CHEMICAL ENGINEERING TRANSACTIONS
VOL. 29, 2012
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at: www.aidic.it/cet
Guest Editors: Petar Sabev Varbanov, Hon Loong Lam, Jiří Jaromír Klemeš

**ISBN** 978-88-95608-20-4; **ISSN** 1974-9791
DOI: 10.3303/CET1229253

# CFD Analysis of a Cement Calciner for a Cleaner Cement Production

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Cement calciners are pyroprocessing units found in modern cement plants. Inside of them occurs a strong endothermic reaction known as the calcination process, and the combustion of pulverized solid fuels. Controlling the mixing of limestone and pulverized fuel particles is of particular importance because it directly affects the energy consumption. The paper analyzes the impact of an axial and a swirl burner on the mixing of the particles, pollutant emissions and the operating conditions of a newly designed cement calciner. All necessary numerical models were developed and implemented into a commercial computational fluid dynamics code FIRE, which is then used for the analysis. This code is used to simulate turbulent flow field, temperature field, concentrations of the reactants and products as well as the interaction of particles with the gas phase, by solving the set of conservation equations for mass, momentum and enthalpy governing these processes. The results gained by these simulations can be used for the optimization of cement calciner's operating conditions.

## 1. Introduction

The cement industry with its high demand for energy is one of the leading producers of anthropogenic greenhouse gases, of which $CO_2$ is the most significant. Cement industry alone, contributes to 5 % of global anthropogenic $CO_2$ emissions, emitting almost 0.81 t $CO_2$/t of cement (Benhelat et al., 2012). Due to the continuous increase in the need for cement and more stringent environmental measures for the cement manufacturers, the dry rotary kiln with preheater and calciner technology has been widely adopted to replace some less energy efficiency kiln processes, e.g. wet rotary kiln process, shaft kiln process etc. (Zhang et al., 2011). Cement calciners are pyroprocessing units found in modern cement plants. Inside of them occurs a chemical process known as the calcination process, which is of particular importance because it directly affects the energy consumption. In recent studies different types of calciners have been investigated. Jianxiang et al. (2012) using the kinetic theory of granular flow and the large eddy simulation approach, simulated the turbulent flow in a cement calciner. This study shows that inlet parameters need to be set up very precisely to have good mixing of particles and a stable production for the simulated calciner. Mujumdar et al. (2007) presented a comprehensive model for the simulation of processes occurring in the pre-heater, calciner, kiln and cooler. This study shows that there is an optimum value for percentage of calcination carried out in calciner, with respect to overall energy consumption in clinker manufacture. For the kiln process in this work, the optimum value of calcination in calciner is about 70 %. Fidaros et al. (2007) demonstrated a mathematical model and a parametric study of flow and transport phenomena in an industrial calciner. This work shows

Please cite this article as: Mikulčić H., Von Berg E., Vujanović M., Priesching P., Tatschl R. and Duić N., (2012), CFD analysis of a cement calciner for a cleaner cement production, Chemical Engineering Transactions, 29, 1513-1518

good prediction capabilities for temperature, velocity and distribution of particles. Iliuta et al. (2002) studied the impact of different operating conditions on the rate of calcination, burn-out of char and NOx emissions of an in-line low NOx calciner. This work made a sensitivity analysis of the model with respect to aerodynamics, char oxidation and limestone decomposition parameters. Huanpeng et al. (2004) studied the effect of different parameters on the dynamics of the two-phase flow in a cement calciner. This work used the kinetic theory of granular flow to describe the transport properties of the solid phase. Hu et al. (2006) using the Eulerian frame for the continuous phase and a Lagrangean frame for the solid phase simulated a 3D model of a dual combustor and calciner, to predict the burn-out of coal particles and the decomposition of limestone. Mikulčić et al. (2012a) demonstrate the potential of CFD to support the design and optimization of calciners. This study shows that from the results obtained by CFD simulations, researchers may gain an in-depth understanding of all relevant thermo-chemical reactions occurring in a cement calciner. But, also all of these studies show that there is still a need for further research of cement calciner's operating conditions, heat and mass transfer and chemical reactions occurring inside the cement calciner.

Since calcination is a strong endothermic reaction, good mixing of limestone and pulverized fuel particles is essential for a more energy efficient, and thus a cleaner cement production. The use of experimental methods to investigate the mixing phenomena is complex and expensive, thus the use of numerical techniques is a more attractive way to obtain the necessary information. Moreover, results gained by the numerical methods give detailed information about the flow and transport processes inside a cement calciner, which is very difficult to obtain experimentally.

