Numerical Modelling and Study of Combustion Behaviour of Rotary Cement Kiln Using Computational Fluid Dynamics

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ABSTRACT

Rotary Cement kiln is one of the key equipment in cement industry used to convert calcineous raw meal to cement clinkers .*Now days Computational fluid dynamics (CFD) is main tool used for conducting researches in different fields in absence of experimental tools or laboratories this paper aims understanding of the flow behaviour what is takes place inside the Cement rotary kilns using Computational fluid dynamics . Both the Primarily and Secondary types of methodologies were used to reach to final point of the research .* The *Computational fluid dynamics* model used in this program solves the Reynolds-averaged Naiver-Stokes (RANS) with K-∈ turbulence model. *The main thermal parameters which are basic for combustion were investigated and confirmed resulted was obtained.*

Keywords: CFD, Combustion, Rotary Cement kiln, Reynolds-averaged Naiver-Stokes (RANS)

1. INTRODUCTION

Cement is a solid product composed of primarily limestone, clay, shale, and silica sand. It has a strong hydraulic binder power and becomes a hard and durable material in a few days by reacting with water. It is used to form concrete (mixture of cement, water, fine sand and coarse aggregates) which is the world’s most commonly used construction material [1].

1.1 **Cement Rotary Kiln systems**

The rotary cement kiln is very large in size, hottest thermal equipment and the heart equipment in cement production. As defined in [2] rotary kiln is one of the key equipment in cement industry used to convert calcineous raw meal to cement clinkers. [3, 4] also defined cement kiln as the most vital part of a cement factory whose outcome is cement clinker.

Rotary kiln has wide range of application such as drying, calcining, iron ore reduction, pyrolysis and titanium dioxide production and recently also rotary kilns for pyrolysis of wastes [5]. In general, the main task of any rotary kiln as described in [2] is to provide high temperature environment to drive solid – solid and solid –liquid reactions for clinker formation.

In cement kiln a lot of reaction are takes place at different temperatures’ in the different zones of the kiln. As described in [6] by referring (Wang et al., 2006), When the kiln feed enters the high-temperature zones in the rotary kiln, a series of chemical reactions occur in which the quicklime, alumina, ferric oxide, silica, and other metal oxides react to form four main compounds of cement namely, CaO.SiO2(C3S), 2CaO.SiO2(C2S), 3CaO.Al2O3(C3A),and 4CaO$Al2O3.Fe2O3 (C4AF).The compounds have their own temperature formation and specific zone of the kiln. Generally, the rotary cement kiln has three main zones.

Table 1: Main zones and Their corresponding reactions [6]

S/N	Zone Name	Chemical reaction	Temperature in (℃)	Explanation
1	**Decomposition Zone**	CaCO3→CaO + CO2	600-900	Calcination occurs in this region, indicating that the limestone, CaCO3, will decompose into calcium oxide (free lime), CaO and carbon dioxide.
		$CaO+Al_2O_3 = CaO.Al_2O_3$	800	
		CaO+Fe2O3 =CaO.Fe2O3	800	
		$CaO+CaO.Fe_2O_3 = 2CaO.Fe_2O_3$	800	
		$3(CaO.Al_2O_3) + 2CaO = 5CaO.3Al_2O_3$	900-950	
2	**Transition Zone**	2CaO+SiO2 =2CaO.SiO2	1000	The key reactions in this zone are exothermic beginning with silica (C2S),(ΔH=+603 kJ/kg C2S) followed by the formation of C4AF (ΔH=+109 kJ/kg C4AF and C3A(ΔH=+37 kJ/kg C3A)
		3(2CaO.Fe2O3)+5CaO.3Al2O3+CaO =3(4CaO.Al2O3.Fe2O3)	1200-1300	
		5CaO.3Al2O3+4CaO=3(3CaO.Al2O3)	1200-1300	
3	**Sintering Zone**	2CaO.SiO2+CaO=3CaO.SiO2	1350-1450	This is the hottest region of the kiln where temperatures can reach above 1350℃ and the solid components begin to liquefy. Coating formation of on the refractory material occurs

1.2 Modeling of the Rotary Cement Kiln System

Sometimes it is difficult to visualize, predict or analyses what is takes place inside the high temperature burners and combustion chamber like cement rotary kiln system, fluidized beds, incinerators and so on by human sense organs. Not only this conducting experiment or testing is also very difficult. Such problems can be easily solved by using tools like Computational Fluid Dynamics (CFD). So in order to understand the physical process and chemical reaction which is takes place inside the rotary kiln CFD is best option. Thus ,here in this research CFD code was used to predict the flow behavior of materials and flue gases ,temperature distribution and pressure profiles in different zones of the kiln ,degree of heating of the fuel(coal) , rate of conversion of mass and energy of fuels and materials ,the combustion characteristics inside a rotary cement kiln etc.

As described by different scholars and researches emphasize that CFD is a multidimensional tool used to analysis systems related to fluid flow, heat transfer and associated phenomena such as chemical reactions, combustions etc. As defined and explained the advantage in [7] CFD is a design and analysis tool that uses computers to simulate fluid flow, heat and mass transfer, chemical reactions, solid and fluid interaction and other related phenomena. The main advantage of CFD over physical experiment is cost saving, timely, safe and easy to scale-up. Thus, CFD codes are virtual laboratory which are run on computers and perform the equivalent numerical experiments conveniently providing insight, foresight and return on investment.

