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CFD Simulation of Flue Gas Recirculation in a Rotary Kiln for NO_x Reduction

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ABSTRACT: The Indian cement industry has to reduce its current emission levels in terms of NO_x emissions to be at par with the newer environment regulations. This paper focuses on simulation of Flue Gas Recirculation system at different recycle ratios for maximum NO_x reduction in an industrial cement rotary kiln while keeping desired temperature at various Rotary Kiln zones. In each simulation, the NO_x emission at Kiln outlet as well as the temperature profile along kiln axis was compared. The results show about 72% reduction of NO_x in given kiln conditions.

KEYWORDS: Computational Fluid Dynamics, NO_x Reduction, Cement, Rotary Kiln, FGR, Flue Gas Recirculation

I. INTRODUCTION

With nearly 390 million tons (MT) of cement production capacity [1], India is the second largest cement producer in the world and accounts for 6.7 per cent of world's cement output, which is expected to reach 407 million tons by FY17.

The process of cement manufacturing due to being a high temperature process favors the formation of nitrogen oxides (NO_x) . NO_x is a major environment pollutant which when released into the atmosphere; dissolve in available moisture to form a weak nitric acid solution which further causes acid rain. Due to this Government of India has made the Environment (Protection) Third Amendment Rules, 2016[2].

Cement Plant with co-processing of wastes			
Oxides of Nitrogen (NO _x) in mg/Nm ³	Concentration not to exceed, in mg/Nm ³		
Commissioned After 25.8.2014	600		
Commissioned 25.8.2014	800 for rotary kiln with In Line Calciner technology.		
	1000 for rotary kiln using mixed stream of ILC,		
	Separate Line Calciner (SLC) and suspension pre-		
	heater technology or SLC technology alone or		
	without calciner.		

Table 1: Environment (Protection) Third Amendment Rules, 2016

A. MOTIVATION

Since the technologies based on secondary mitigation of NO_x such as SCR, SNCR etc. require either high capital or operating expenses an existing technology called Flue Gas Recirculation seems a suitable solution. Though there are onetime costs involved in duct work, and small power (fan power), this technology doesn't involve use of any hazardous reagents. The typical cement plant flue gas consists of about 14% to 19% CO₂ (from limestone calcination and fuel oxidation) depending upon the fueland raw material characteristics, about 4% to 7% Oxygen (depending upon the false air) and remaining is atmospheric Nitrogen. The idea behind the technology is to create inert zones i.e. absence of oxidization zones inside flame. This reduces formation of thermal NO_x. Also, by reducing percentage of Nitrogen in overall mixture, the probability of NO_x formation decreases.



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Another, benefit of using flue gas recirculation is that it increases CO_2 fraction in the flue gas, this can be very helpful for efficient carbon capture possibilities for sustainability of the industry.

The purpose of this study is to establish the most effective configuration by which NO_x reduction can be efficiently achieved without highly affecting kiln temperature profile. For this, an existing rotary kiln system along with a multichannel burner was modeled using actual flow rates of fuel and air. In later stage a secondary oxidizer stream was introduced in the kiln geometry for introducing flue gas in the system. The reduction efficiency as well kiln temperature profile was plotted for different flue gas recirculation ratio.

II. THEORY

2.1. NO_x generation: NO_x is a major environment pollutant which when released into the atmosphere, dissolve in available moisture to form a weak nitric acid solution which further causes acid rain, moreover when it mixes with volatile organic compounds and sunlight forms photochemical smog. The nitrogen oxides (NO and NO_2) or NO_x are produced during the combustion process where nitrogen and oxygen gases in the air combine to form oxides of nitrogen when exposed to extremely high heats (>1500°C).

Five major mechanisms for formation of NO_x are as follows [3]:

2.1.1. The Thermal Mechanism: also referred to as the extended Zeldovich mechanism, can be simplified to the following elementary reactions:

$O + N2 \Leftrightarrow NO + N$	(1)
$N + O2 \Leftrightarrow NO + O$	(2)
$N + OH \Leftrightarrow NO + H$	(3)

The rate-limiting reaction is equation (1) due to its relatively high activation energy of 319050 kJ/kmol. With the assumptions that the N_2 , O_2 , O and OH concentrations are at their equilibrium values, the NO concentrations are much less than their equilibrium values and the N atoms are in steady state, the following expression can be obtained:

$$\frac{d[NO]}{dt} = 2 k_1[O]eq[N_2]eq$$
(4)

here [] denote concentrations and k_1 , the rate coefficient in equation (2-1), is given by:

$$K_1 = 1.8 . \ 1011. \ \exp\left[\frac{-38370}{T(K)}\right] = \left[\frac{m^3}{kmol-s}\right]$$
(5)

From equation (4) and (5), it can be seen that the thermal NO formation can be controlled by the O and N_2 concentration, temperature and residence time. Thus by preventing hot spots, reducing oxygen rich zones at high temperatures and reducing time of exposure at high temperatures can lower the NO_x production. In the literature, thermal NO_x is said to be unimportant for temperatures below 1800 K [4, 5].

