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SIMULATION OF THE DOLOMITE THERMAL DECOMPOSITION BASED ON THE GRANULE MODEL

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ABSTRACT. In this paper the mathematical model of thermal decomposition for a dolomite granule has been developed and studied. The model offers the possibility to estimate the distribution of the over heated oxide obtained from dolomite and unreacted dolomite core for given operating conditions of the kiln. The mathematical equations of the model are presented and the simulator is implemented using MATLAB and FEMLAB software package.

Mathematical Model

The mathematical model, as basis for the dynamic simulator development, aims at studying different possibilities of reducing the fuel consumption of the kiln. According to data reported in literature, the dolomite decomposition process was considered and implemented on the assumption of the unreacted core model, firstly developed by Kunii. The model for the dolomite thermal decomposition was chosen in order to reflect the real process behaviour, in a better way. In order to define the mathematical equations, the geometrical shape of the dolomite granule has to be specified. Spherical dolomite granules [1] with initial radius R have been considered, figure 1. The decomposition process begins on the dolomite surface. The reaction takes place on the interface surface situated at a distance r_m from the centre. The solid reactant is assumed to lie within the r_m radius sphere. The reaction zone moves toward the centre of the granule. During the decomposition process the unreacted core (dolomite) decreases with time changing velocity.

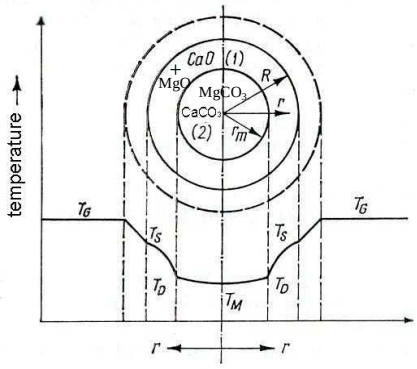

Fig. 1 The unreacted core model for dolomite granule

The mathematical model of the dolomite granule decomposition is built considering the following assumptions [1, 2]:

- dolomite granules are spherical and present initial homogeneous properties: equal diameter, uniform temperature on the external surface and radial propagation of the reaction in each granule;
- gaseous phase properties have been considered constant.

Thermal decomposition of dolomite considers the following phenomena:

- heat transfer from the gaseous phase to the solid surface;

- heat transfer through the reacted product;
- reaction on the surface;
- diffusion of the carbon dioxide from the solid phase to the gaseous phase;
- heating the dolomite unreacted core up to the reaction temperature;
- heating the resulted layer.

The mathematical equations for thermal the decomposition of dolomite are [1,3,4]:

- heating the granule core by conduction

$$\frac{\partial T_2}{\partial t} = a_2 \cdot \left(\frac{\partial^2 T_2}{\partial r^2} + \frac{2}{r} \cdot \frac{\partial T_2}{\partial r}\right)$$

- heating the reacted layer

$$\frac{\partial T_1}{\partial t} = a_1 \cdot \left(\frac{\partial^2 T_1}{\partial r^2} + \frac{2}{r} \cdot \frac{\partial T_1}{\partial r}\right) + \frac{M_{CO2} \cdot Cp_{CO2} \cdot \rho_2}{M_{dolomite} \cdot Cp_m \cdot \rho_1} \cdot \frac{r_m^2}{r^2} \cdot \frac{dr_m}{dt} \cdot \frac{dT_1}{dr}$$

- the heat transferred between gaseous phase and the solid surface:

$$\frac{\partial T_G}{\partial t} = k_T \cdot S_v \cdot \rho \, (v_S / W_G) \cdot (T_G - T_{sp})$$

The initial and boundary conditions taken into consideration are:

$t = 0$, $0 \le r \le R$; $T_1 = T_2 = T_0$

$t > 0$; $r = R$, $T_1 = T_s$ $\lambda_1 \frac{\partial T_1}{\partial r} = k_T (T_G - T_{sp})$

$r = r_m$; $T_1 = T_2 = T_d$

$$\lambda_1 \frac{\partial T_1}{\partial r} + \Delta H_R \cdot \rho_2 \cdot \frac{dr_m}{dt} = \lambda_2 \cdot \frac{\partial T_2}{\partial r}$$

The mathematical model of the process was implemented using FEMLAB software package [5]. A special developed application opens up possibilities of approaching the moving boundary problem and solving the involved PDEs.