Combustion of pulverized fuel is a very important mode of fuel utilization. To ensure the adequate conditions for successful combustion of pulverized fuels appropriate burners need to be used. There are two types of burners that can be used in cement calciners, axial and swirl burners. The advantage of swirl burners over axial burners is their favourable effect on stabilization of the combustion process and reduction of $CO_2$, NOx, SOx and other emissions. The aim of this paper is to simulate the cement calciner with an axial burner and a swirl burner, to better understand the mixing of limestone and pulverized coal particles and the influence the type of a burner has on the limestone conversion rate. A three dimensional geometry of a cement calciner is simulated with a commercial finite volume based CFD code FIRE. This code is used to simulate turbulent flow field, temperature field, concentrations of the reactants and products as well as the interaction of particles with the gas phase. In this study a previously developed mathematical model for calcination process (Mikulčić et al., 2012b), taking into account the effects of temperature, decomposition pressure, diffusion, and pore efficiency, is used to investigate the rate of limestone conversion and a two stage coal combustion model treating pyrolysis and heterogeneous oxidation is applied.

Based on the modelling interactions between swirling introduction of limestone and coal dust firing are studied, e.g., regarding cooling effects in the near wall regions, distribution of gaseous species are analysed and particle trajectories of limestone and fuel are discussed. The results gained by these simulations can be used for optimization of cement calciner's operating conditions.

## 2. Numerical models

To investigate the mixing of particles inside the cement calciner and the operating conditions of a cement calciner, all relevant thermo-chemical reactions must be treated. The decomposition of limestone and the process providing the reaction enthalpy, e.g., the combustion of pulverized coal are the two main thermo-chemical reactions that occur in the cement calciner. In this study the Lagrangian formulation is used for the motion and transport of solid particles through the cement calciner, and the Eulerian formulation is used for the continuous phase. The developed mathematical models used for the pulverized coal and calcination calculation are treated in the Lagrangian spray module, where thermo-chemical reactions occur inside a particle as well as between the particle and the gas phase. The developed models, as well as a particle radiation model, were integrated into the CFD code, and applied together with additional user functions for providing thermo-physical properties of coal and limestone particles to simulate the calcination and combustion processes (FIRE Manual, 2011).

**2.1 Pulverized coal combustion**

The pulverized coal combustion is modelled as a two stage process. The coal particle, which is composed of pit-coal, sulphur and ash, is first undergoing the pyrolitic decomposition into volatiles and char particle. Pyrolysis is the most important physico-chemical change in the coal particle. During this stage a significant loss of weight occurs, because of the release of volatile matter, the quantity and composition of which depend on the ingredients of coal (see Eq. 1). Parallel to the pyrolysis, the char is oxidized to CO and $CO_2$ taking into account a mechanism factor depending on coal particle size and temperature (see Eq. 2). A complex composition, represented via chemical formula $C_{50}H_{18}O_6N_2$, for the pit coal is assumed, which has been chosen to meet the elemental composition of a typical coal as given in literature (Schnell, 1991). The treated heterogeneous chemical reactions are:

$$C_{50}H_{18}O_6N_2 \longrightarrow 5CO + H_2O + CH_4 + H_2 + HCN + NH_3 + 37C + C_6H_6, \quad (1)$$

$$C + \frac{1}{f_m}O_2 \xrightarrow[-110kJ/mol]{-395kJ/mol} \left(2 - \frac{2}{f_m}\right)CO + \left(\frac{2}{f_m} - 1\right)CO_2. \quad (2)$$

$$S + O_2 \longrightarrow SO_2 \quad (3)$$

Here $C_6H_6$ was chosen as tar representative, and $f_m$ denotes the mechanism factor (Görner, 1991), which ranges between 1 and 2, causing predominant production of $CO_2$ for temperatures below about 900 K and predominant generation of CO for higher temperatures. Named heterogeneous reactions (Eq. 1, 2 and 3) cause mass transfer sources and sinks to the gas phase and particles, which are described by rate equations for pit coal consumption, char production from pyrolysis and consumption from oxidation.

