors.

- A further benefit of enhancing the pyrolysis rate and higher local temperatures is that flame stability is likely to be improved through higher reaction rates. The effect of oxygen of improving flame stability is well understood in other applications and may be considered as being related to an increase in burning rate or flame speed. The effect of enhancing flame stability leads to the potential for running the combustor locally at reduced stoichiometries and hence raising the potential to stage the combustor more deeply and effectively, thus reducing thermal NOx.

- Further benefits potentially arise from elevating the temperature and heating rate of the coal particle through the use of oxygen. Coal particle fragmentation may be enhanced through the rapid evolution of volatiles and thermal shock, this again improving flame stability and, as above, leading to the potential for reducing NOx and reducing grinding requirements. There is also the potential to use lower grades of coal than would previously be possible through the improvement in flame stability.

Given these mechanisms it was postulated that if implemented correctly, oxygen enrichment in coal-fired systems has the potential to reduce NOx emissions levels. The Combustion Test Facility (CTF) at WRI was used to assess the viability of the technique and determine the quantities of oxygen required for NOx reduction from coal-fired boilers. In addition to the experimental work a series of CFD simulations were made of the CTF under comparable conditions.

WRI COMBUSTION TEST FACILITY

The WRI coal combustion test facility (CTF) is a nominal 30-pph, balanced-draft system designed to replicate a pulverized coal-fired utility boiler. In its present configuration (Figs. 1 and 2), the unit has been set up to simulate a tangential-fired boiler, but may be easily adapted to wall-fired or other configurations. The fuel feed system consists of screw-based feeders and pneumatic transport to four burners inserted in the corners of a refractory-lined firebox. The burners can be angled to attain different tangential flow characteristics in the firebox. The unit is equipped with appropriately sized heat-recovery surfaces such that the time/temperature profile of a utility boiler can be replicated, and includes provisions for preheating the combustion air to mimic a utility air preheater. The system also includes over-fire air injection ports for combustion staging. The unit is equipped with a bag filter and solids and gas sampling.

Figure 1 CTF Facility at WRI

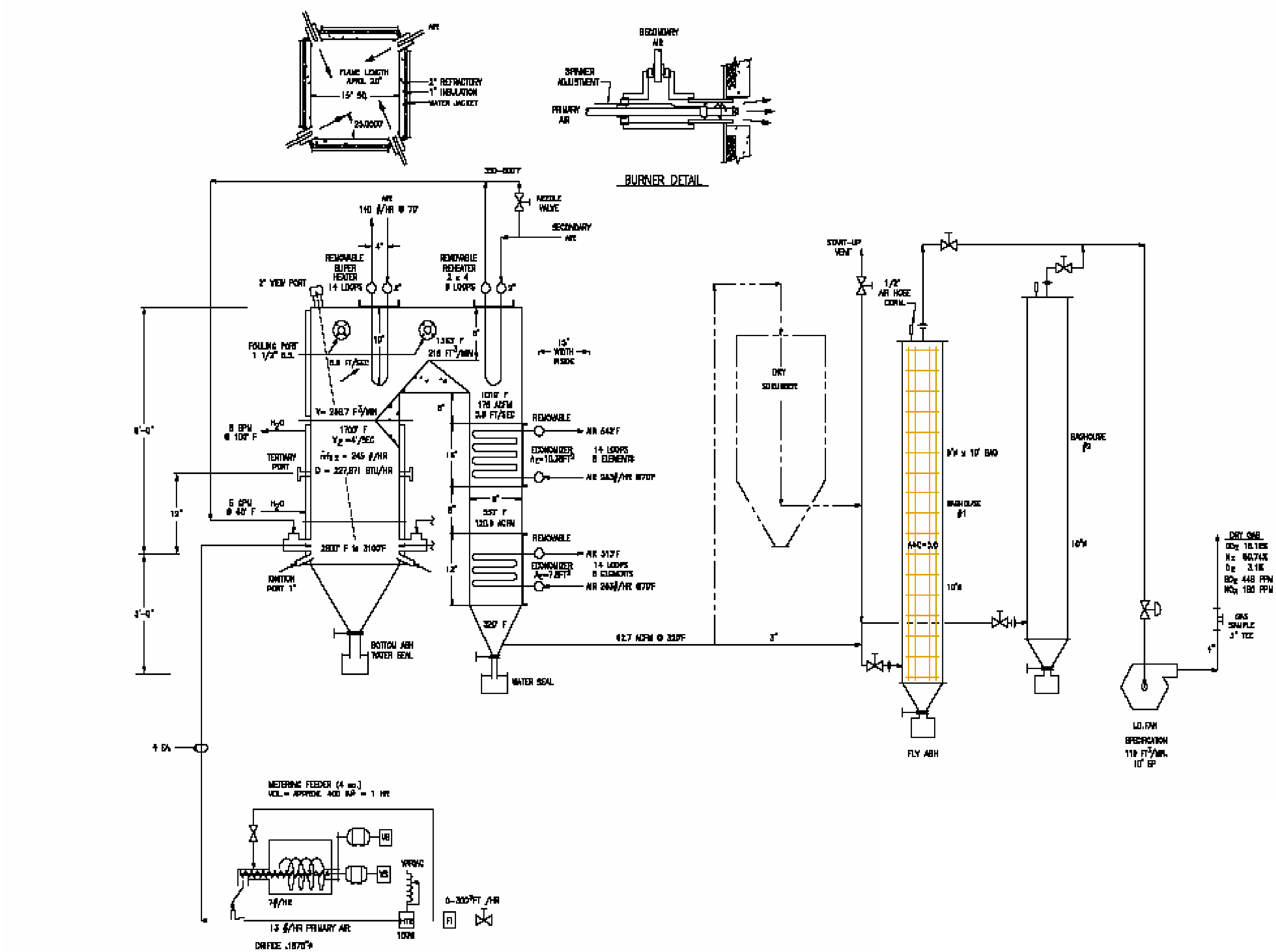


Figure 2 CTF Schematic

EXPERIMENTAL

A series of oxygen enrichment tests was performed using the CTF. In these tests, oxygen was injected into one of the following streams: (i) the primary air (PA), (ii) the secondary air (SA), and (iii) the combined primary and secondary air. Emissions data were collected for all tests, and compared with the corresponding data from the baseline cases, where no oxygen was injected. Lee Ranch coal was used for all trials with properties determined from Wyoming Analytical Laboratory (Table 1)

Table 1 Lee Ranch Coal Analysis

		As received wt%	dry wt%	daf wt%
Proximate				
	Moisture	7.56		
	Ash	17.33	18.75	
	Volatiles	38.36	41.50	51.08
	Fixed Carbon	36.75	39.75	48.92
	Total	100	100	100
Ultimate				
	Moisture	7.56		
	H	3.56	3.85	4.74
	C	58.61	63.4	78.03
	N	0.95	1.03	1.27
	S	0.84	0.91	1.12
	O	11.15	12.06	14.84
	Ash	17.33	18.75	
	Total	100	100	100
Heating Value (Btu/lb)		10,445	11,299	13,906

A key test parameter was the burner stoichiometry ratio (Burner SR), defined as the air/fuel ratio of the burners normalized against the air/fuel ratio required for stoichiometric combustion. The Burner SR was adjusted by changing the amount of overfire air (OFA) entering the CTF downstream of the burners. Increasing (decreasing) the OFA flowrate had the effect of decreasing (increasing) the Burner SR. Conditions were generally contained to the range indicated in Table 2, which lists the test parameters and their corresponding ranges. Enrichment levels were intentionally kept to low levels due to the desire to identify cost effective emissions reductions with small amounts of oxygen enrichment and the desire to maintain oxygen levels below 25% for safe operation.

Table 2 Test parameters and their corresponding ranges

Test Parameter	Range of Conditions
Burner stoichiometry	0.45-0.95
Fraction of air replaced with oxygen	6- 10%
Oxygen injection location	PA, SA, PA+SA

Initial experiments focused on the effect of the effect of secondary air at different OFA levels. In order to evaluate the effect of oxygen replacement, each enriched condition was preceded by the comparable air-fuel condition. Results from this series of trials are detailed in Table 3 and depicted in Figure 3 in terms of lbNOx/MMBtu as a function of burner stoichiometry. As expected for each data set there is a reduction in the amount of NOx as the near burner conditions become more reducing. While there is a fair amount of scatter in the data, there also appears to be a definite reduction in the amount of NOx emitted when oxygen is added. Oxygen appears to be most effective at reducing NOx at higher burner stoichiometries with reductions in the order of 11% being feasible, however its efficacy is significantly less as the OFA level is increased.

