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MODELING AND SIMULATION OF THE LIMESTONE THERMAL DECOMPOSTION IN THE VERTICAL LIMEKILN

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ABSTRACT. A mathematical model of the limestone thermal decomposition process has been developed in order to determine the evolutions of temperature, solid and gaseous products distribution in the vertical limekiln.

The modeling approach considers the kiln divided into four different subsystems: the gas phase, two solid phases (limestone and coke) and the kiln wall. The model incorporates a detailed mathematical description for the two phases presented into the system, also taking into account the heat transfer through the kiln wall. The gas phase, solid phases and kiln wall have been modeled using mass and heat balance equations for counter-current flow systems. Both time and spatial distribution for gaseous and solid components are described revealing the interactions between different subsystems considered.

A variability study has been used to point out the main process variables and material properties included in the dynamic model. The dynamic model has been compared and fitted with process data collected from an industrial limekiln resulting in a dynamic simulator able to show the evolution of the main process variables versus time and space.

1. INTRODUCTION

Calcium oxide (lime) is one of the most used raw materials for different industries: constructions, steel manufacture, chemical processes, environmental protection etc. In soda ash manufacture, both process products are needed: gaseous flow (carbon dioxide) and solid flow (lime). The lime manufacture process is performed in vertical kilns.

The decrease of energy consumption and efficient use of raw materials for the decomposition process of the limestone in the vertical lime kiln may result in important economic benefits.

Mathematical modeling and simulation in dynamic conditions of the vertical lime kiln represent a valuable tool for studying different construction design approaches, operating strategies and control system design configurations.

2. MATHEMATICAL MODEL

The vertical lime kiln is divided in three zones. The first zone is the heating zone for the solid phase (a mixture of limestone and coke) and at the same time the cooling zone for the gaseous phase. The second zone is the thermal decomposition zone of the limestone and coke combustion. The third zone is the cooling zone for the solid phase (lime) and the heating zone for the gaseous phase (air) that enters into the kiln.

The kinetics of the endothermic decomposition reaction of calcium carbonate decomposition:

$$CaCO_3 \rightarrow CaO + CO_2$$

is considered to follow first order Arrhenius' law.

The coke combustion was modeled using the overall reaction scheme of Amundson in which both CO and CO_2 are recognized as primary products:

$$2\frac{\eta+1}{\eta+2}C + O_2 \xrightarrow{k_C} 2\frac{\eta}{\eta+2}CO + \frac{2}{\eta+2}CO_2$$

where η-is the primary production ratio $\eta = 70 \cdot e^{-3070/T}$ [1].

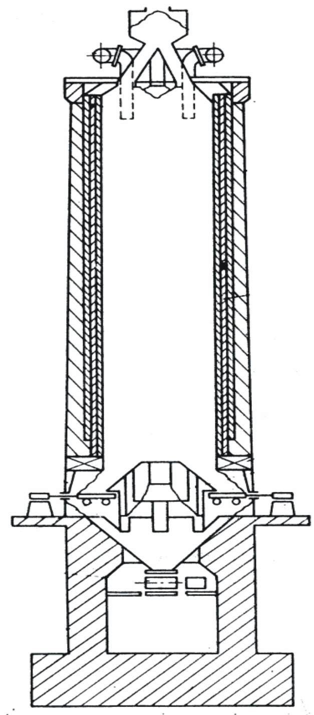

Figure 1. Limekiln

Assumptions:

- Model parameters are constant in the radial cross section of the kiln;
- Limestone is uniformly distributed across the kiln section;
- Flowing regime is ideal for both phases (plug flow);
- Both gas and solids velocity is considered constant.

The modeling approach considers the lime kiln divided into four different subsystems: the gas phase, two solid phases (limestone and coke) and the kiln wall.

The model incorporates a detailed mathematical description for the different phases describing also the heat transfer through the kiln wall.

The gas phase, solid phases and kiln wall, have been modeled using mass and heat balance equations for counter-current flow systems. The mathematical equations of the model are presented below [2-5].

The mathematical equations for heating and cooling zones:

$$\frac{Q_i c_{p_i}}{v_i} \cdot \frac{\partial T_i}{\partial t} = -Q_i c_{p_i} \frac{\partial T_i}{\partial z} + S_{energ}$$

$$M_p \cdot c_{p_p} \cdot \frac{\partial T_p}{\partial t} = S_{energ}$$

where:

c_p - specific heat, [kcal/(kg K)]
M - mass per unit height of vertical kiln, [kg/m]
Q - flow rate, [kg/h]
T - temperature [K]
v - gas and solids velocity, [m/h]
i - gas, limestone and respective coke
S_{energ} – energy source terms.