2.1.2. The Prompt Mechanism: also known as the Fennimore mechanism is directly linked to the combustion of hydrocarbons. Hydrocarbon radicals react with molecular nitrogen to form hydrocyanic acid (HCN). These compounds are then converted to intermediate compounds that form NO. The quantity of HCN formed increases with the concentration of hydrocarbon radicals, which in turn increases with equivalence ratio. The prompt mechanism can be described with the following equations [3]:

$$\begin{array}{ll} N_2 + CH \Leftrightarrow HCN + N & (6) \\ HCN + O \Leftrightarrow CO + H & (7) \end{array}$$

(6) and (7) will ultimately react to form NO, and the chemistry becomes more complex with higher equivalence ratio. As the equivalence ratio increases, prompt NO_x production increases at first, then passes a peak, and finally decreases due to a deficiency in oxygen.



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2.1.3. The N_2O -intermediate mechanism: increases in importance under fuel-lean, low temperature and high pressure conditions. The following three reactions are involved in the N_2O -intermediate mechanism:

$O + N_2 + M \Leftrightarrow N_2O + M$	(8)
$H + N_2O \Leftrightarrow NO + NH$	(9)
$O + N_2O \Leftrightarrow NO + NO$	(10)

This mechanism becomes important in lean premixed combustion, but may also contribute to the NO_x -production in rich premixed combustion.

2.1.4. The NNH mechanism: is a route forming NO by the oxidation of NNH radicals proposed by Bozzelli and Dean in 1995. They suggested that significant amounts of nitrogen oxide can be produced in flames from N_2 via NNH formed in the reactions:

$$\begin{array}{ll} N_2 + H \Leftrightarrow NNH & (11) \\ NNH + O \Leftrightarrow NH + NO & (12) \end{array}$$

This route is said to be of importance in rich flames and in lean mixtures up to moderately high (1900 K) temperatures.

2.1.5. Fuel NO_x: If nitrogen is a part of fuel molecule, it can form NO_x, the Fuel NO_x can contribute as much as 50% of total emissions, when combusting oil and as much as 80% when combusting coal.

The mechanism consists of three reaction steps:

HCN-NO formation: HCN + O₂ \longrightarrow HCO +NO (13) HCN-NO destruction: HCN + NO \longrightarrow HCO + N₂ (14) HCO oxidation: HCO + $\frac{3}{4}$ O₂ \longrightarrow CO₂+ $\frac{1}{2}$ H₂O (15)

The rate law of formation of nitric oxide:

$$[NO] = k \int [N]^{\alpha} [O_2]^{\beta} d\theta$$
(16)

2.2. NO_x Reduction Technologies

The NO_x reduction technologies can be broadly divided into two categories, Combustion modification or Primary Mitigation and Post-combustion treatment or secondary mitigation. Secondary mitigation technologies either require too much operating costs (SNCR) or high capital expenses (SCR)

2.2.1. Combustion Modification: These are some of the technologies available for primaryNO_x reduction:Lox-NO_x Burners,Overfire Air, Reburnings,Flue Gas Recirculation, and Operationalmodifications.

2.2.2. Post-Combustion Treatment: Selective Catalytic Reduction (SCR), Selective Non-catalytic Reduction (SNCR).

III. CFD ANALYSIS

The existing burner was modeled using CFD software to obtain measured value of NO_x emissions. CFD technology mainly consists of three parts. The first part is the physical models which are a set of conservation equations of mass, momentum, energy, state equation, turbulent equations, etc. The second part is a series of solution approaches for



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solving these physical models, and the third part is the preprocessor of discretization of computational domain and the postprocessor of visualization of numerical results.

A. MODELING OF EXISTING KILN SYSTEM

3.1.1. Geometry

The burner consists of several separate channels for Petcoke, primary air (axial& swirl). A 2d geometry of burner along the kiln was built in Ansys Design Modeler Software. A structured quad mesh was created in Ansys Meshing Module.