The homogeneous reactions of volatiles, tar, and CO oxidation (Görner, 1991), NOx formation and the combustion of methane, which is treated via the four step Jones-Lindstedt mechanism (Jones and Lindstedt, 1988), are treated within the gaseous phase reactions module of the CFD code. Eq. 4 and Eq. 5a-5d represent the CO oxidation and the four step Jones-Lindstedt mechanism for methane combustion, whereas Eq. 6 represents the tar ($C_6H_6$) oxidation.

$$CO + \frac{1}{2}O_2 \longrightarrow CO_2 \quad (4)$$

$$CH_4 + \frac{1}{2}O_2 \longrightarrow CO + 2H_2 \quad (5a)$$

$$CH_4 + H_2O \longrightarrow CO + 3H_2 \quad (5b)$$

$$CO + H_2O \longleftrightarrow CO_2 + H_2 \quad (5c)$$

$$H_2 + \frac{1}{2}O_2 \longrightarrow H_2O \quad (5d)$$

$$C_6H_6 + 3O_2 \longrightarrow 6CO + 3H_2 \quad (6)$$

The extended Zeldovich mechanism has been used to describe the thermal NOx formation (Görner, 1991):

$$O + N_2 \longleftrightarrow NO + N, \quad (7a)$$

$$O + NO \longleftrightarrow N + O_2, \quad (7b)$$

$$H + NO \longleftrightarrow OH + N. \quad (7c)$$

Fuel NOx formation is treated via HCN release from pit-coal during pyrolysis and HCN oxidation and NO reduction by HCN in gas phase (Görner, 1991):

$$4HCN + 5O_2 \longrightarrow 4NO + 4CO + 2H_2O, \quad (8a)$$

$$4HCN + 6NO \longrightarrow 5N_2 + 4CO + 2H_2O, \quad (8b)$$

and the De Soete mechanism (De Soete, 1975) is used to describe the fuel NOx formation from the NH3 released from the pit-coal during the pyrolysis:

$$NH_3 + O_2 \longrightarrow NO + H_2O + 0.5H_2, \quad (8a)$$

$$NH_3 + NO \longrightarrow N_2 + H_2O + 0.5H_2. \quad (8b)$$

**2.2 Calcination process**

In general the calcination process can be presented by the following equation:

$$\mathrm{CaCO_3(s)} \xrightarrow{+\ 178\ kJ/mol} \mathrm{CaO(s) + CO_2(g)}. \quad (9)$$

The developed model of the calcination process takes into account the effects of decomposition pressure, temperature, diffusion, and pore efficiency. The model is detailed enough to contain the relevant physical and chemical processes, yet simple enough for detailed CFD simulations. The model of the calcination process was thoroughly tested and validated in our previous studies (Mikulčić et al., 2012b). The model was validated by simulating experiments performed in the International Flame Research Foundation pipe reactor, for which measurements of limestone decomposition exist. The comparison with the experimental conversion rates showed that the model chosen predicted very well the influence of all of the relevant process parameters (temperature, $CO_2$ content, mass flow, etc.).

## 3. Computational details

The modelled calciner consists of two vertical cylinder parts and a cylinder connecting them. In the first vertical cylinder the burner is positioned, and in the second vertical cylinder the hot gas stream from the rotary kiln is used to enhance the calcinations process. At the bottom of the second vertical cylinder a converging-diverging section is used to increase the velocity of the incoming hot stream from the rotary kiln. The entire model is 24 m high, with the diameter of the first cylindrical part of 5.5 m, and with the diameter of the second cylindrical part of 4.5 m. The connecting cylinder is positioned at 60° angles and is 4 m in diameter. At the top of the first vertical cylinder two limestone and two tertiary air inlets are positioned diametrically opposite each other.

To discretize the computational domain used in the simulation of the cement calciner, 47,000 cells were employed. The differencing scheme used for momentum, continuity and enthalpy balances was MINMOD Relaxed, and for the turbulence and scalar transport equations, an Upwind scheme was applied. Turbulence was modelled by the standard $k-\varepsilon$ model. The tertiary air entered the domain with the mass flow of 49,600 kg/h, limestone with 73,950 kg/h. Burner primary air entered the domain with the mass flow of 16,200 kg/h, burner secondary air with the mass flow of 33,065 kg/h, and coal with 14,811 kg/h. Hot gas stream from the rotary kiln entered the domain with the mass flow of 110,600 kg/h, and static pressure of $10^5$ Pa was used for the outlet boundary condition.

## 4. Results and discussion

Figure 1 shows the limestone and char particle distribution inside a calciner with an axial burner, and inside the calciner with a swirl burner. The 'empty' regions are where conversion of limestone to lime and char to CO and $CO_2$, to a large extent, has already been completed. Also, it can be seen that the particles are distributed in the same manner in both cases, however, with somewhat delayed conversion in case of the swirl burner.