Now a day CFD is the popular investigation tool in different research areas. As mentioned in [8] different researchers use CFD program to predict fluid flow behavior, heat and mass transfer, chemical reactions (e.g. devolatilization, combustion), phase changes (e.g. vapor in drying, melting in slagging), and mechanical movement (e.g. rotating cone reactor) .In addition to this researchers have been using CFD also to simulate and analyze the performance of thermochemical conversion equipment such as fluidized beds, fixed beds, combustion furnaces, firing boilers, rotating cones and rotary kilns. Researcher's such as [9] used CFD to understanding chemical reactions, the heat exchange processes and fluid flow, different cement Calciners. Thus, a lot of researchers and scholars have been used computational fluid dynamics (CFD) as a tool to study, model and simulate rotary kiln from different perspectives. Few of the published that applies CFD to model the cement rotary kiln process is presented in the following paragraphs. For example [10] uses CFD to model three-dimensional steady state model to predict the flow and heat transfer in a rotary kiln.

Others like [11] used commercial CFD code Fluent-6.3.26 to model and carried out for a full scale rotary cement kiln with multi-channel coal burner. The study included developing and combining the models of gas-solid flow and modeling of pulverized coal combustion.

A three-dimensional mathematical model based on the Eulerian approach and the kinetic theory of granular flow is developed to predict the granular flow in rotary kiln was studied in [12]. Thus, particle flow behavior in axial direction, Velocity vector of particle and Velocity profiles at four different locations, Granular temperature etc. have been analysed. Finally, the CFD results where compared with experimental results and reasonable agreement was obtained.

Still others have utilized [13] CFD to Model the Waste Heat recovery On the Rotary Kiln System in the Cement Industry. This study has used CFD fluent code analysis to show the flow of heat absorbed by air from the surface of the kiln wall, air inlet temperature profile, input heat energy to the system components, air outlet temperature profile in outlet shell, temperature distributions at each position on the kiln shell width.

Meat and bone meal (MBM) combustion and coal combustion in a rotary cement kiln were simulated .here in this study Contours of O_2 , CO and CO_2 mass fraction for meat and bone meal(MBM), static temperature for MBM, Coal char and MBM mass fraction variation of ten random 20 µm particle, Mass-weighted average oxygen mass fraction along the kiln in different diameter of kiln and other parameters have predicted using CFD in [14].

Not only research articles but also some projects were also used CFD to simulate the rotary cement kiln. For examples [15] uses A general purpose three-dimensional CFD model for rotary lime kilns .From this the project undertaken it has been concluded that the developed CFD model can be used as a powerful tool to study the detailed flame characteristics and burner design parameters for a rotary lime kiln and to examine the impacts on the kiln performance due to varied kiln operation parameters and firing conditions. The evaluation of the developed CFD model against the in-plant measurements shows that the predicted results from the CFD modelling agree reasonably well with the in-plant measured data.

1.6 Combustion Modeling Using CFD for Cement Rotary Kiln

Combustion is the conversion of reactants called a fuel into chemical compounds known as products of combustion by combination with an oxidizer. The combustion process is an exothermic chemical reaction. Combustion may be represented symbolically as follow:

Fuel + Oxidizer $\longrightarrow$ Products of combustion + Energy

Combustion is one of the most important processes in engineering, which involves turbulent fluid flow, heat transfer, chemical reaction, radiative heat transfer and other complicated physical and chemical processes [16].

Combustion must consider a number of complex, simultaneous and interdependent processes such as gas and particle phase dynamics, turbulence, heat transfer, pollutant formation and heterogeneous and homogenous chemical reactions [6].

Rotary cement Kiln is normally a counter-flow heat exchanger type in which the direction of the flow flue gases and raw feed materials is opposite as shown in figure 2. Different authors and researchers were used different fluid flow models to analyse the combustion process inside the rotary cement kiln. For instance, reference [6] was used the Eulerian–Lagrangian model to describe the flow of the gas and particle phases, and RNG - k epsilon model took into account the rotational effect of material in the kiln. The SIMPLEC algorithm was chosen for the pressure–velocity coupling. As stated in [11,17] CFD codes applied to rotary kiln combustion modeling consist of "renormalization group" (RNG) k-ε turbulent model for gas phase and, in the case of pulverized combustion particles, the statistical (stochastic) trajectory model for homogeneous volatile and heterogeneous solid-phase char combustion.

As we stated above rotary kiln is counter flow heat exchanger. Thus, the mathematical model of gas-solid equation is describing as follow.

1.6.1 Gas-Phase Conservation Equations Used in CFD Modeling of Rotary kiln

The set of conservation equations that are solved in most CFD analyses are as including the stress generation are presenting in equation (6-12) [17]. Every flow model in FLUENT solves the conservation of mass and momentum So as illustrated in [19] literature the governing equation of continuity and momentum of gas phase is described below in equation 6 and equation 8 respectively.

$$\frac{\delta\rho}{\delta t}+\frac{\delta}{\delta xi}=Sp \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (6)$$

However, if, the system is considered as steady state condition equation 6 becomes as follow.

$$\frac{\delta}{\delta xi}=Sp \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (7)$$

Where Sp is the source term resulted from combustion particles.

$$\frac{\delta\rho}{\delta t}(\rho ui)+\frac{\delta}{\delta xi}(\rho uiuj)=-\frac{\delta p}{\delta xj}+\frac{\delta\tau ij}{\delta xj}+\rho gi+Fi+Sp\ldots\ldots\ldots\ldots\ldots\ldots (8)$$

Where P, τ ρg and F pressure and turbulent shear stresses, gravitational force and force respectively

The **τ**ij term in equation (8) represents Reynolds stress as follow.

$$- \rho uiuj = \mu t\left(\frac{\delta ui}{\delta xj}+\frac{\delta uj}{\delta xi}\right)-\frac{2}{3}\delta ij(\rho k+\mu t\frac{\delta ui}{\delta xi} \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots (9)$$

Turbulence modelling is implemented as a closure model for the Reynolds stress with the most commonly used k-ε turbulence model.

k-equation

$$\frac{\delta}{\delta t}(\rho k)+\frac{\delta}{\delta xi}(\rho kui)=\frac{\delta}{\delta xj}\left[\left(\mu+\frac{\mu t}{\sigma k}\right)\frac{\delta k}{\delta xj}\right]+G-\rho\varepsilon \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots ..(10)$$

where the generation of turbulence denoted by G comprises two terms, (I) the generation of turbulence kinetic energy due to the mean velocity gradients, and (II) that due to the generation of turbulence kinetic energy due to buoyancy.

