Annotation. *The computer model that enables investigate of the limestone endothermic calcination process in the industrial cyclone-calciner furnace has been proposed. The model was compiled based on terms of heat transfer, chemical kinetics, mass transfer and limestone properties. Numerical experiments confirmed that the proposed method can be used for calculations of calcinations processing modes. The results will be used to optimizing of furnace operation modes.*
Keywords*: CFD – modeling, calcination, cyclone furnace, chemical kinetics*

Анотація. *Запропонована комп'ютерна модель, яка дозволяє досліджувати процес декарбонізації вапняку в циклонній печі промислового типу. Модель була складена на основі процесів теплопередачі, хімічної кінетики, масоперенесення і властивостей вапняку. Моделюванням підтверджено, що запропонований метод може використовуватися для розрахунку режимів обробки матеріалу. Результати будуть використані для оптимізації режимів роботи печі.*
Ключові слова: *CFD – моделювання, декарбонізація, циклонна піч, хімічна кінетика*

Аннотация. *Предложенная компьютерная модель, которая позволяет исследовать процесс декарбонизации известняка в циклонной печи промышленного типа. Модель была составлена на основе процессов теплопередачи, химической кинетики, массопереноса и свойств известняка. Моделированием подтверждено, что предложенный метод может использоваться для расчета режимов обработки материала. Результаты будут использованы для оптимизации работы печи.*
Ключевые слова: *CFD – моделирование, декарбонизация, циклонная печь, химическая кинетика*

Introduction

Limestone is the basic raw material for the production of lime and carbonation gas in metallurgy, construction, chemical and food industries.

Currently, more than 60 million tons of limestone is produced in Ukraine in a year. The lime manufacturing processes include firing raw materials in furnaces of various designs: shaft furnaces, rotary kilns, fluidized bed furnaces and cyclone furnaces. Particle size distribution of limestone from quarries is generally between 40 and 200 mm. Before limestone is put into the furnaces, it should be clean of clay, sorted and crushed.

Preparation of raw materials in the traditional technological schemes inevitably creates considerable dust dispersed solids.

This is mainly a particle size from 20-150 microns to 1-2 millimeter, which can be up to 30% by weight of dry material. For a long time, these materials are dumped in the dumps. In Ukraine, these dumps occupied fertile land with total area of 48-50 thousand hectares.

In practice, these problems can be solved by using the cyclone-type furnace for lime manufacturing. Processes based on the use of cyclone furnaces are of particular interest because these furnaces are characterized by high thermal efficiency; low operating costs provide high quality of finished product and occupy small production area.

For the wide industrial introduction of these furnaces, it is necessary to develop new methods of calculating them. These methods should be based on the furnace modes, aerodynamics and calcination reaction kinetics.

To solve these problems CFD (computational fluid dynamics) methods are widely used. CFD provide an accurate means to model and simulate many processes in chemical engineering, reduce time and cost of progressive prototype creation and testing, analyze the performance of the proposed apparatus. This approach has been used in our work based on ANSYS Fluent version 15.

Problem formulation

In the previous studies, two operation modes were presented for the various inlet velocities of the flows [1] and chemical combustion reaction in the cyclone calciner furnace [2]. In order to examine the effects of these models on the calcination of limestone, multiple simulations have been run.

Limestone decomposition is a gas-solid reaction in which the solid is a reactant. The reaction for thermal decomposition of limestone can be expressed as:

$$CaCO_3(s) = CaO(s) + CO_2(g)$$

It is a highly endothermic reaction, requiring 3.16 MJ of heat input to produce 1 kg of lime (CaO).

The endothermic decomposition behavior is determined by three processes: heat transfer by convection from the surrounding gas phase to the solid surface and by conduction from the surface to the reaction front through the oxide shell, chemical reaction at the front, mass transfer of the gas CO_2 by diffusion from the reaction front to the surface through the pours oxide layer and the boundary layer of the gas phase [3, 4]. In a calcination process, limestone particles (< 150 μm) are rapidly calcined in an counter-flow furnace at the temperature between 823 and 1,023 K.

The particles residence time in the furnace is a few seconds. Therefore, mathematical description of the considered processes requires joint consideration of all above phenomena.