The source terms in the heat balance equation include: heat fluxes from gas to solids and wall and from solids to wall.

The mathematical equations for reaction zone:

- Total Mass Balance Equation:

$$\frac{1}{v_i} \cdot \frac{\partial Q_i}{\partial t} = -\frac{\partial Q_i}{\partial z} + S_{mass}$$

- Components Mass Balance Equations:

$$\frac{1}{v_s} \cdot \frac{\partial \left(Q_m x_j\right)}{\partial t} = -\frac{\partial \left(Q_m x_j\right)}{\partial z} + S_{comp\,j}$$

$$\frac{1}{v_g} \cdot \frac{\partial \left(Q_g x_k\right)}{\partial t} = -\frac{\partial \left(Q_g x_k\right)}{\partial z} + S_{comp\,k}$$

- Heat Transfer Equations:

$$\frac{Q_i c_{p_i}}{v_i} \cdot \frac{\partial T_i}{\partial t} = -Q_i c_{p_i} \frac{\partial T_i}{\partial z} + S_{energ}$$

$$M_p \cdot c_{p_p} \cdot \frac{\partial T_p}{\partial t} = S_{energ}$$

where:

c_p - specific heat, [kcal/(kg K)]
M - mass per unit height of vertical kiln, [kg/m]
Q - flow rate, [kg/h]
T - temperature [K]
v - gas and solids velocity, [m/h]
x - component concentration
Indices:
i - gas, limestone and respective coke
j - $CaCO_3$ and CaO
k - O_2, CO_2, CO and N_2
S_{mass}, S_{comp}, S_{energ} - source terms.

Extra source for mass (S_{mass}) are due to limestone thermal decomposition reaction and coke combustion.

Carbon dioxide and carbon monoxide are transferred from the solids phases to gas phase (S_{comp}).

S_{energ} terms include: reactions heat (endothermic limestone decomposition reaction and exothermic coke combustion), heat fluxes from gas to solids and wall and from solids to wall.

For the simulation the thermal decomposition process of the limestone in a vertical limekiln, the parameters presented in the table 1 were used.

Table 1.

Parameters of the model

Limekiln parameter: Height Diameter	 H = 16 m D = 4.5 m
Input flows: Air flow Limestone flow Coke flow	 Q_g = 9676 kg/h Q_m = 10500 kg/h Q_c = 1000 kg/h
Feed composition: Air Limestone Coke	 X_{O2} = 0.233; X_{N2} = 0.767; X_{CaCO3} = 0.98 X_C = 0.8
Input feed temperature	T_0 = 20 + 273K
Velocity: Solid phases Gas phase	 v_s = 0.4062 m/h v_g = 1.5 m/s

3. RESULTS AND DISCUSSIONS

The mathematical model of the limestone decomposition process was simulated using MATLAB software package (version 7).

The simulation of the mathematical model of the limestone thermal decomposition process reveals the evolutions (both in time and space) of temperature, solid and gaseous products distribution in a vertical lime kiln.

Some of the most representative simulation results are presented in the figures below. The limestone is the principal raw material of the process, the feed of limestone is on the top of lime kiln, so that in the figures below the bench mark "0" is the top of lime kiln.

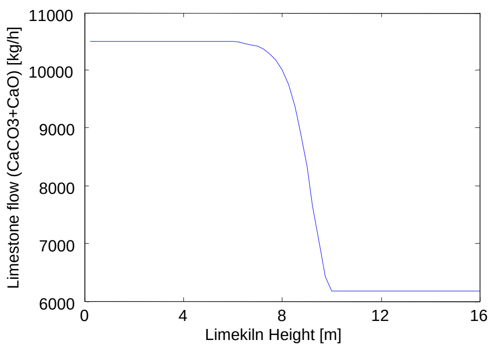

Figure 2. Limestone flow profile along the kiln height

In the figures 2, 3 and 4 the limestone, gas and coke flow profiles along the kiln height are presented. The flows are constant in the heating and cooling zones of the kiln. The decompositon of calcium carbonate and coke burning processes lead to decreased of solid flows in the reaction zone. Also, the gas flow is increased along the reaction zone because of carbon dioxide and carbon monoxide formation in those two processes.