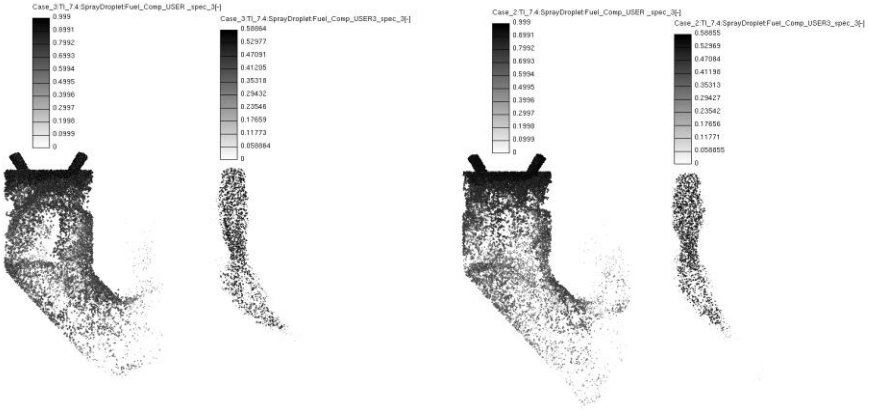

*Figure 1: Distribution of limestone and char mass fractions in the particles: Calciner with an axial burner(left); Calciner with a swirl burner(right).*

Figure 2 shows the temperature field and NO mass fraction inside a calciner with an axial burner, and inside the calciner with a swirl burner. It can be seen that when an axial burner is used, a higher concentration of NO close to the burner occurs.

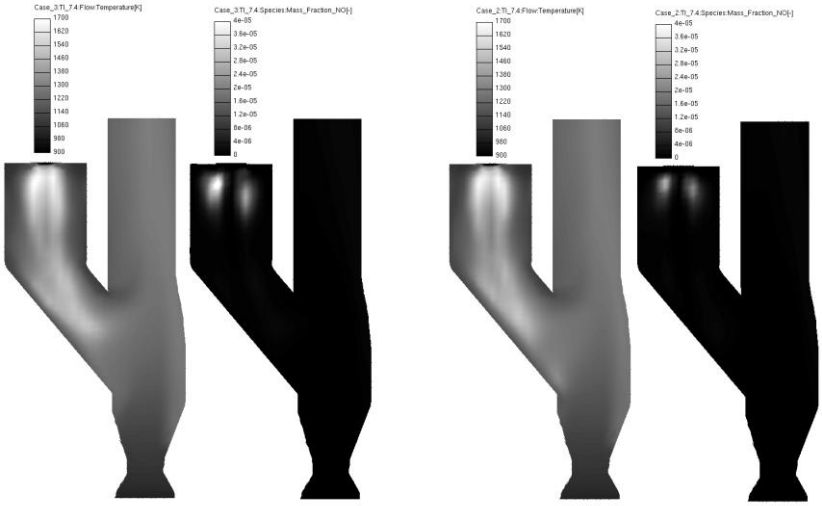

*Figure 2: Temperature field and NO mass fraction: Calciner with an axial burner(left); Calciner with a swirl burner(right).*

Interestingly in the simulation results shown the swirl burner is less favourable in terms of pollutants and conversion grade of limestone, since it causes a more efficient combustion along the centre lines, while for process control reasons a more pronounced radial distribution of heat release towards the region of high limestone concentration would be desirable. By variation of geometric parameters and inlet conditions different scenarios can be explored to support a final design decision.

## 5. Conclusion

Due to the increased environmental awareness and the need for a more sustainable cement manufacturing process, cement manufacturers are trying to lower their pollutant emissions. To satisfy the continuous increase in the need for cement and more stringent environmental measures, more and more cement calciners are included in the production process. The present paper demonstrates that it is possible to numerically simulate different thermo-chemical processes inside a cement calciner. Furthermore, it demonstrates that CFD can be used as a tool for the analyses and improvements of the understanding of the mixing of particles, and the thermo-chemical reactions that occur in cement calciners. The results gained by these simulations can be used for the decision which burner is to be used and furthermore, the gained results can be used for the optimization of cement calciner's geometry and operating conditions. By using appropriate burners and by optimizing cement calciner's operating conditions, a reduction of pollutant emissions can be achieved, resulting with a more efficient and ecologically compatible cement production.

**Acknowledgements**

The authors wish to thank Dr. H. Maier for useful discussions and for providing the calciner's geometry for a CFD calculation. Authors also wish to thank A TEC for the input data needed for the calculation.

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