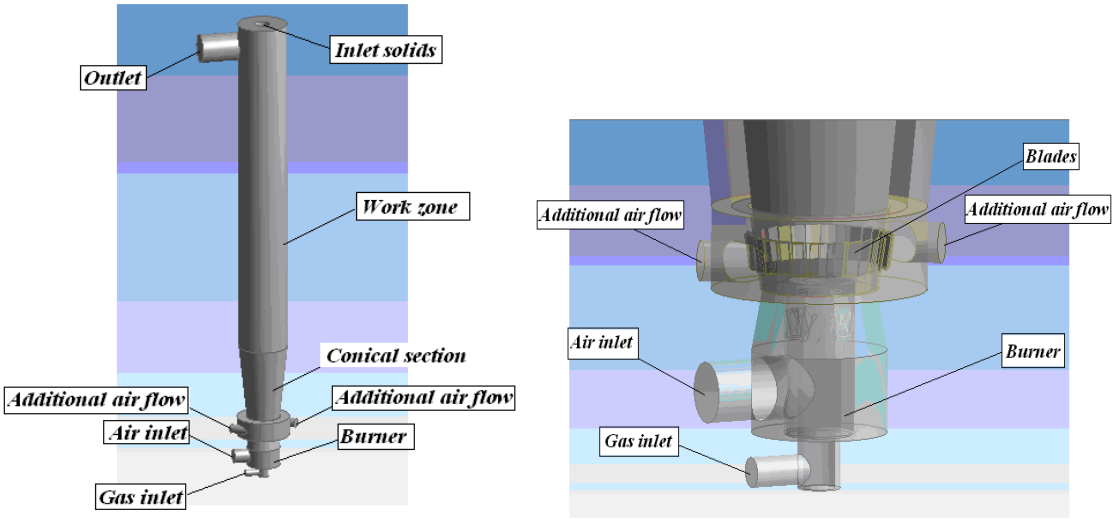
A large number of mathematical models have been developed to study limestone decomposition. Models were developed based on chemical reaction mechanism, heat and mass transfer and the diffusion process. According to these models, the thermal processes and chemical kinetics are the limiting to limestone decomposition reaction for small particle size [5]. This approach has been used in our studies and presented in this work.

The main objective of this research is to investigate the kinetics of limestone calcination and to determine the impacts of furnace operating conditions on the percentage of $CaCO_3$ decomposed to CaO.

Obtaining these results is very important for theoretical and experimental studies to help to predict limestone calcination behavior in furnace and provide design data to optimize existing design.

Analysis research

The three-dimensional geometry of the furnace was used for numerical simulations. The modeled cyclone-calciner furnace is shown in Fig. 1, a, b. The computational mesh was built using mesh generation ANSYS Meshing CFD and consisted of near 2 mln. cells.



a b

Fig. 1. Cyclone-calciner furnace geometry:
a - general view of furnace; b - burner location

In the CFD-code used in this study, there are the basic equations of hydrodynamics, namely the continuity equation; it expresses the law conservation of mass in the elementary volume, and the equation of momentum conservation. These equations represent the basic model of the medium flow. To simulate the turbulence flow, the "Realizable" k-ε model of turbulence was used. [6]

To simulate the diffusion methane-air combustion in a turbulent flow, the most popular approach eddy-dissipation model was used. The combustion was modeled using a global one-step reaction mechanism, assuming complete conversion of the fuel (methane) to CO_2 and H_2O. This mechanism gives the average value of enthalpy and is applicable to estimate the distribution of the main products of combustion (CO_2, H_2O) and temperature fields.

To simulate the particles distribution in cyclone-calciner furnace, Discrete Phase Model was used. For each particle, the trajectory is calculated based on the forces balance equation acting on the particle. According to the experimental data, the particle size distribution is presented in the Rosin-Rammler format and it is assumed that all the particles are spherical.

The reaction kinetics of limestone decomposition with different particle sizes presented in the Rosin-Rammler format was performed based on the single kinetic rate devolatilization model presented in the CFD-code Fluent 15.

The single kinetic rate devolatilization model assumes that the rate of devolatilization is first-order dependent on the amount of volatiles remaining in the particle [6]:

$$-\frac{dm_p}{dt} = k[m_p - (1 - f_{v,0})(1 - f_{w,0})m_{p,0}] \quad (1)$$

where m_p – particle mass (kg), $f_{v,0}$ – mass fraction of volatiles initially present in the particle, $f_{w,0}$ – mass fraction of evaporating material, $m_{p,0}$ – initial particle mass, k – kinetic rate.