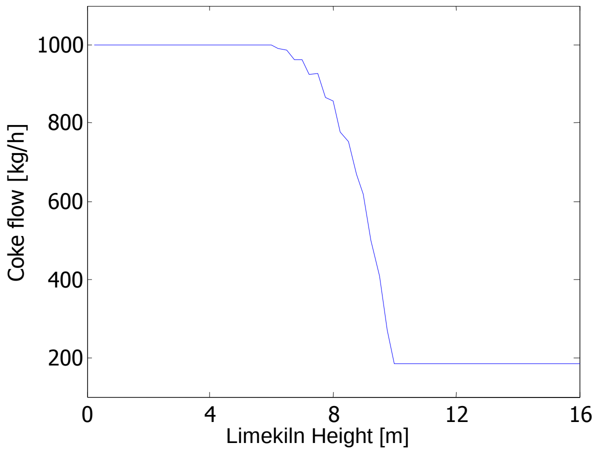

Figure 3. Coke flow profile along the kiln height

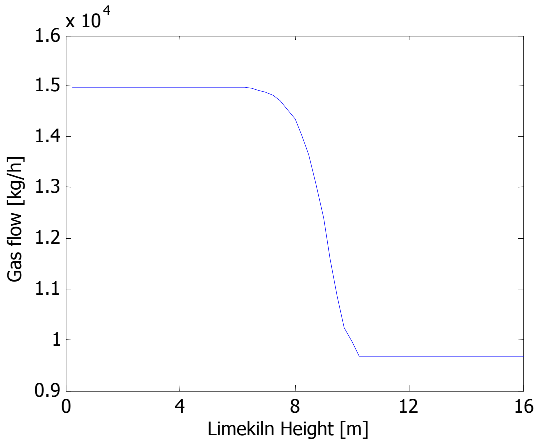

Figure 4. Gas flow profile along the kiln height

The figure 5 shows that the calcium oxide concentration increases along the reaction zone (from top to bottom of the limekiln) at value 89.43 % [weight %] what is corresponded to 95.7 % conversion of limestone.

In figure 6, the carbon dioxide concentration profile on the vertical limekiln is presented. The concentration of the carbon dioxide on the top of the limekiln obtained by simulation has value 38.2% [volume %] and is comparable with the one obtained in the real plant (38-41% [volume %]).

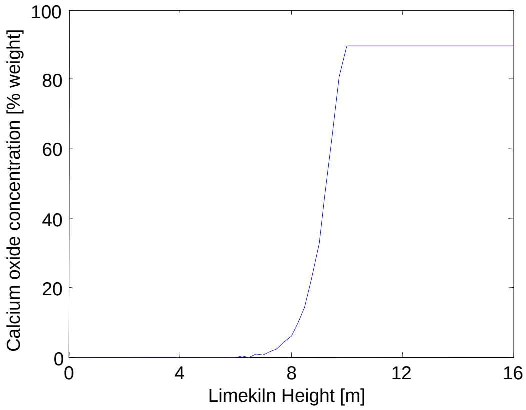

Figure 5. Calcium oxide concentration profile along the kiln height

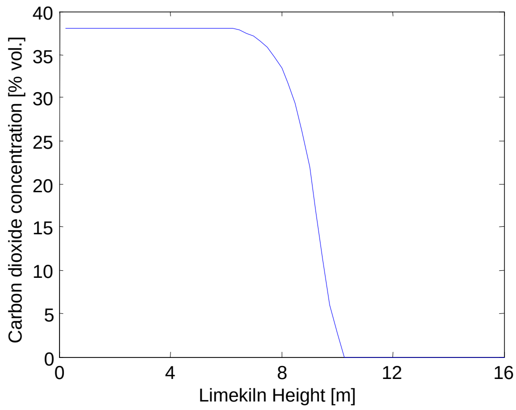

Figure 6. Carbon dioxide concentration profile along the kiln height

The limestone ($CaCO_3$ + CaO) T_m, coke T_c, gas T_g and inside kiln wall T_p temperatures profiles are presented in the figure 7.

The figure 7 shows that the solids temperatures increase in the heating zone. The limestone and coke introduced on the top of the kiln are heated by the warm gaseous phase, leaving the reaction zone, up to the point when limestone thermal decomposition and cook burning begin. The lime resulted in the decomposition zone is cooled in the third zone with the gaseous phase (air) introduced at the bottom of the kiln. The maximum of temperatures are in the second zone where the coke's burning reaction takes place in parallel with thermal decomposition of the limestone. The wall temperature profile follows the gaseous and solid phases profiles.

In the table 2, the simulation results of the limekiln are compared with real plant operation data in order to validate the application developed for simulation of the process.