Model Dimensions				
Body	Length, n	nm i	Radius, mm	
Kiln	48000		1300	
Burner	950		280	
Burner Dimensions				
Burner Design	D2, mm	D1, mm	Area, mm ²	
Swirl Air Inlet	130	117	2522	
Fuel Inlet	173	141	7892	
Axial Air Inlet	222	210	4072	

Table 2: Kiln and Burner dimensions

Mesh Statistics			
Nodes	38408		
Elements	37743		
Mesh Metric	Orthogonal Quality		
Min	0.99993		
Max	1.		
Average	0.99999		
Standard Deviation	9.8195e-006		

Table 3: Mesh Quality Details

Following six Named Selections were created in order to provide boundary conditions in solver: SYMMETRY, SECONDRY_INLET, WALL, PRESSURE_OUTLET, B_PIPE_WALL, B_WALL, AXIAL_INLET, FUEL_INLET, SWIRL_INLET

3.1.2. Solver Settings

The Boundary Conditions, General solver settings and Physics used in simulations are as follows:

Boundary Conditions			
Boundary	Mass Flow Rate, Kg/hr Gauge Pressure, mm		
Fuel	2500	3000	
Axial Air	2650	3250	
Swirl Air	2650	3250	
Secondary Air	28450	-5	
Pressure Outlet		-25	

Table 5: Boundary conditions



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General solver settings		
Solver Type	Pressure-based	
Velocity Formulation	Absolute	
Time	Steady	
2 d space	Axisymmetric Swirl	
Energy	On	
Viscous Model	Standard k-epsilon turbulence model	
Radiation	P1	
Wall Treatment	Standard Wall Functions	
Species	Non-Premixed Combustion	
NO _x	On	
Pressure velocity coupling scheme	SIMPLE	
Spatial discretization Gradient	Least square cell based	
Pressure	PRESTO!	
Upwind Scheme	First Order Upwind	

Table 4: General solver settings and Physics

B. FLUE GAS RECIRCULATIONSYSTEM [4]

3.2.1 Theory

A flue gas recirculation system uses gases exhaust gases from the pyro system and injects them back with secondary air, this helps in reduction of flame temperature by temperature dilution as well as creation of inert zones inside the flame as the flue gas is deficient in Oxygen content (4% to 5% in Pre-Heater exhaust in Cement Industry) as compared to fresh air (20.9 %).

The flue gas is introduced through an inlet normal to the kiln axis similar to secondary air in vicinity of burner. For this an annular segment of 130 mm is drawn in the geometry (over the burner).

The Geometry was meshed again and the newly created Flue gas injection inlet was provided with *named selection* FGR_INLET.



Figure 1: Rotary Kiln Geometry for Flue Gas Recirculation

3.2.2 Description of the Equilibrium Mixture Fraction/ PDF Model

To provide the composition of secondary inlet the mean mixture fraction[4] was calculated using the following method:



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Figure2: Using the Non-Premixed Model with Flue Gas Recycle

$$f_{\text{exit}} = \frac{\dot{m}_{\text{fuel}}}{\dot{m}_{\text{fuel}} + \dot{m}_{\text{ox}}} \tag{17}$$

Where, \mathbf{f}_{exit} is the exit mixture fraction (and the mixture fraction at the flue gas recycle inlet), \mathbf{m}_{ox} is the mass flow rate of the oxidizer inlet, \mathbf{m}_{fuel} is the mass flow rate of the fuel inlet.

The NO_xgeneration was calculated atdifferent recirculation ratios by providing Mean Mixture Fraction =0.06896.

IV. RESULTS

Both the case files were compared in CFD Post Module of Ansys Workbench (Academic 16.2). The graph plotted below shows the temperature profile along the Kiln length. There is reduction of about 1.5% and 3.6% in temperature for 2% and 5% recirculation ratio respectively.



Figure 3: Temperature Profile along kiln length

Significant reduction in NO_x formation is evident from figure 4. It shows the mass fraction of Pollutant along the kiln axis at 0%, 2% and 5% recirculation ratio. At 5% recirculation ratio, without too much decrease in flame temperature there is reduction in NO_x generation.



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Figure 4: NO_x emission along kiln length

The results can be further summarized as shown in table 6 which shows Pollutant NO_x , CO, O_2 and Temperature at Kiln outlet at various Recirculation ratios. At 5% recirculation ratio there is significant reduction in NO_x .

Recirculation Ratio	NO _x , PPM	CO, %	O ₂ , %	T, °C
0%	229	0.0282	0.815	1506
2 %	139	0.0211	0.812	1483
5%	65	0.0150	0.810	1452

Table 6: Comparison between Original and Low NO_x design

V. CONCLUSION

In the present study, the effect of Flue gas Recirculation was investigated at different Recycle Ratios in an existing Cement Rotary Kiln System by using commercial CFD software ANSYS –FLUENT (Version 16.2 Academic). The results show about 72% reductions at 5% and 39% at 2% Recirculation Ratio. The effect on temperature profile was also determined which shows 1.5% and 3.6% on 2% and 5% recirculation ratio respectively. This shows Flue gas recirculation is a promising technology for effective mitigation of NO_x without significant capital and operating expenses.

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