The kinetic rate, k, is defined by input of an Arrhenius type pre-exponential factor A and activation energy E:

$$k = Ae^{-(E/RT)} \quad (2)$$

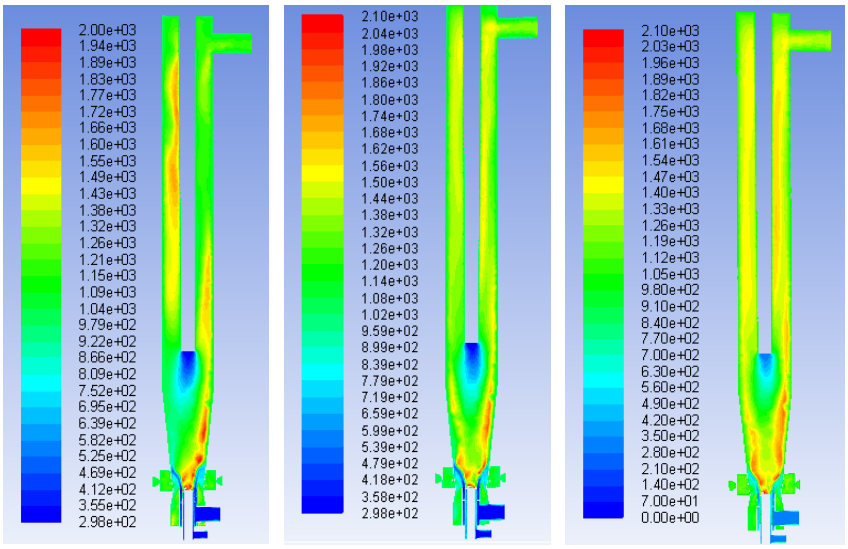
The values of the Arrhenius parameters used for this study was E = $2{,}05 \cdot 10^8$ J/(kg·mo1) and A =$3.81 \cdot 10^8$. The operation modes of the furnace are: inlet air, 17- 22 m/s; inlet gas, 7 m/s. All the geometric data and the initial and boundary conditions were supplied by "Pustomyty lime plant", Ukraine.

For limestone calcination reaction, the effects of temperature distribution in the furnace, trajectories of CaCO3 particles, as well as particles residence time and particles volatile mass fraction were taken into account.

Fig 2. shows the calculated temperature distribution of the gaseous phase in vertical cross section. In Fig. 2 higher temperatures are observed in the conical section of the furnace where the burner location is.

Under the central pipe location where the particles entrance is and in the work zone of the furnace there is no high temperature because of intense calcination, resulting to high heat absorption. The high temperatures are in the regions where higher velocities prevail and there are no CaCO3 particles.

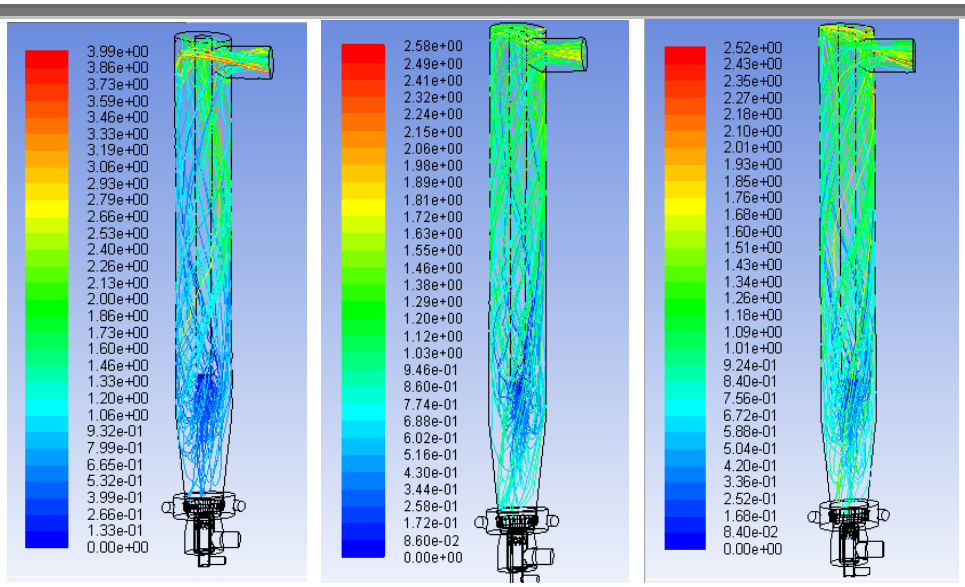
This is also confirmed by the results presented in Fig. 3 where particles residence time are shown. According to these results, the average particle residence time is 1 or 2 s while the longest 5 s for different input parameters, respectively. This residence time should be sufficient to calcination of all the particles in the furnace.