ε-equation

$$\frac{\delta}{\delta t}(\rho\varepsilon)+\frac{\delta}{\delta xi}(\rho\varepsilon ui)=\frac{\delta}{\delta xj}\left[\left(\mu+\frac{\mu t}{\sigma\varepsilon}\right)\frac{\delta\varepsilon}{\delta xj}\right]+C1\varepsilon\frac{\varepsilon}{k}-C2\varepsilon\frac{\varepsilon^2}{k}+S\varepsilon \dots \dots \dots \dots \dots \dots . \dots \dots \dots .(11)$$

Where the term Sε is the turbulence source term in the turbulent Naiver Stokes equations

In order to include temperature distribution, the Navier Stokes equations are accompanied by an energy equation that solves for enthalpy (h=cpT). The balance equation for enthalpy is

$$\frac{\delta}{\delta t}(\rho h)+\frac{\delta}{\delta xi}(\rho uih)=(\mathbb{\Gamma} h\frac{\delta h}{\delta xj}+Sh \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots ..(12)$$

. The source term,Sh, includes combustion, that is, the heat source and the heat transfer within the system that affect temperature. In rotary kilns, the dominant heat transfer mode is radiation .

1.6.2 Particle-Phase Conservation Equations Used in CFD Modeling of Rotary kiln system

As stated in [18] Coal combustion has been modeled using the eddy dissipation model of Fluent. The particle phase is treated by solving the Lagrangian equations for the trajectory of a statistically significant sample of individual particle, which represents a number of the real particles with the same properties. In present work, coal particles following a Rossin-Rammler size distribution are tracked in Lagrangian frame of reference using stochastic trajectories model with gravity effect on as shown in equation 13.

$$M_p\frac{duip}{\delta t}=C_D\frac{Ap}{2}(uig-uip)|uig-uip|Mpgk \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (13)$$

Combustion processes of coal are treated as de-volatilizing first and then char burning. Combustion of volatile is rapid and the combustion is said to be mixing-controlled, complex, and often unknown, chemical kinetic rates can be safely neglected[11]. Again, as described in [rr2] by refereeing the work of Magnussen and Hjertager. The net rate of production of species due to reaction r, Ri,r, is given by the smaller (i.e., limiting value) of the two expressions below equations (14 & 15):

$$R_{i,r}=V'_{i,r}\ M_{w,r}A\rho\frac{\varepsilon}{k}\min_R\left(\frac{YR}{V'i,r\ \ Mw,R}\right) \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots .. \dots \dots \dots \dots \dots \dots \dots \dots .(14)$$

$$R_{i,r} = V'_{i,r} \; M_{w,r} A B \rho \frac{\varepsilon}{k} \frac{\sum P Y P}{\sum_{J}^{N} V''_{i,r} \; M_{w,j}} \quad \text{..........} (15)$$

Where Yp , is the mass fraction of any product species, YR is the mass fraction of a particular reactant, A is an empirical constant equal to 4.0 & B is an empirical constant equal to 0.5.

2. MATERIALS AND METHODS

2.1 Description of Rotary Kiln

Messebo cement factories have currently two main production lines. Here the rotary kiln of line -I which also known as old line was studied. The kiln burning system is composed of a Φ3.75x57m with inline calciner and a single five stage preheater