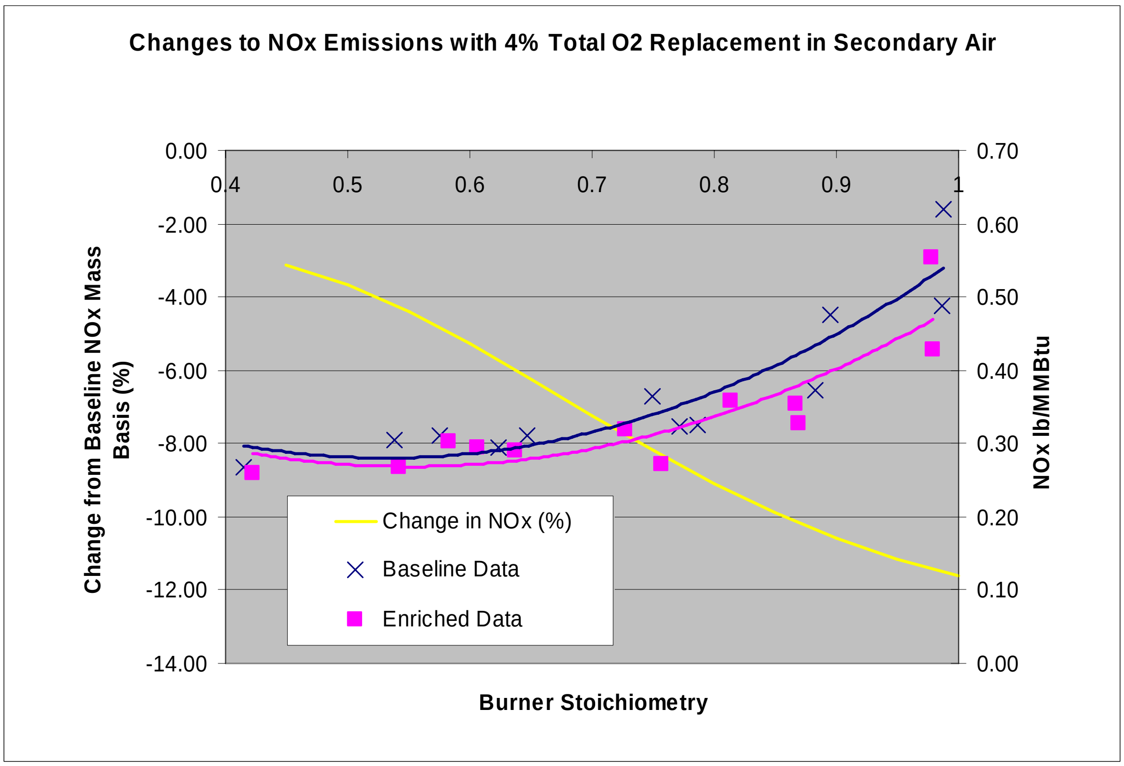


Figure 3 NOx Reduction due to Secondary Air Enrichment

A further series of trials were performed in which both the primary and secondary air streams were enriched with oxygen. Adopting this approach allowed greater amounts of oxygen to be added without excessively high oxygen levels in the feed streams. As can be seen in Figure 4, even with the increased total amount of oxygen added, enrichment of both primary and secondary air streams produced NOx reductions only at high burner stoichiometries, with very poor performance at appreciable OFA levels.

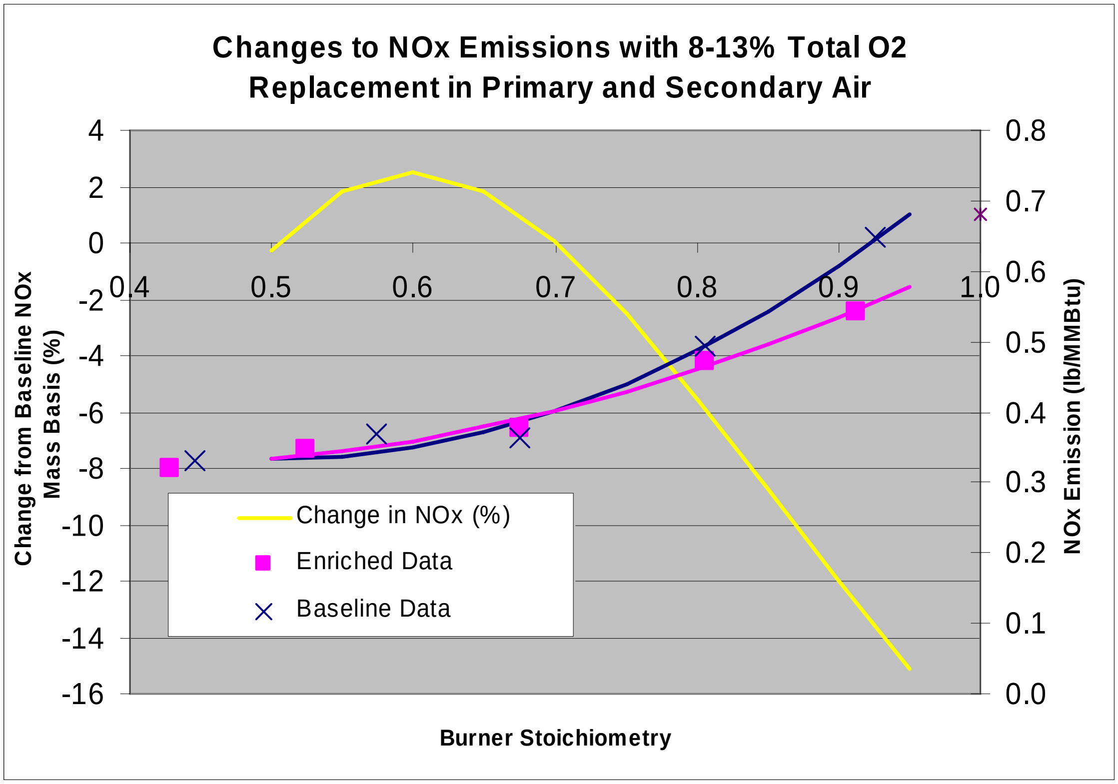


Figure 4 NOx Reduction due to combined Primary and Secondary Air Enrichment

The existing burner enrichment options were further pursued by examining the effect of enriching only the primary air i.e. the coal transport air (Table 5). In this case the observed NOx reductions were seen to be more consistent, but with an average reduction of only 7.3% (Fig. 5).

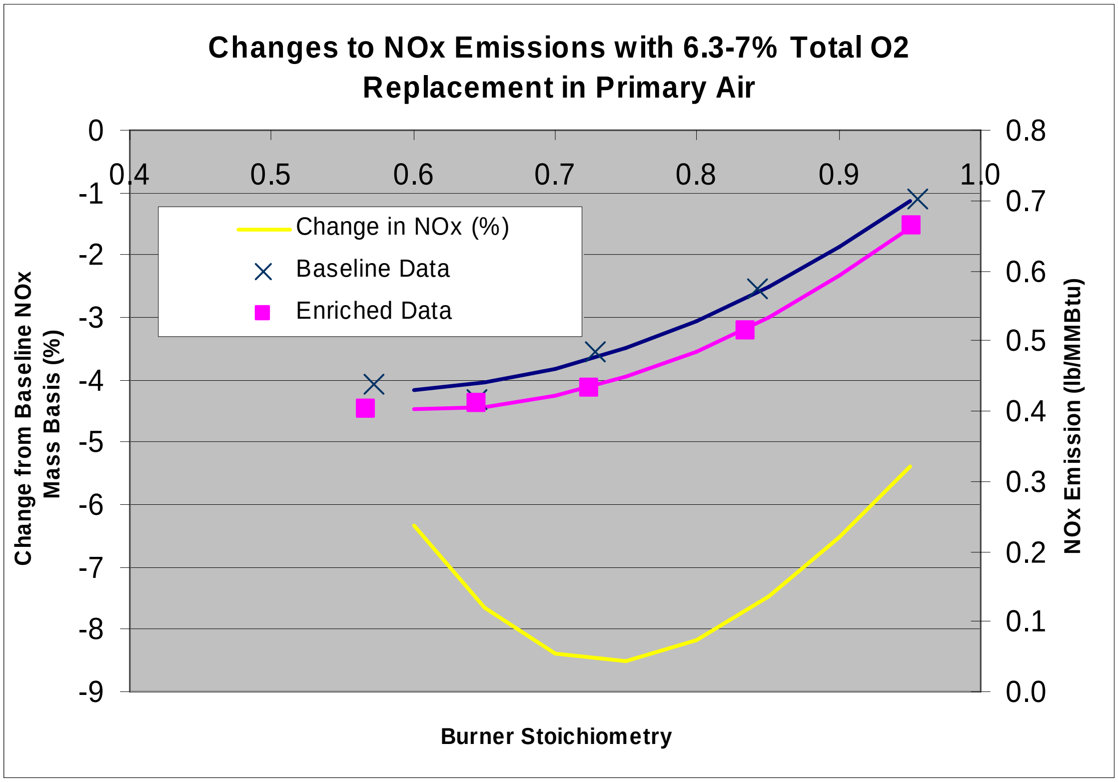


Figure 5 NOx Reduction due to Primary Air Enrichment.

Given that the fairly low average NOx reductions of 7.4% observed in above experiments are significantly lower than the 25-50% reductions reported by others in the literature [1,2], it was felt prudent to utilize the remaining experimental time available exploring the effect of burner design and firing patterns. The experimental burner used here was of a simple tube-in-tube design, which would lead to rapid primary/secondary air mixing compared to practical low NOx burners that are carefully staged to maintain a large fuel rich zone. Two separate modifications were made to the burners in an attempt to retard primary and secondary air mixing and form a larger fuel-rich core. The two modifications were:

(i) Installing inserts on the burner tips to delay mixing between the primary air/coal and the secondary air.

(ii) Adjusting the secondary and primary tangential injection angles such that the primary air/coal was injected closer to the center, and the SA closer to the walls.

Despite these modifications, as can be seen in Table 6, the NOx results were not particularly different from those of the previous primary air enrichment tests, i.e. ~10% reduction with 7% of the air replaced with O_2.