a) b) c)

Fig. 2. Contours of temperature:
a) inlet air 17 m/s; b) inlet air 20 m/s; c) inlet air 22 m/s

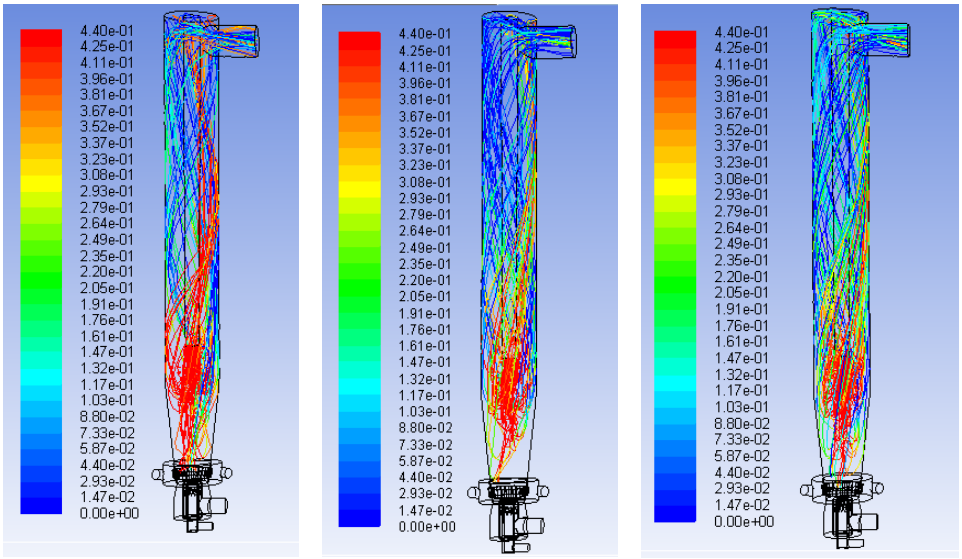
But the results presented in Figure 4 show that particle decarbonisation process depends on residence time and temperature field in the furnace. In Fig. 4 the red color in the start of the particles trajectory corresponds to 44% of the CO_2 volatile mass fraction in the limestone. The blue color in the end of the trajectory shows the 0% of the CO_2 in the lime.



a) b) c)

Fig. 3.Particle residence time:
a) inlet air 17 m/s; b) inlet air 20 m/s; c) inlet air 22 m/s

Calcination is noticeable in the zones which agree with the temperature field. The maximum predicted calcination reaches 85,6 % and is realised in all the active furnace height.



a) b) c)

Fig. 4.Particle calcination reaction:
a) inlet air 17 m/s; b) inlet air 20 m/s; c) inlet air 22 m/s

To verify the accuracy of the modeling approach, the numerical predictions were compared with experimental data. According to the experimental data, calcination reaches 82%.

Conclusion

The approach to evaluate the effect of temperature and hydrodynamic flow on the calcination reaction in the industrial cyclone-calciner furnace has been presented. This

approach was based on Eddy-Dissipation combustion model with the single kinetic rate devolatilization model for calcination reaction.

The comparison of the calculation results with the experimental data shows that the simplified approach based on CFD simulation of the calcination reaction described in the article can be used to optimize design of cyclonic furnace in chemical engineering.

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КОМПЬЮТЕРНОЕ МОДЕЛИРОВАНИЕ ВЛИЯНИЯ ДАВЛЕНИЯ В РЕАКТОРЕ НА ХИМИЧЕСКИЕ ПРЕВРАЩЕНИЙ В ВОДНО-СОЛЕВЫХ ПЛАЗМОРЕАКТОРНЫХ СИСТЕМАХ

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КОМП'ЮТЕРНЕ МОДЕЛЮВАННЯ ВПЛИВУ ТИСКУ У РЕАКТОРІ НА ХІМІЧНІ ПЕРЕТВОРЕННЯ У ВОДНО-СОЛЬОВИХ ПЛАЗМОРЕАКТОРНИХ СИСТЕМАХ

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COMPUTER SIMULATION THE EFFECT OF PRESSURE IN THE REACTOR TO CHEMICAL REACTIONS IN AQUEOUS-SALT PLASMA-REACTOR SYSTEMS

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