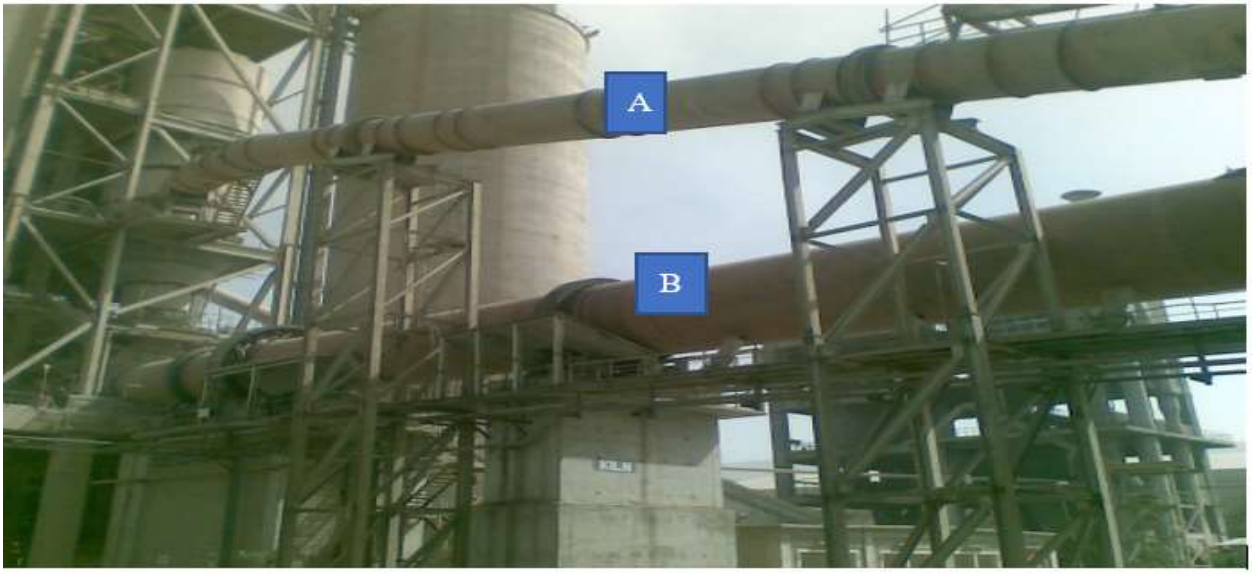


Figure 1: Tertiary duct (A) and kiln of line -I (B) of the company

Table 1: Different kiln zones, their corresponding lengths, surface temperature and calculated areas using cylinder formula

Kiln zone	Length (m)	Diameter(m)	Surface area $2\pi r^2 + 2\pi rh$ in m	MaxSurface Temp (℃)	Min Surface Temp (℃)
In let zone	16.5	3.7	213.187	291	149
Transition zone	33	3.7	404.88	298	151
Higher burnin zone	1.5	3.7	38.97	300	161

In the reference plant the Pre calcined raw material is then fed to the Rotary kiln where a series of physical & chemical process take place to form the clinker. Hot clinker is then led to the cooler. The energy requirement for clinker formation is met by burning fuel (coal, oil, gas) at the lower end of the kiln through multichannel burner. Primary air at ~ 70- 80°C is injected from the channels of the burner as swirl & axial air. Secondary air at ~ 1000 °C is drawn from the cooler through the annular opening between burner and the wall of the kiln. Heat transfer between flue gas and charge takes place through radiation and convection. Flue gas from the kiln flows out of the upper end of kiln into the pre calciner. The solid material (i.e. Clinker) coming out of the Rotary kiln is at around 1300-1450 °C and is cooled to 100-120 °C using ambient air. Look figure 3 below.

Figure 2: General Description of the rotary kiln Material and flue gas flow

2.3 CFD Process Flow Modeling and Features

A rotary kiln with 57m long including the burner and 3.7 diameter of Computational Domain Size was investigated. Solid work 2020 was used to draw the 3D geometry of the rotary kiln and ANSYS FLUENT, version 19.0, was used for modeling and simulation of the combustion process inside a rotary cement kiln. Three-Dimensional (3D) domain of gas-solid flow in rotary kiln with steady state has been considered. In order to reduce the mesh complexity and meshing time 1:10 was used.

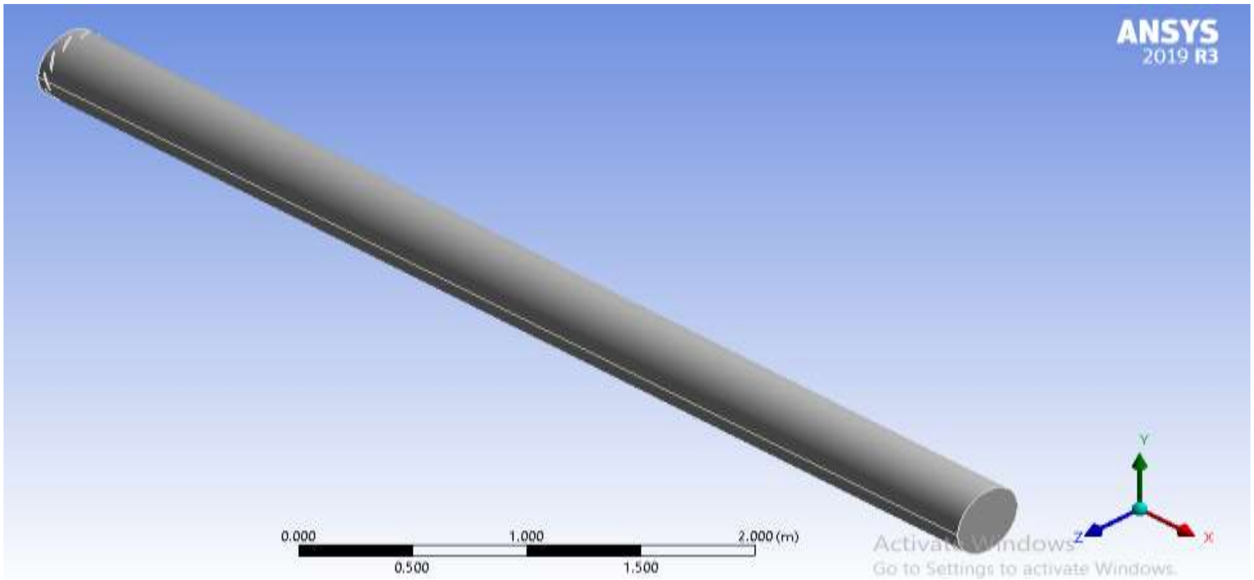
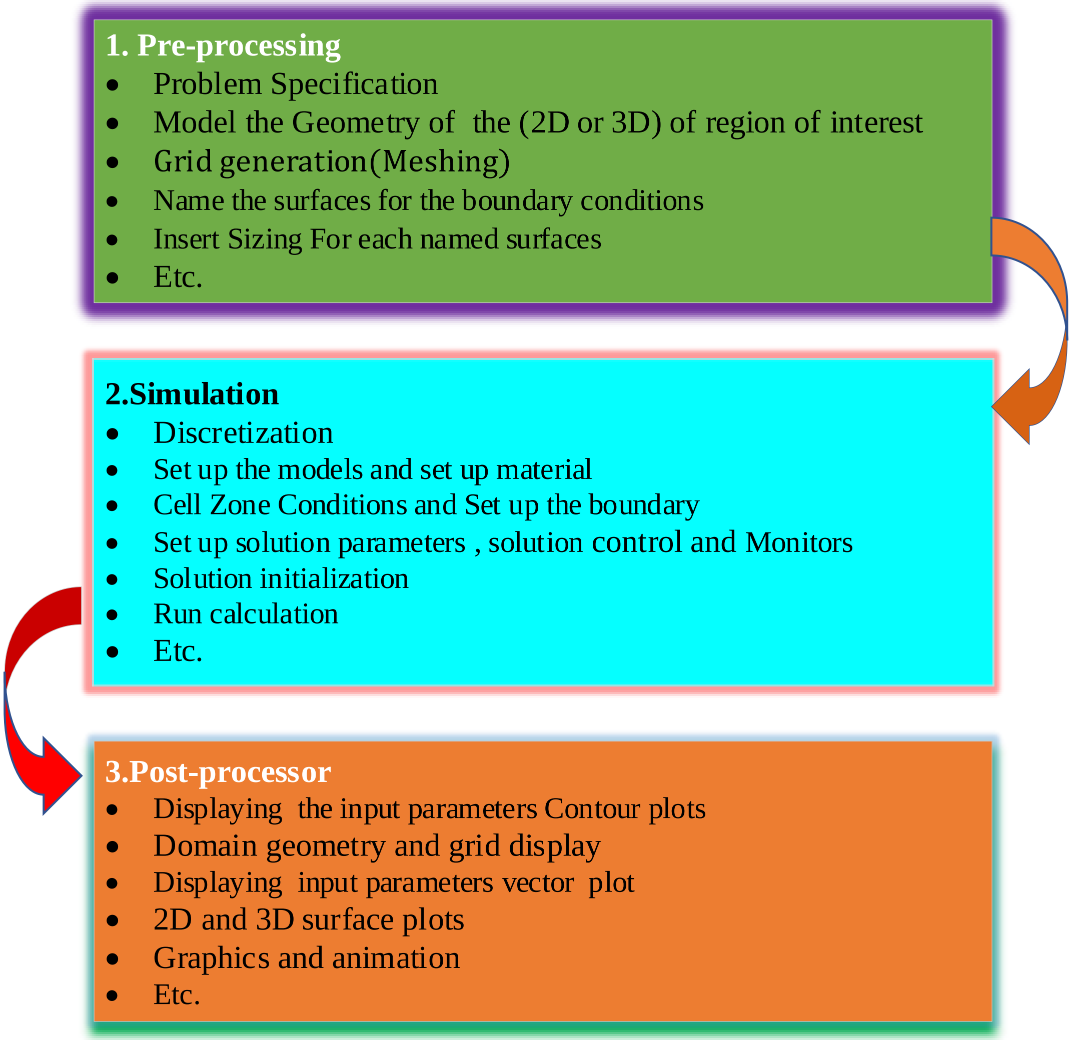