Table 3 Secondary Air Enrichment

Date	Coal lb/hr	PA Scfm	SA scfm	OFA scfm	OFA %	Air Scfm	**Burner SR**	O2 Scfm	**O2 % replaced**	O2 in SA	O2 in tot air	O2 %	SO2 ppm	CO ppm	NOx ppm	**NOx lb/MM Btu**	**NOx Red.**
10/13/2004	16	9.1	17.3	4.33	14.1%	30.7	**0.99**	0	**0.0%**	20.90%	20.90%	3.1	615	208	476	**0.62**	
10/13/2004	16	9.0	14.5	4.33	15.6%	27.8	**0.98**	0.28	**4.4%**	22.43%	21.70%	3.3	609	140	441	**0.55**	**10.8%**
10/13/2004	15.8	9.1	14.4	6.69	22.2%	30.1	**0.89**	0	**0.0%**	20.90%	20.90%	3.4	600	25	364	**0.47**	
10/13/2004	15.8	9.0	10.6	6.69	25.4%	26.3	**0.87**	0.28	**4.4%**	22.98%	21.74%	2.9	597	67	262	**0.33**	**30.8%**
10/13/2004	15.6	9.0	10.5	9.05	31.6%	28.6	**0.79**	0	**0.0%**	20.90%	20.90%	3	619	91	250	**0.33**	
10/13/2004	15.6	9.0	11.8	9.05	30.3%	29.9	**0.81**	0.28	**4.7%**	22.77%	21.64%	3.4	588	180	285	**0.36**	**-10.0%**
10/14/2004	16.2	9.0	12.3	11.37	34.8%	32.6	**0.75**	0	**0.0%**	20.90%	20.90%	3.3	624	76	280	**0.37**	
10/14/2004	16.2	9.0	9.5	11.37	38.1%	29.8	**0.73**	0.28	**4.1%**	23.24%	21.64%	3.3	602	77	254	**0.32**	**12.4%**
10/14/2004	16	8.5	9.1	13.73	43.8%	31.4	**0.65**	0	**0.0%**	20.90%	20.90%	3.5	628	55	238	**0.31**	
10/14/2004	16	7.4	8.6	13.73	46.2%	29.7	**0.64**	0.28	**4.3%**	23.46%	21.65%	3.1	582	61	231	**0.29**	**6.4%**
10/14/2004	16.2	7.3	8.8	16.09	50.0%	32.2	**0.58**	0	**0.0%**	20.90%	20.90%	3.1	614	92	239	**0.31**	
10/14/2004	16.2	7.3	8.2	16.09	51.0%	31.5	**0.58**	0.28	**4.2%**	23.61%	21.60%	3.3	635	91	240	**0.30**	**2.9%**
10/18/2004	16	9.0	17.2	4.33	14.2%	30.5	**0.99**	0	**0.0%**	20.90%	20.90%	3.3	597	26	374	**0.49**	
10/18/2004	16	9.0	14.9	4.33	15.3%	28.2	**0.98**	0.23	**3.6%**	22.12%	21.54%	3.4	630	76	339	**0.43**	**12.1%**
10/18/2004	15.6	8.9	13.2	6.69	23.2%	28.8	**0.88**	0	**0.0%**	20.90%	20.90%	3.5	590	16	286	**0.37**	
10/18/2004	15.6	9.0	10.6	6.69	25.4%	26.3	**0.87**	0.23	**3.8%**	22.61%	21.59%	3.2	586	192	280	**0.35**	**5.3%**
10/18/2004	15.6	9.0	9.5	9.05	32.9%	27.5	**0.77**	0	**0.0%**	20.90%	20.90%	3.3	600	136	248	**0.32**	
10/18/2004	15.6	7.7	8.8	9.05	35.3%	25.6	**0.76**	0.23	**4.0%**	22.96%	21.61%	3.1	614	231	215	**0.27**	**16.2%**
10/19/2004	15.8	7.3	9.0	13.73	45.8%	30.0	**0.62**	0	**0.0%**	20.90%	20.90%	3.4	627	225	225	**0.29**	
10/19/2004	15.8	7.3	7.2	13.73	48.7%	28.2	**0.61**	0.23	**3.7%**	23.43%	21.55%	3.5	597	379	233	**0.29**	**-0.4%**
10/19/2004	16	7.1	7.1	16.09	53.1%	30.3	**0.54**	0	**0.0%**	20.90%	20.90%	3.3	623	357	233	**0.30**	
10/19/2004	16	6.4	7.1	16.09	54.5%	29.5	**0.54**	0.23	**3.6%**	23.47%	21.52%	3.3	634	361	212	**0.27**	**11.7%**
10/19/2004	16	6.4	4.5	19.36	64.0%	30.3	**0.41**	0	**0.0%**	20.90%	20.90%	3.4	605	143	205	**0.27**	
10/19/2004	16	6.4	4.0	19.36	65.1%	29.7	**0.42**	0.23	**3.6%**	25.45%	21.51%	3.5	600	97	205	**0.26**	**2.9%**

Table 4 Secondary and Primary Air Enrichment

Date	Coal	PA	SA	OFA	OFA	Air	Burner	O2	O2	O2	O2	O2	SO2	CO	NOx	NOx	NOx
	lb/hr	scfm	scfm	scfm	%	Scfm	SR	scfm	% of total	in PA/SA	in tot air	%	ppm	ppm	ppm	lb/MM Btu	Red.
11/9/2004	12.0	7.3	14.5	5.28	19.5%	27.1	0.93	0	0.0%	20.90%	20.90%	3.3	N/A	263	469	0.647	
11/9/2004	12.0	5.9	11.8	5.28	22.9%	23.0	0.91	0.66	13.7%	23.84%	23.17%	3.1	N/A	156	436	0.542	16.2%
11/9/2004	12.0	5.9	12.2	7.74	30.0%	25.8	0.81	0	0.0%	20.90%	20.90%	3.0	N/A	232	357	0.493	
11/9/2004	12.0	5.3	10.6	7.74	32.7%	23.7	0.81	0.59	11.9%	23.83%	22.87%	3.2	N/A	146	376	0.473	4.1%
11/10/2004	12.0	5.0	10.0	10.56	41.3%	25.6	0.67	0	0.0%	20.90%	20.90%	3.2	1500	232	264	0.364	
11/10/2004	12.0	5.0	8.0	10.56	44.8%	23.6	0.67	0.53	10.8%	24.12%	22.68%	3.3	1627	159	297	0.377	-3.6%
11/10/2004	12.0	5.0	8.0	13.02	50.0%	26.0	0.57	0	0.0%	20.90%	20.90%	3.5	1568	199	268	0.370	
11/10/2004	12.0	5.0	4.2	13.02	58.7%	22.2	0.52	0.46	9.9%	24.86%	22.54%	3.4	1596	93	272	0.348	5.9%
11/10/2004	12.0	5.0	4.8	15.49	61.2%	25.3	0.45	0	0.0%	20.90%	20.90%	3.1	1552	142	239	0.330	
11/10/2004	12.0	5.0	2.7	15.49	66.7%	23.2	0.43	0.39	8.0%	24.89%	22.23%	3.4	1548	181	246	0.319	3.3%

Table 5 Primary Air Enrichment

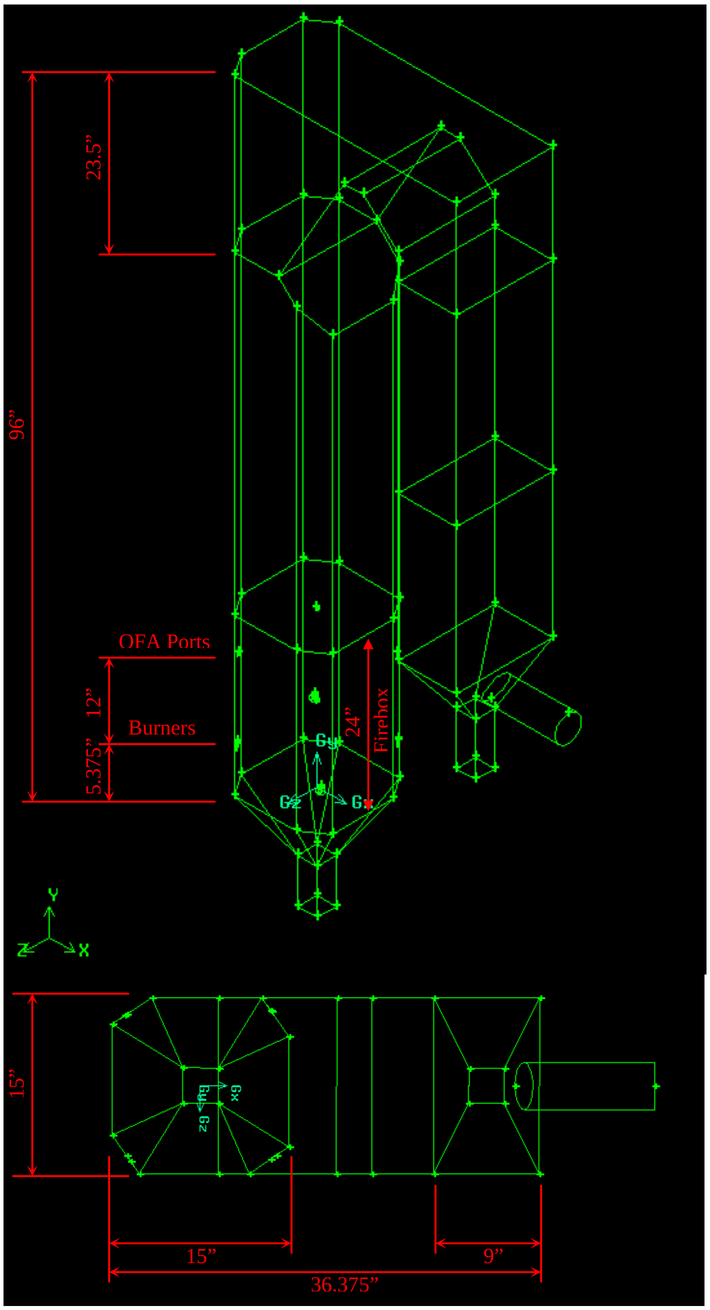
Date	Coal lb/hr	PA scfm	SA scfm	OFA scfm	OFA %	Air Scfm	Burner SR	O2 scfm	O2 % of total	O2 in PA	O2 in tot air	O2 %	SO2 ppm	CO ppm	NOx ppm	NOx lb/MM Btu	NOx Red.
11/17/2004	11.6	7.3	13.5	4.58	18.0%	25.4	**0.96**	0	**0.0%**	20.90%	20.90%	3.5	1434	261	509	**0.702**	
11/17/2004	11.6	5.7	12.7	4.58	19.9%	23.0	**0.95**	0.33	**6.9%**	25.21%	22.02%	3.6	1556	172	508	**0.665**	**5.4%**
11/22/2004	11.6	7.3	10.8	7.04	28.0%	25.1	**0.84**	0	**0.0%**	20.90%	20.90%	3.6	1422	193	417	**0.575**	
11/22/2004	11.6	5.7	9.6	7.04	31.4%	22.4	**0.84**	0.33	**7.0%**	25.21%	22.05%	3.6	1583	105	394	**0.515**	**10.5%**
11/22/2004	11.6	7.3	8.4	9.50	37.8%	25.1	**0.73**	0	**0.0%**	20.90%	20.90%	3.6	1497	116	351	**0.484**	
11/22/2004	11.6	5.7	7.7	9.50	41.4%	23.0	**0.72**	0.33	**6.9%**	25.21%	22.02%	3.7	1521	89	330	**0.432**	**10.9%**
11/23/2004	11.6	7.3	7.3	11.62	44.4%	26.2	**0.64**	0	**0.0%**	20.90%	20.90%	3.4	1505	266	301	**0.415**	
11/23/2004	11.6	5.7	7.3	11.62	47.2%	24.6	**0.64**	0.33	**6.4%**	25.21%	21.95%	3.6	1582	210	314	**0.412**	**0.8%**
11/23/2004	11.6	7.3	6.2	14.08	51.1%	27.5	**0.57**	0	**0.0%**	20.90%	20.90%	3.6	1499	141	318	**0.439**	
11/23/2004	11.6	5.7	5.1	14.08	56.6%	24.9	**0.57**	0.33	**6.3%**	25.21%	21.93%	3.6	1590	89	306	**0.402**	**8.4%**