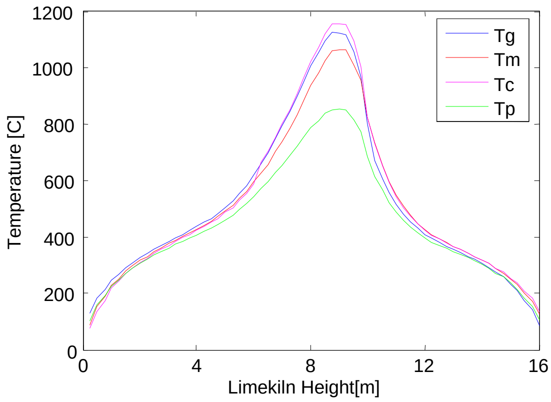

Figure 7. Temperatures profile along the kiln height

Tabel 2.

Comparison of simulation results with real plant data

Parameter	Real plant dataparameters	Process simulation results
Reaction zone temperature	1050 – 1200°C	1159°C
Output gas temperature	80 – 160°C	130°C
Gas composition [volume %]:		
CO_2	38 – 41%	38.2 %
O_2	0.4 – 1.5 %	1.12 %
CO	0.5 – 2.5 %	0.58 %
Output lime temperature	50 – 120°C	120°C
Lime composition [weight %]:		
$CaCO_3$	< 10 %	7.16 %
CaO	> 80 %	89.43 %
Efficiency of limestone decomposition	91 – 96 %	95.7 %
Thermal efficiency of limekiln	75 %	76 %

From the comparison of simulation results with data collected from the real plant a close similarity can be observed. This fact validates the mathematical model of the process and the simulation results obtained using MATLAB software package.

The dynamic behavior of the lime kiln was also investigated in the presence of the typical process disturbances (e.g. limestone flow variation). Some of the representative results are presented in the figures 8 and 9.

The process response at a step increase of $\Delta Qm=+10\%$ are characterized by the oscillation of parameters. The oscillation amplitude of parameters is decreasing in time, needing more than 20 hours to attend a new stationary phase.

The simulation results were compared with real plant operation data in order to validate the application developed for the process. From the comparison of the simulation results with data collected from real plant operation a close similarity can be noticed. This fact validates the mathematical model of limestone decomposition process in a vertical kiln.

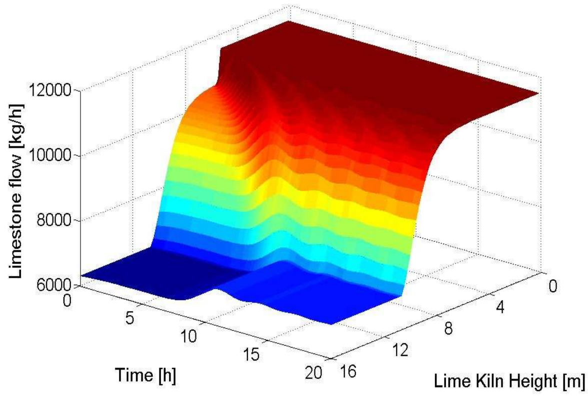

Figure 8. Dynamic response of limestone flow for a step increase of ΔQm=+10%

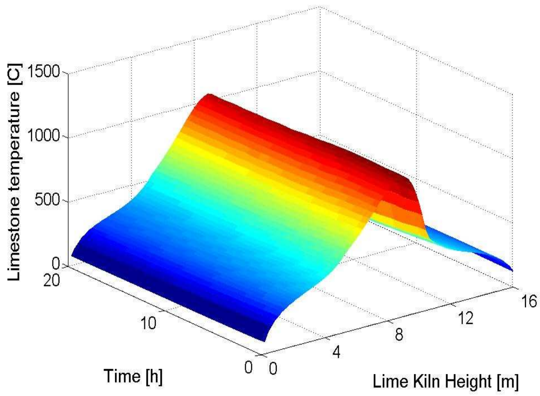

Figure 9. Dynamic response of limestone temperature for a step increase of ΔQm=+10%

4. CONCLUSIONS

Modeling and simulation of the thermal decomposition of limestone in the vertical limekiln was done using MATLAB software.

The evolutions in both time and space of the process parameters (solid and gaseous flows, composition of the streams, temperatures) were studied during the limestone decomposition process. The simulation results were compared with real plant operation data in order to validate the application developed for the process.

The mathematical model of the limestone thermal decomposition can be used to study the behavior of the process in changing operating conditions and the influence of different disturbances on the thermal decomposition of limestone. The process simulation results can be very useful to establish the optimal operation conditions and to design the control system for the plant.

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