Figure3: Screenshot of the 3D model of the rotary kiln with swirler burner inside

By default, the combustion is turbulent type of reaction because turbulence is among the 3T' parameter's (i.e. time, temperature and turbulence) which are very important to have good combustion. So, calculating Reynolds number is not need here to know the behavior of gases (i.e. laminar or turbulent) inside the rotary kiln. The main reaction takes place in the rotary kiln is the reaction between pre calcined materials' (solid phase) and flue gases (gaseous phase) generating from secondary air and pulverized coal. The general flow work of CFD process is described in the figure 4 below.



1. Pre-processing

- Problem Specification
- Model the Geometry of the (2D or 3D) of region of interest
- Grid generation(Meshing)
- Name the surfaces for the boundary conditions
- Insert Sizing For each named surfaces
- Etc.

2.Simulation

- Discretization
- Set up the models and set up material
- Cell Zone Conditions and Set up the boundary
- Set up solution parameters , solution control and Monitors
- Solution initialization
- Run calculation
- Etc.

3.Post-processor

- Displaying the input parameters Contour plots
- Domain geometry and grid display
- Displaying input parameters vector plot
- 2D and 3D surface plots
- Graphics and animation
- Etc.

Figure 4: General flow work of CFD process

A Suitable computational grids or mesh for the discretisation technique based on standards and different scholars and researcher's recommendation, regular structure or topology mesh was used. Ansys fluent, which is based on the finite volume approach, is used for solving the set of governing equations. As recommended and described in [19, 20] the two-equation turbulence models gained popularity and formed the basis for much of the turbulence simulations over the

Past 40 years and it is most suitable model for combustion. The boundary condition (BC) used here was, an inflow of mass flow rate, Pressure out let (Flue gases) as outlet, Circular Swirl. Wall Boundary conditions with “no slip” was used. Since the current flow case was incompressible, the pressure-based solver is selected. A segregated algorithm called Semi-Implicit Method for Pressure Linked Equations abbreviated as “SIMPLE” was selected for the pressure-velocity coupling. The first order upwind spatial discretization scheme was used. Finally, Iterative convergence, residuals and under-relaxation factors were carefully adjusted to ensure solution convergence. For the level of accuracy, the limited residual values for the solution convergence (minimum values reached), when the residuals equation reach $10e^{-2}$ for velocity components and $10e^{-4}$for (k –ε) as shown in figure 6 .Thus it meets the minimum convergence criteria as recommended by different scholars and researcher like [21]