Table 6 Primary Enrichment – Modified Firing Configuration

Date	Coal lb/hr	PA scfm	SA scfm	OFA scfm	OFA %	Air Scfm	Burner SR	O2 scfm	O2 % of total	O2 in PA	O2 in tot air	O2 %	SO2 ppm	CO ppm	NOx ppm	NOx lb/MM Btu	NOx Red.
Inserts on PA Tips																	
12/3/2004	11.0	7.3	8.4	9.50	37.8%	25.1	**0.71**	0	0.0%	20.90%	20.90%	3.1	1487	241	387	**0.532**	
12/3/2004	11.0	5.7	8.4	9.50	40.3%	23.6	**0.71**	0.33	6.7%	25.21%	21.99%	3.2	1574	229	387	**0.505**	**5.1%**
12/3/2004	11.0	7.3	7.6	11.62	43.8%	26.5	**0.65**	0	0.0%	20.90%	20.90%	3.2	1506	186	383	**0.528**	
12/3/2004	11.0	5.7	7.4	11.62	47.0%	24.7	**0.64**	0.33	6.4%	25.21%	21.94%	3.3	1600	148	377	**0.493**	**6.8%**
Modified Injection Angles																	
12/10/2004	11.6	7.3	15.6	9.50	29.3%	32.4	**0.85**	0	0.0%	20.90%	20.90%	4.2	1459	341	336	**0.486**	
12/10/2004	11.6	5.7	14.5	9.50	32.0%	29.7	**0.84**	0.33	5.3%	25.21%	21.77%	4.2	1610	208	313	**0.430**	**11.5%**
12/10/2004	12.0	7.3	14.3	11.62	35.0%	33.2	**0.74**	0	0.0%	20.90%	20.90%	3.1	1700	149	282	**0.387**	
12/10/2004	12.0	5.7	14.5	11.62	36.5%	31.8	**0.75**	0.33	5.0%	25.21%	21.71%	3.3	1672	197	298	**0.396**	**-2.1%**

COMPUTATIONAL FLUID DYNAMIC MODELING OF COMBUSTION TEST FACILITY

A three dimensional model of the interior of the CTF was made incorporating the combustion chamber, convection and economizer sections as shown in Figure 6. The geometry was meshed using a hybrid mesh of approximately 600,000 hexahedral and tetrahedral elements.



4 x OFA Ports:

- 0.4” Diameter
- 45º angle from sidewall

4 x Coal Burners

- PA: ID 0.405” OD 0.500”
- SA: ID 1.049” OD 1.315”
- PA & SA pipes flush with wall
- 35º angle from sidewall

Figure 6 Geometric Representation of the CTF

The mesh was read into the Fluent 6.2.16 code and a series of models performed to investigate the behavior of the furnace. The following general settings were made:

- Segregated steady state solver
- *k-ε* turbulence model with standard wall functions
- P-1 radiation model
- Discrete phase model for coal particle tracking and char combustion
    - Updated every 20 flowfield iterations
    - Particles tracked for 4000 steps with a 2" step length
    - Particle –radiation interaction allowed for
    - Particles released from surface of primary air tube
        - Flow vectors to account for burner angle
        - Initial temperature 300K
        - Rosin Rammler size distribution
            - Dmin: 1e-5m
            - Dmax: 5e-5m
            - Dmean: 2.5e-5m
            - Spread: 4.52
            - # Size Ranges: 5
    - Turbulent dispersion through stochastic tracking discrete random walk model: 3 trajectories/particle with 0.15 time constant.
- Coal combustion model – modified from Fluent's medium volatile coal model to match properties of coal in experiment. Incorporates devolatilization of coal particle to form a char that continues to combust in the combusting particle model and a volatile species that undergoes gas phase reaction.
    - Combusting Particle
        - Density: 1300 kg/m3
        - Cp: 1000 kg/m3
        - Thermal Conductivity: 0.0454 w/m-k
        - Vaporization Temperature: 400K
        - Volatile component fraction: 0.415
        - Binary Diffusivity: 4e-5
        - Particle Emissivity: 0.9
        - Particle Scattering Factor: 0.6
        - Swelling Coefficient: 2
        - Burn-out Stoichiometric Ratio: 2.67
        - Combustible Fraction: 0.3975
        - Heat for Reaction for Burnout: 3.2789e7 J/kg
        - Heat of Reaction Fraction absorbed by Particle: 0.3
        - Devolatilization Model (1/s): Single Rate
            - Activation Energy: 31811.54 Btu/lbmol
            - Pre-Exponential Factor: 492000
        - Combustion Model: Kinetics/Diffusion Limited
            - Mass Diffusion Limited Rate Constant: 5e-12

        - Kinetics-Limited Rate Pre-Exponential Factor: 0.002
        - Kinetics-Limited Rate Activation Energy: 33960.97

  - Volatiles (Gas Phase)

	Reactants			Products	
	mols	Rate Exp.		mols	Rate Exp.
Volatiles	1	1	CO_2	1	0
O_2	1.293	1	H_2O	0.962	0

    - Species considered in gas phase:
        - N2, O2, CO2, H2O, Volatiles
    - Volatile species generated (match physical properties/close energy/mass balances) with:
        - Cp: 1500 J/kg-K
        - Mol Wt.: 19.95112 kg/kgmol
        - Standard State Enthalpy: 4624.387 btu/lbmol
    - Standard mixture calculations for density, Cp etc…
- NO Model
  - Turbulence interaction with temperature through 10 point Beta PDF
  - Thermal NO
    - Partial Equilibrium calculations for [OH] and [O]
  - Fuel NO
    - Route though HCN intermediate
    - Char N converts direct to NO
    - BET Surface Area 25000 m^2/kg
    - Char and volatile with equal N mass fraction

The following common boundary conditions were also applied

- Walls: reflect discrete phase particles
  - Emissivity: 1
  - Firebox (combustion chamber) walls: zero heat flux
  - Nose, convection, economizer walls: convection
    - Heat transfer coefficient: 20 W/m2-K
    - Free Stream Temperature: 400K
- Primary Air: 350K, 21 mol% O2
- Secondary Air: 600K
- OFA: 600K, 21 mol% O2

A series of models were devised to mimic the initial experiments in which the secondary air alone was enriched with 4% of the total oxidant supplied with pure oxygen. For these models the overall equivalence ratio was maintained at 1.06 and the flowrates of primary air and coal were maintained at 0.005152 and 0.001991 kg/s respectively. Three overfire air levels (10%, 22.5% and 45%) with corresponding burner equivalence ratios of 0.95, 0.82 and 0.58 were considered at both 4% enrichment and for air operation. Details of the changes to flows through the secondary and OFA ports necessary to attain the desired OFA levels and enrichment levels are given in Table 7.

GENERAL MODEL FEATURES

Each model exhibited certain common features that might be expected in this firing configuration. These may be appreciated by considering images taken from the air and enriched 22.5% OFA cases (Figures 7-14) and the general conditions within the 'firebox' (Table 8.) A relatively compact high temperature rotating toroidal flame is formed approximately at the coal burner elevation. In this region the rapidly evolved volatile component and resultant char undergo rapid mixing and combustion with the co-injected oxygen. Typically a fuel rich core, manifest by the presence of unreacted volatile species, is formed at the center of the torus and extends down to the bottom of the furnace. The rotating fuel rich column rises and interacts with a central oxygen rich region formed by the OFA ports to complete the burnout.

Two main expected trends may be observed between the cases:

- The lower regions become increasingly fuel rich with increasing OFA level (higher volatile concentrations)
- Higher temperatures within the firebox and in the toroidal flame

There are slight changes in the flowfield between cases, chiefly as a result of the reduced momentum of the flames in the enriched cases which affects the mixing between PA/SA and OFA and leads to some spurious trends in the low oxygen concentrations within the firebox.

DISCUSSION ON NOx RESULTS

It is very much evident that the reactions that form NOx are essentially complete within the firebox and that local temperatures and oxygen availability affect the results. In these simulations the firebox temperatures are on average some 40 K higher with oxygen enrichment, but have comparable local oxygen concentrations. As one might expect this leads to a predicted increase in NO formation (average across cases of 340 ppm vs. 310 ppm) within the firebox. These results correlate closely with the conditions at the exit of the model furnace (Table 9) as little further reaction takes place throughout the furnace.

Considering the NOx determined at the furnace exit we can see that while the model correctly predicts the trend of reducing NOx with increasing OFA, it also predicts a 2-4% increase in NOx with oxygen enrichment as opposed to the decrease observed in the experiment. A further disparity is in the magnitude of the emissions with the experiment having an average emission rate of 0.35 lbNOx/MMBtu, while the model predicts emission rates around 0.19 lbNOx/MMBtu.

The second disparity presents less of a problem than the first and may be largely attributed to inaccuracies in the replication of the temperature field in the model. The formation rate of NO is strongly affected by temperature and wall thermal boundary assumptions will have a significant affect on the predicted temperature and NO formation. A more reasonable approach would be to impose fixed wall temperatures that could be measured through experiment. In a practical water wall boiler, as the wall temperatures are typically low and radiation path lengths are high it may be possible to assign an assumed value without an error of similar magnitude.

The first disparity is more problematic as it relates to the fuel NO model. Not only is their debate over the correct mechanism to use (e.g. NH_3 route or HCN route), there is no facility within Fluent to predict how much fuel bound N evolves with the volatiles and how much stays with the char for later release. In the absence of data in this simulation the fuel nitrogen content was arbitrarily distributed with equal mass fractions in the volatiles and char, however there is no reason to argue that this is by necessity the case. The hypothesis was that increasing the heating rate through higher ambient temperatures would drive more volatiles and N out of the coal into a fuel rich region, which would not be favorable for NOx generation. Without model development in this area we cannot predict fuel NO accurately. If such a model were available, more detailed coal characterization would be required to determine the rate at which volatiles are evolved with temperature and heating rate, and the nitrogen components in said volatiles.

CONCLUSIONS

Experimental evidence indicated that oxygen enrichment does appear to be able to reduce NOx levels from coal combustion, especially when operated at low OFA levels. The reductions observed however are significantly smaller than that reported by others (7-8% vs. 25-50%), questioning the economic viability of the technique. If NOx can only be reduced by the small amounts seen in this experiment through oxygen enrichment then a much more reasonable approach is the current practice of increasing the OFA levels. It is possible that burners with clearly defined fuel-rich flame stabilization zones may exhibit better NOx reductions. It is also possible that this technique may find favor with fuels that are difficult to burn or stabilize at high OFA and produce excessive LOI.

While Fluent appears to predict NO amounts in the correct order of magnitude and the correct trend with staging, it is sensitive to thermal conditions and an accurate thermal prediction is essential. Furthermore, without development, Fluent's fuel-NO model cannot account for a solution sensitive fuel-N distribution between volatiles and char and thus cannot predict the trends seen in the experiment.

Case 1 - Low OFA%

	Each(kg/s)	Total(kg/s)	O2 massF	kg O2/s
Primary Flowrate	0.001288	0.005152	0.233	0.001200
Secondary Flowrate	0.002558	0.010230	0.233	0.002384
OFA	0.000427	0.001709	0.233	0.000398
Total		0.017091		0.003982
% OFA				10.00%
Burner Flow		0.015382		0.003584
Coal kg/s	0.000498	0.001991		
1 kg coal requires	1.8953	kg O2		
Overall ER				1.06
Burner ER				0.95

Case 2 - Med OFA%

	Each(kg/s)	Total(kg/s)	O2 massF	kg O2/s
Primary Flowrate	0.001288	0.005152	0.233	0.001200
Secondary Flowrate	0.002038	0.008153	0.233	0.001900
OFA	0.000947	0.003786	0.233	0.000882
Total		0.017091		0.003982
% OFA				22.15%
Burner Flow		0.013305		0.003100
Coal kg/s	0.000498	0.001991		
1 kg coal requires	1.8953	kg O2		
Overall ER				1.06
Burner ER				0.82

Case 3 - High OFA%

	Each(kg/s)	Total(kg/s)	O2 massF
Primary Flowrate	0.001288	0.005152	0.233
Secondary Flowrate	0.001062	0.004248	0.233
OFA	0.001923	0.007691	0.233
Total		0.017091	
% OFA			
Burner Flow		0.009400	
Coal kg/s	0.000498	0.001991	
1 kg coal requires	1.8953	kg O2	
Overall ER			
Burner ER			

Case 4 - Low OFA% - 4% O2 Replaced Through Secondary

	Each(kg/s)	Total(kg/s)	O2 massF	kg O2/s
Primary Flowrate	0.001288	0.005152	0.233	0.001200
Secondary Flowrate	0.002387	0.009546	0.233	0.002224
Secondary Oxygen	3.982E-05	0.000159	1	0.000159
OFA	0.000427	0.001709	0.233	0.000398
Total		0.016566		0.003982
				1
% OFA				10.00%
Burner Flow		0.014698		0.003584
Coal kg/s	0.000498	0.001991		
1 kg coal requires	1.8953	kg O2		
Overall ER				1.06
Burner ER				0.95
O2 Replaced				4%
O2 Replaced (kg/s)				0.000159
Mass Fraction O2 in Combined Secondary				0.2456
% O2 in Combined Secondary				22.17%

Case 5 - Med OFA% - 4% O2 Replaced Through Secondary

	Each(kg/s)	Total(kg/s)	O2 massF	kg O2/s
Primary Flowrate	0.001288	0.005152	0.233	0.001200
Secondary Flowrate	0.001867	0.007470	0.233	0.001740
Secondary Oxygen	3.982E-05	0.000159	1	0.000159
OFA	0.000947	0.003786	0.233	0.000882
Total		0.016566		0.003982
				1
% OFA				22.15%
Burner Flow		0.012621		0.003100
Coal kg/s	0.000498	0.001991		
1 kg coal requires	1.8953	kg O2		
Overall ER				1.06
Burner ER				0.82
O2 Replaced				4%
O2 Replaced (kg/s)				0.000159
Mass Fraction O2 in Combined Secondary				0.2490
% O2 in Combined Secondary				22.49%

Case 6 - High OFA% - 4% O2 Replaced Through Secor

	Each(kg/s)	Total(kg/s)	O2 massF
Primary Flowrate	0.001288	0.005152	0.233
Secondary Flowrate	0.000891	0.003565	0.233
Secondary Oxygen	3.982E-05	0.000159	1
OFA	0.001923	0.007691	0.233
Total		0.016566	
% OFA			
Burner Flow		0.008716	
Coal kg/s	0.000498	0.001991	
1 kg coal requires	1.8953	kg O2	
Overall ER			
Burner ER			
O2 Replaced			
O2 Replaced (kg/s)			
Mass Fraction O2 in Combined Secondary			
% O2 in Combined Secondary			