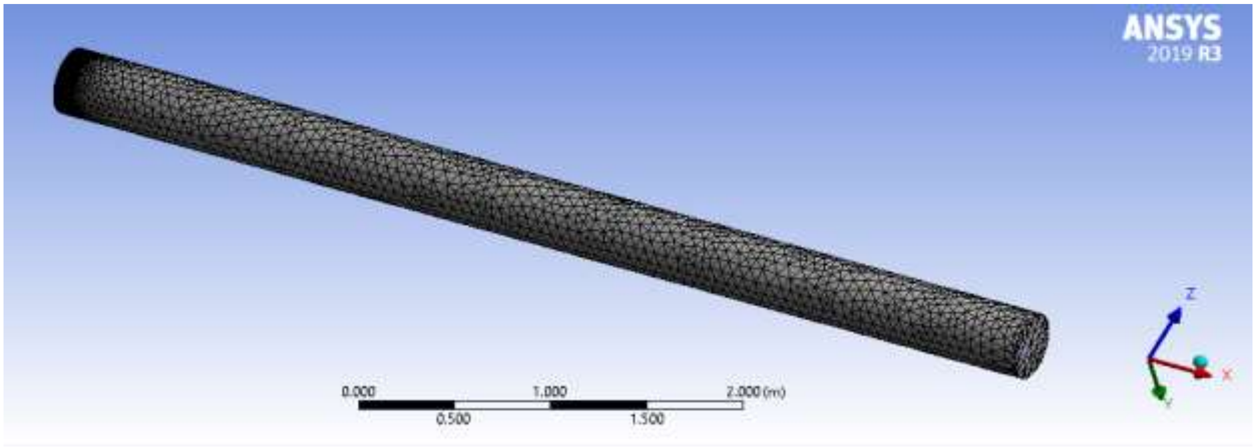


Figure 5: Screenshot of the mesh (Grid Development for 3D Model of Rotary Kiln)

3. RESULT AND DISCUSSION

3.1 Convergence criteria

As shown in Figure 6 the solution is converged (minimum values reached), when the residuals equation reach $10e^{-2}$for x, y, z-velocity components and $10e^{-4}$for (k –ε). Thus it meets the minimum convergence criteria [21].

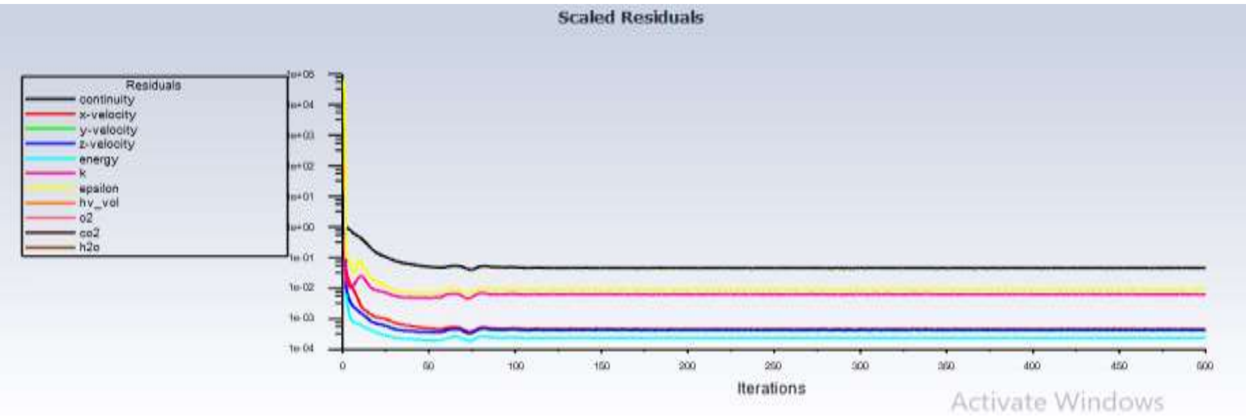


Figure 6: Convergence of the residuals

3.1 CFD Simulation Results of Flow Modelling

Velocity streamline, pressure and Temperature counter lines plots for the different air streams are shown in the following figures

The Velocity streamline for the three different starting conditions (firing conditions) were investigated .Because this is non-premixed type of burner. Even if there are a lot mixing probabilities (possible conditions) inside the burner. Here only four possible conditions were simulated (tasted). These conditions are adding the primary air and fuel at the same and the then add secondary air, secondly mixing the fuel and secondary air inside the burner then add primary air, feed the primary and secondary then feed the fuel in to the burner and lastly adding the materials at the same time. So it conclude that adding the Secondary after mixing the fuel with primary have great contribution to take place turbulent combustion due to its high temperature with aid air swirled as shown figure8.

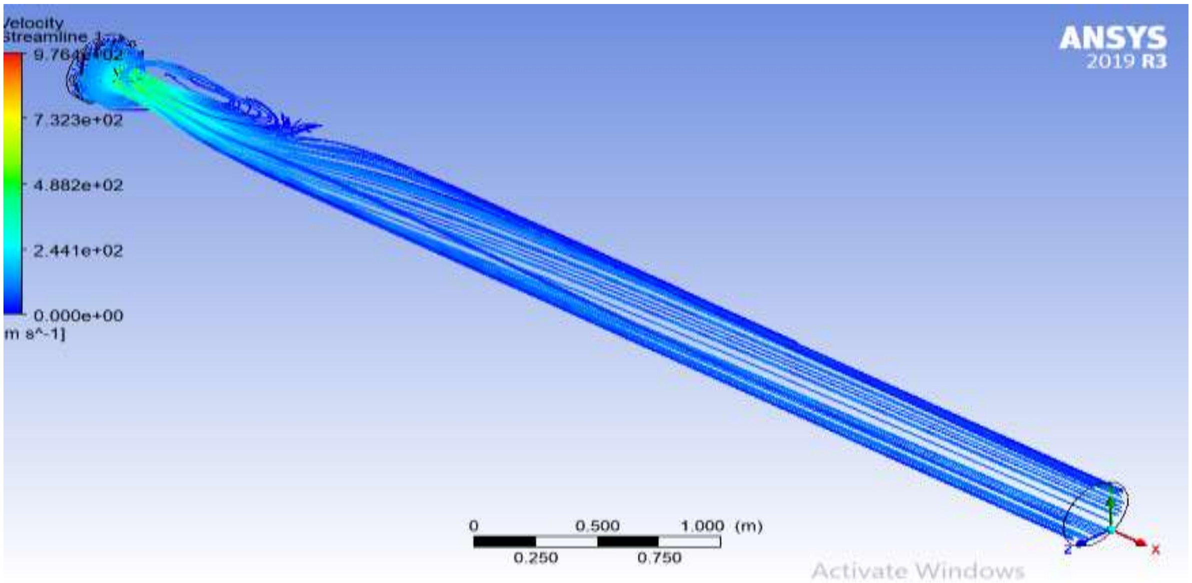


Figure 7:Velocity flow of stream line starting from primary air

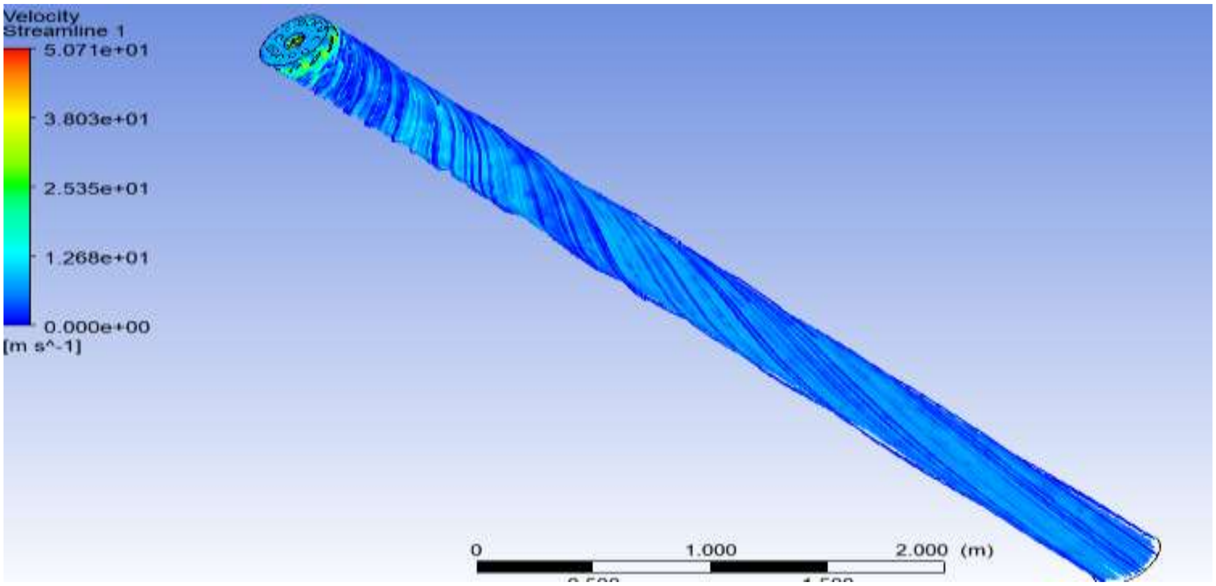


Figure 8:Velocity flow of stream line starting from Secondary air

As in the figure 7 shown starting from inlet of burner till the out let of kiln the presence of Swirler is clearly seen to have high turbulence and great circulation of air velocity during combustion .Thus high turbulence is among the basic parameters which highly affect the combustion process. So in figure 7 high velocity exists in the entrance of burner which due to high temperature of secondary air which around 1000℃ .So having high velocity helps to facilitate the mixing process of the fuel (in our case is coal) or to having good mixing of fuel with the different air streams.