Table 7 Model Flowrates

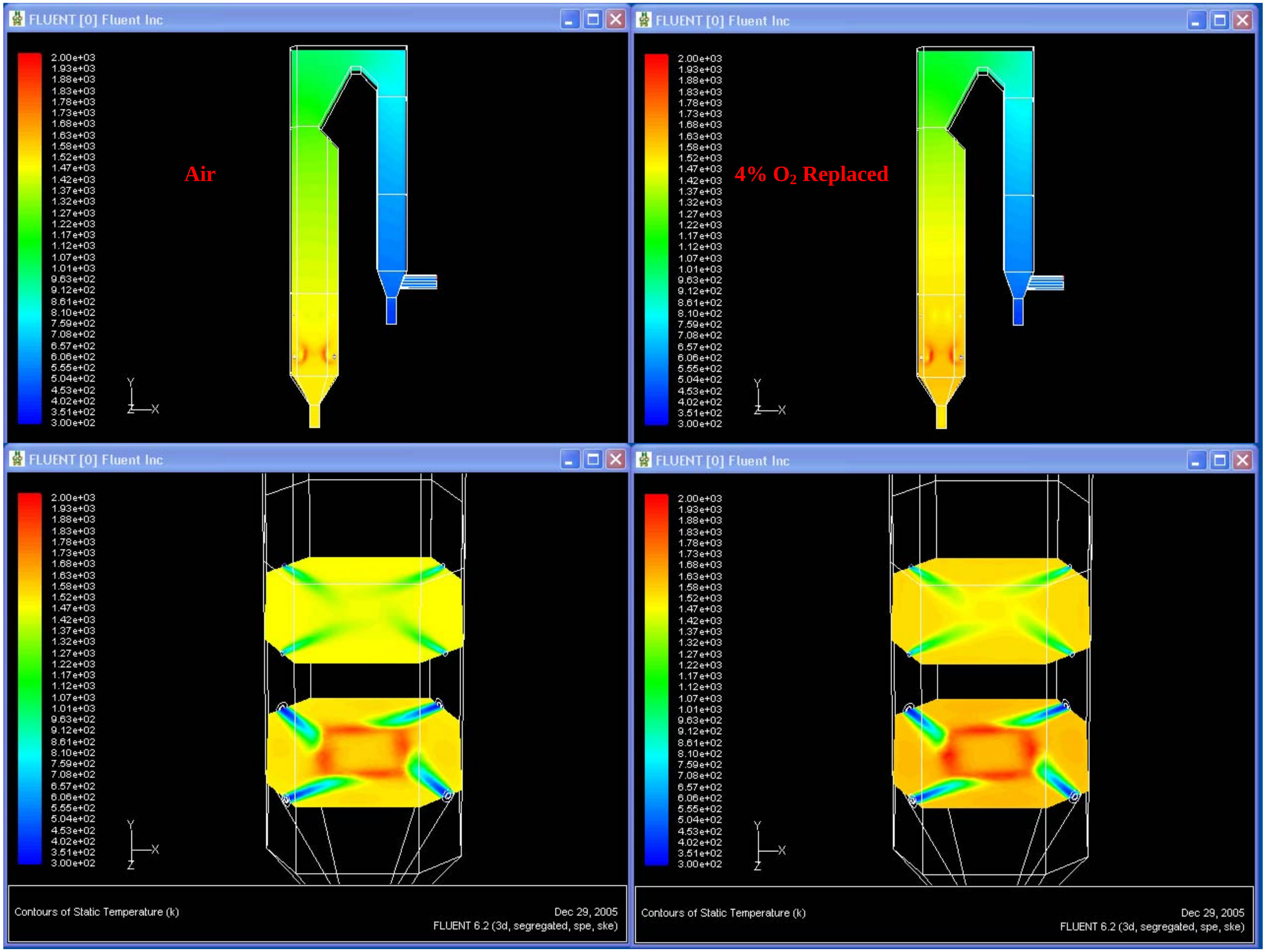


Figure 7 Temperature Profiles for 22.5% OFA Cases

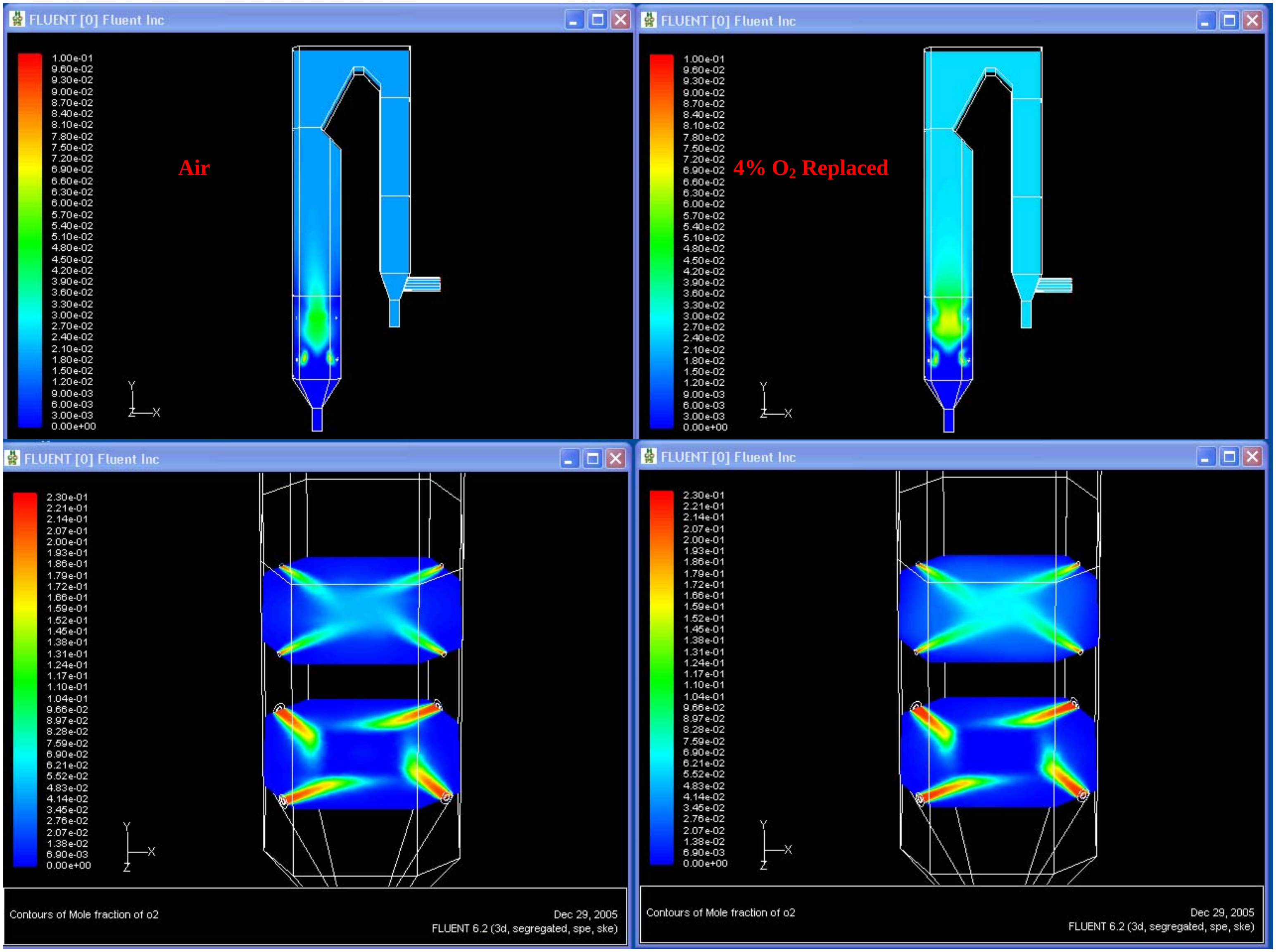


Figure 8 Oxygen Profiles for 22.5% OFA Cases

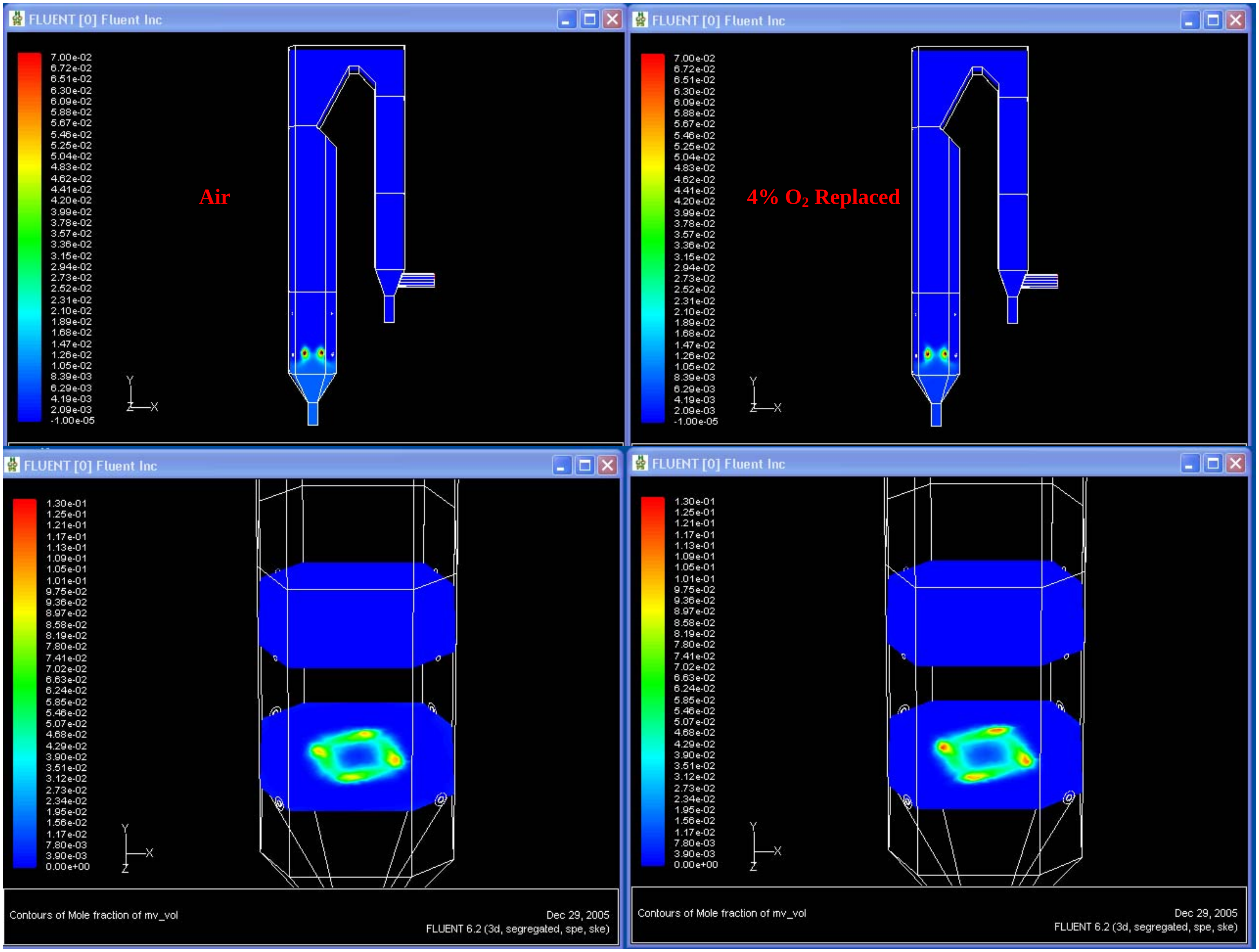


Figure 9 Volatile Concentration for 22.5% OFA Cases

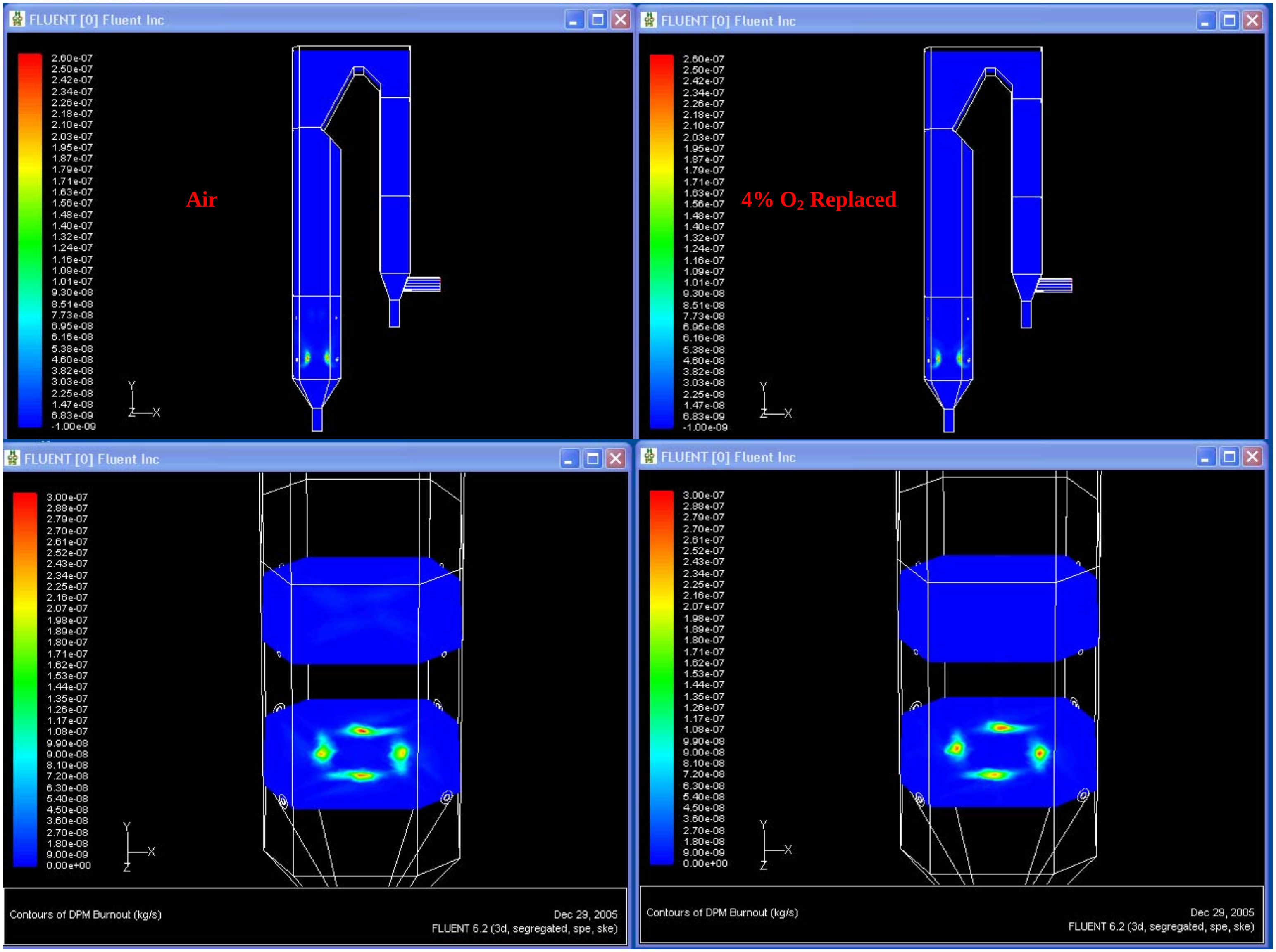


Figure 10 Discrete Phase (Coal) Concentration for 22.5% OFA Cases

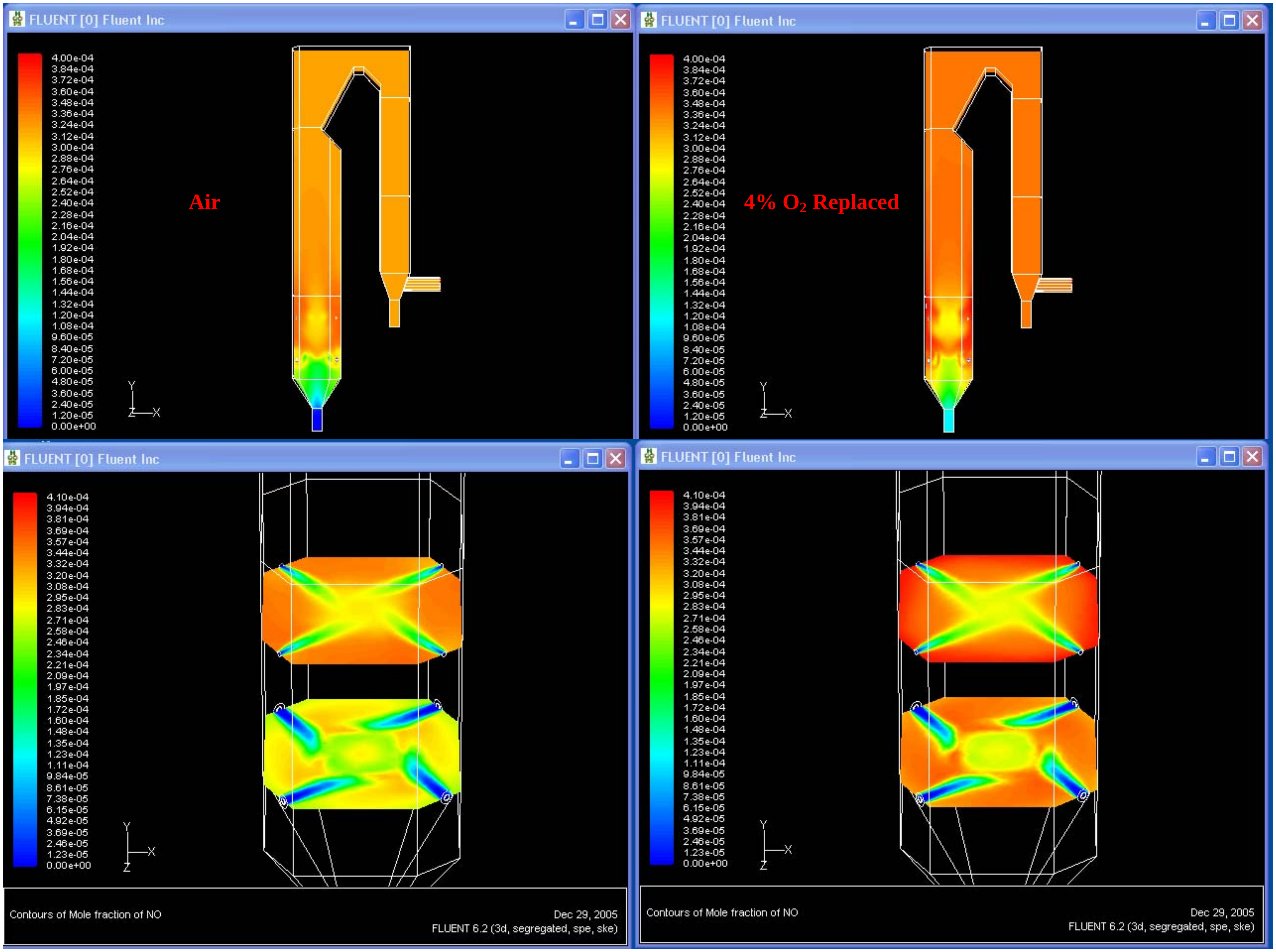


Figure 11 NOx Concentration for 22.5% OFA Cases

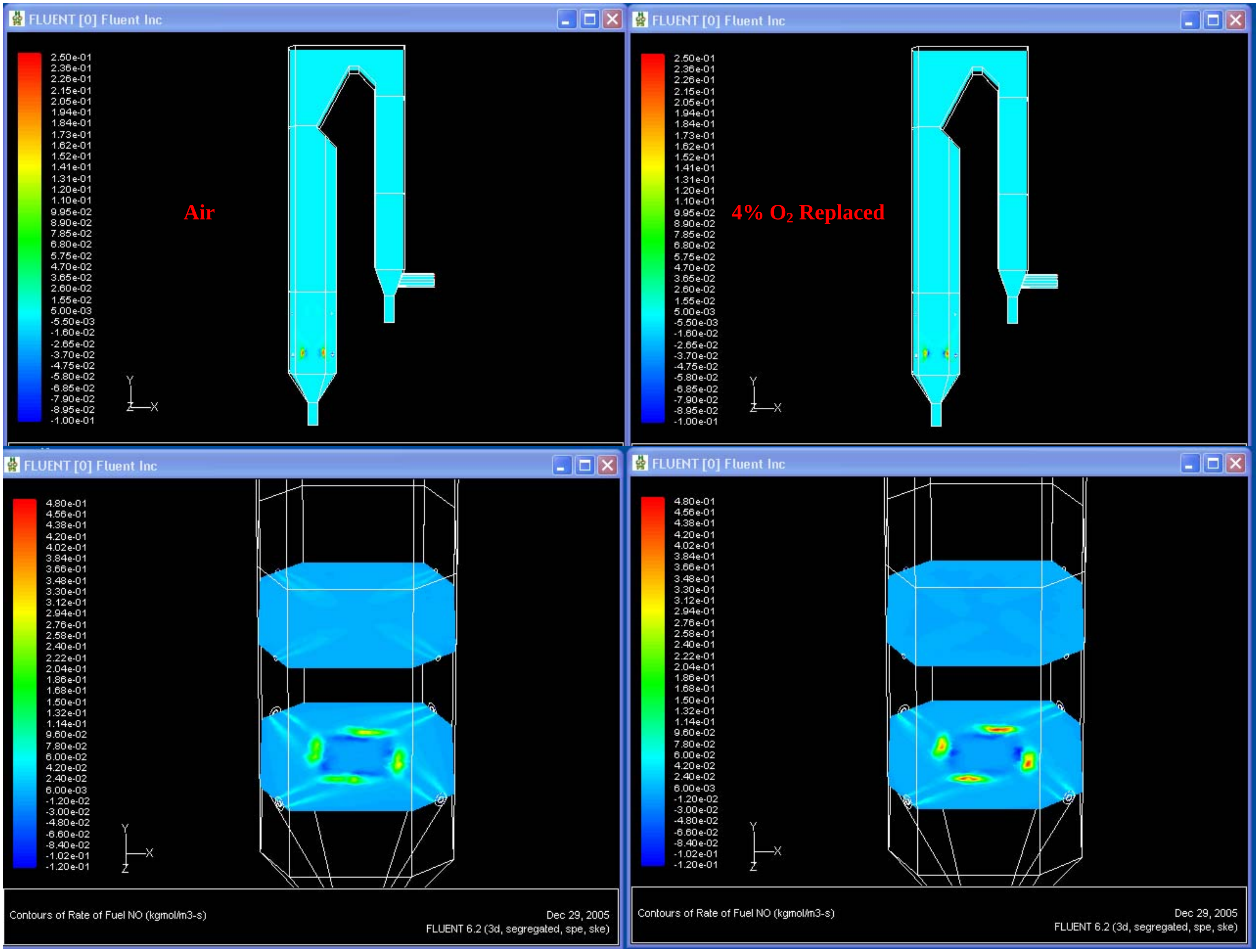


Figure 12 Rate of Fuel NO for 22.5% OFA Cases

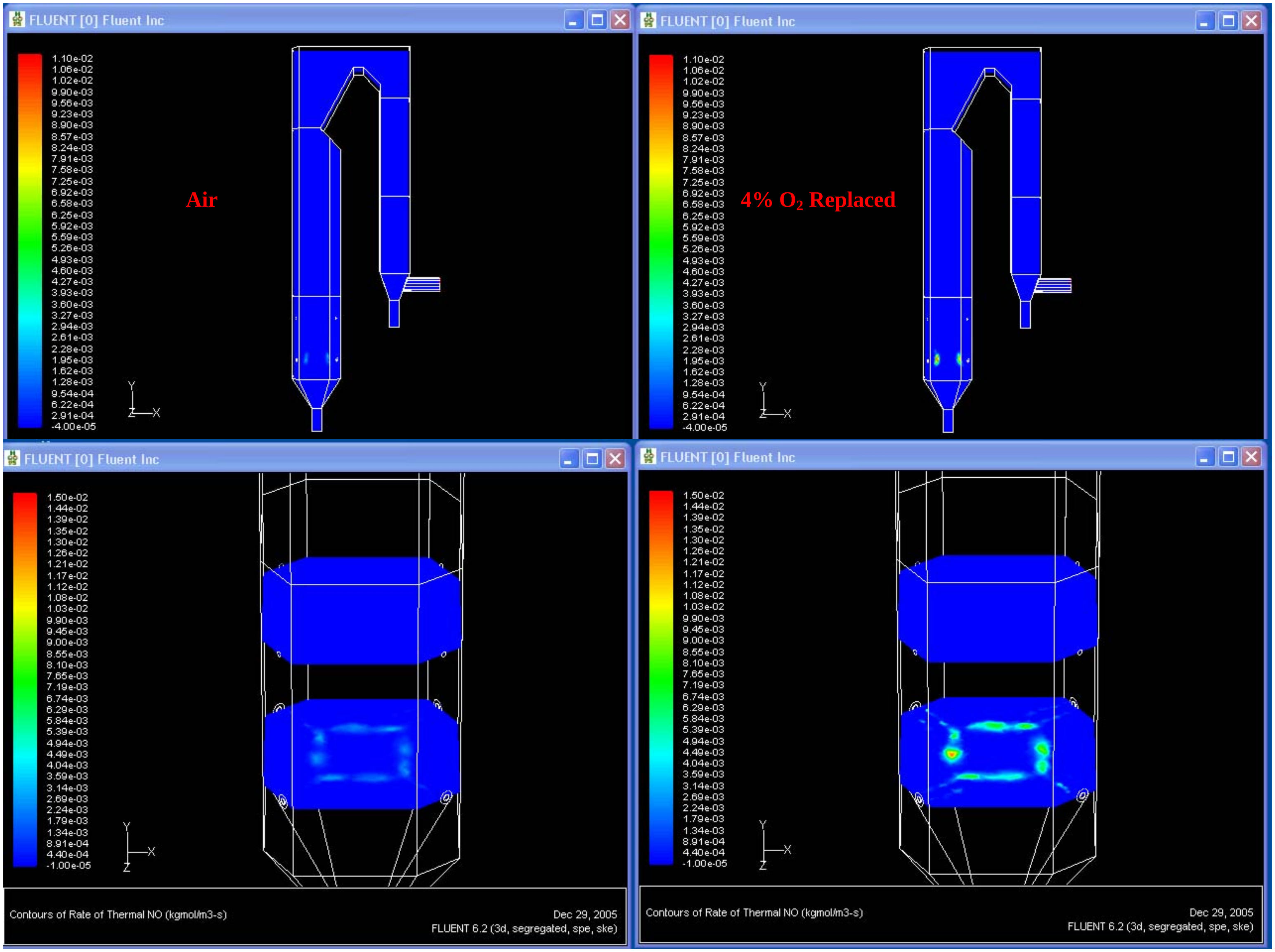


Figure 13 Rate of Thermal NO for 22.5% OFA Cases

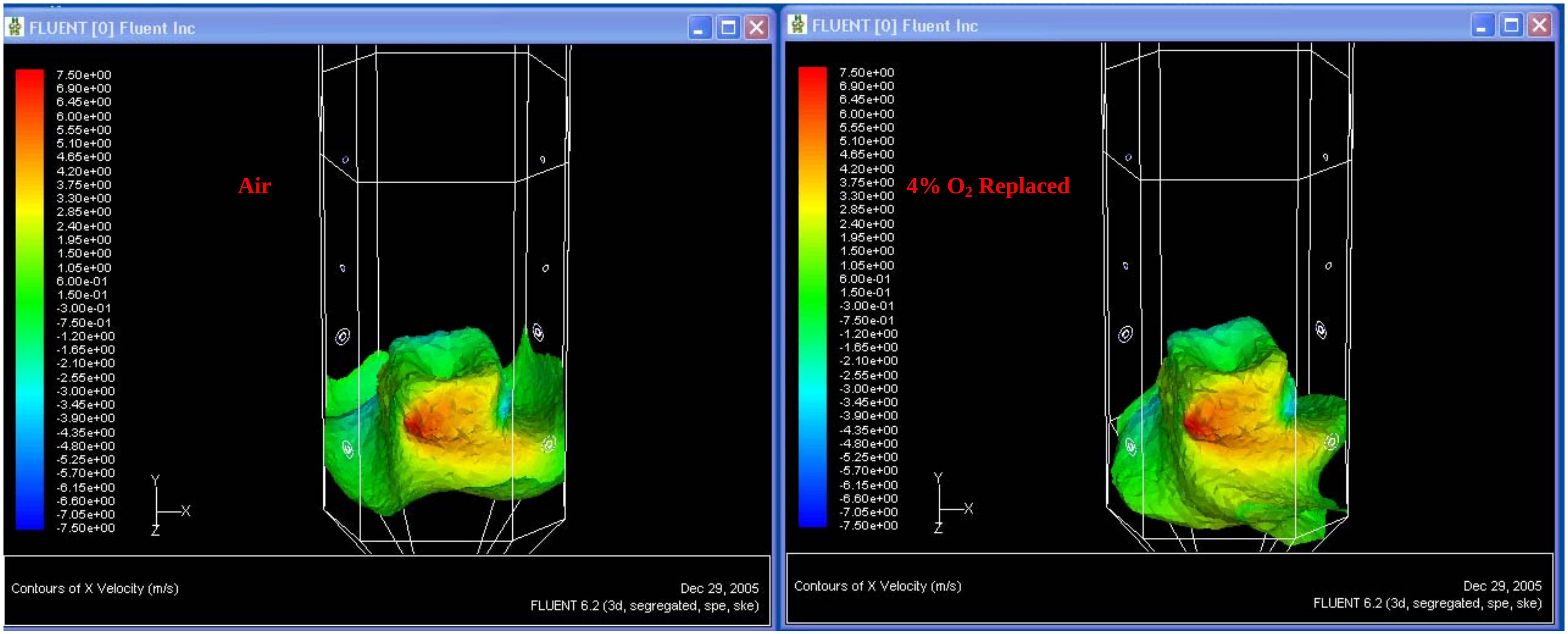


Figure 14 Rotating Fuel Rich Core for 22.5% OFA Cases (Contours of x-velocity on surface of [volatiles]=0.005)

Table 8 Firebox Conditions

Temperature (K)	Air	4% O2