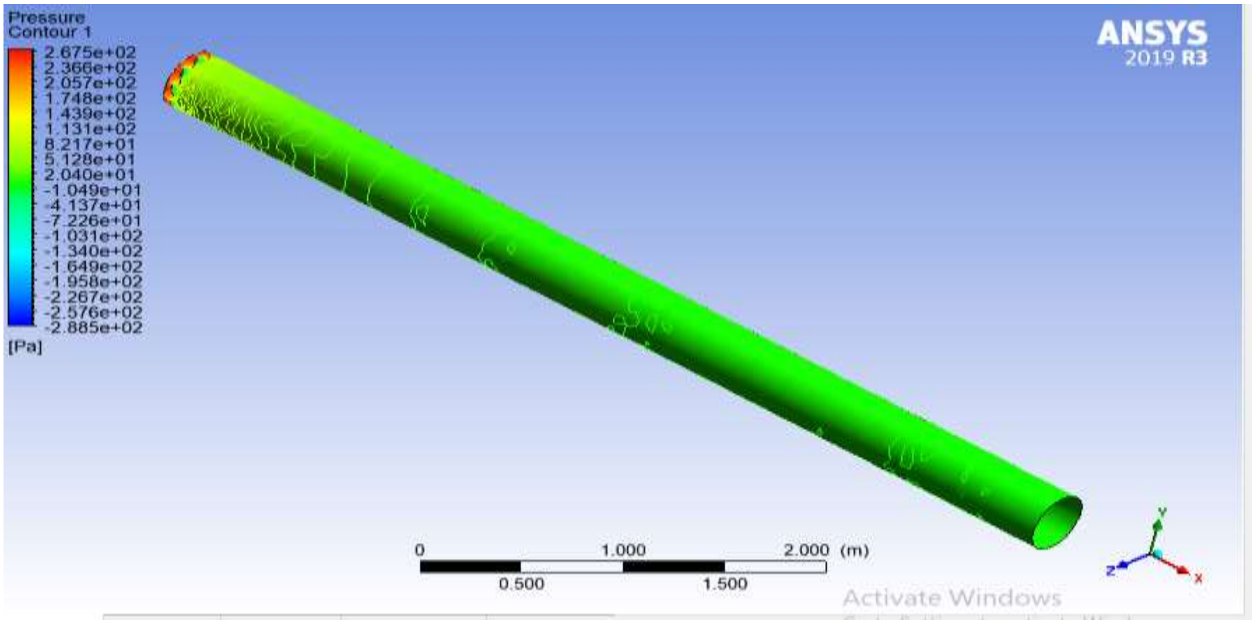


Figure 9: Pressure counter lines

From figure 9 of the above the pressure is high at inlet portion of fuel, secondary air ,primary air or at outlet of calcined material and lower at inlet of the material to be calcined or at out let of flue gases.

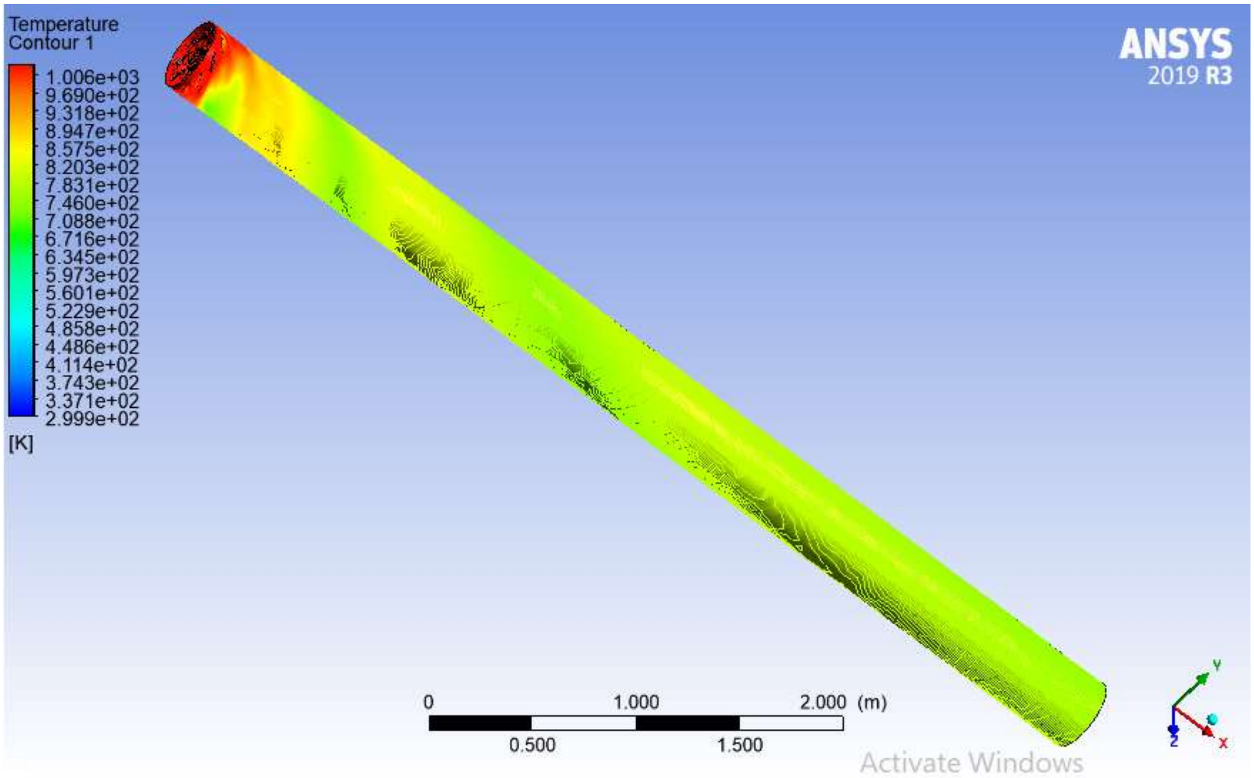


Figure 9: Temperature counter lines

Temperature contours as shown in figure 10 the condition of flame inside the kiln staring from burner inlet until it mixes with in coming material to be heated. Normally in the reference the maximum temperature of the kiln reaches around 1450℃(1723K) in higher burring zone of kiln .And here the maximum simulated (predicted using the CFD software) is shown in figure 9 which is around 1600℃(1873K). Thus as we can read from figure and the legend the temperature is high at out let of calcined material, medium in the transition zone and minimum in inlet zone which indicated by green colour in the legend and it is as expected with the actual kiln.

4. CONCULSION

The simulation was conducted with the use of a commercial CFD program, ANSYS Fluent 2019 R3.0. The computational domain was drawn in Solid work 2020 by reducing the actual dimension of the length and diameter with of ratio of 1:10. The CFD model used in this program solves the Reynolds-averaged Naiver-Stokes (RANS) with K-∈ turbulence model. Thus, the solution was converged (minimum values were reached), when the residuals of the continuity equation and the conservation of momentum equation reach 10e-2, for x, y, z-velocity components: 10 e^{-4}. For (k –ε). All simulated parameters were confirmed(validated) by comparing with actual data. The air Swirler have great role to facilitate combustion .The pressure and Temperature are high at inlet of fuel, secondary and primary air.

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