Low OFA (10%, ER 0.95)	1574	1588
Med OFA (22.5%, ER 0.82)	1504	1575
High OFA (45%, ER 0.58)	1525	1557

[O2]	Air	4% O2
Low OFA (10%, ER 0.95)	0.017	0.017
Med OFA (22.5%, ER 0.82)	0.012	0.020
High OFA (45%, ER 0.58)	0.014	0.015

[Volatiles]	Air	4% O2
Low OFA (10%, ER 0.95)	0.0014	0.0014
Med OFA (22.5%, ER 0.82)	0.0024	0.0021
High OFA (45%, ER 0.58)	0.0046	0.0042

[NO]	Air	4% O2
Low OFA (10%, ER 0.95)	0.00036	0.00038
Med OFA (22.5%, ER 0.82)	0.00031	0.00034
High OFA (45%, ER 0.58)	0.00026	0.00029

Table 9 Model Exhaust NOx Results

Mole Fraction NO	Air	4% O2
Low OFA (10%, ER 0.95)	0.000356	0.000375
Med OFA (22.5%, ER 0.82)	0.000321	0.000342
High OFA (45%, ER 0.58)	0.000309	0.000330

Mass Fraction NO	Air	4% O2
Low OFA (10%, ER 0.95)	0.000355	0.000373
Med OFA (22.5%, ER 0.82)	0.000319	0.000341
High OFA (45%, ER 0.58)	0.000308	0.000328

Mass Flow (kg/s)	Air	4% O2
Low OFA (10%, ER 0.95)	0.0186	0.0181
Med OFA (22.5%, ER 0.82)	0.0186	0.0181
High OFA (45%, ER 0.58)	0.0186	0.0181

Mass NO (kg/s)	Air	4% O2
Low OFA (10%, ER 0.95)	6.614E-06	6.74E-06
Med OFA (22.5%, ER 0.82)	5.945E-06	6.15E-06
High OFA (45%, ER 0.58)	5.739E-06	5.94E-06

Fuel Flow 0.001991 kg/s 4.96E-05 MMBtu/s

Mass NOx (kgNO/MMBtu)	Air	4% O2
Low OFA (10%, ER 0.95)	0.2044	0.2084
Med OFA (22.5%, ER 0.82)	0.1838	0.1901
High OFA (45%, ER 0.58)	0.1774	0.1836

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[1] Bool, L., and Bradley, J., "Demonstration of Oxygen-Enhanced Combustion at the James River Power Station, Unit 3", The Mega Symposium, Washington D.C., May 20, 2003.

[2] Chatel-Pelage, F., Pranda, P., Perrin, N, Farzan, H., and Vecci, S.J., "Oxygen-Enrichment for NOx Control in Coal-Fired Utility Boilers," The 29th International Technical Conference on Coal Utilization & Fuel Systems, April 18-22, 2004, Clearwater, FL.