Simulation Results

Diagrams have been obtained for a dolomite granule of 16-mm diameter at 1000 ^oC gaseous phase temperature.

As it can be noticed from the above figures the granule surface reaches the decomposition in approximate 17-20 min. Heat exchange between the dolomite granule surface and gaseous phase depends on the partial heat transfer coefficients and the temperature gradient.

Profiles of the temperature versus time and radius of the granule at different moments of time, t=3 and t=7 min, are presented in figures 2 and 3.

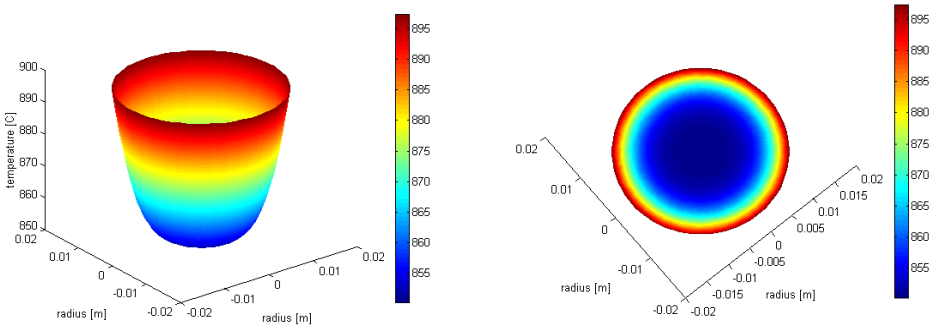

Fig 2. a) Representation of the temperature profile in a granule section, after 3 min (3-D), b) Temperature profile in a granule section, after 3 min (2-D).

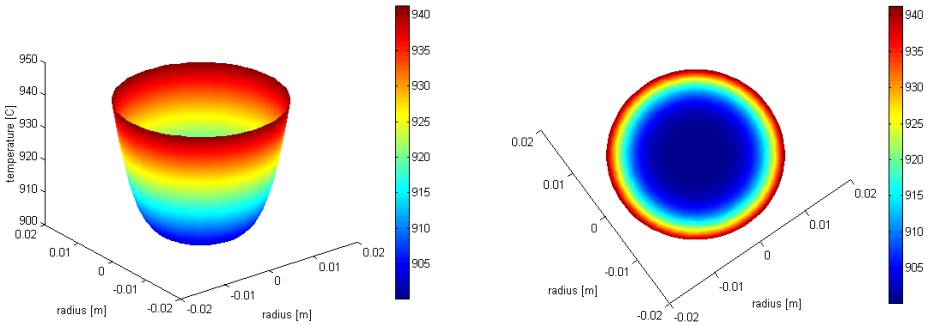

Fig 3. a) Representation of the temperature profile in a granule section, after 7 min (3-D), Temperature profile in a granule section, after 7 min (2-D).

A good agreement between the process simulation results and the experimental data results may be noticed. The decomposition time is of about 17-20 min, both for the simulation of dolomite decomposition and for the experimental data. The temperature evolutions on the solid surface and the temperature in the core (experimental data results) are presented in figure 4.

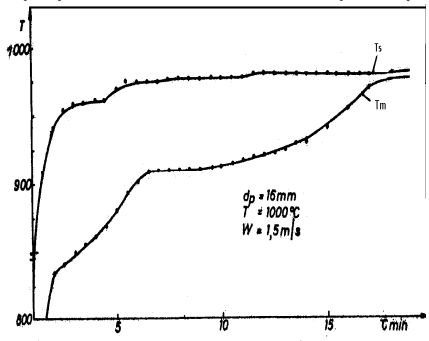

Fig. 4 Time dependence of the temperature on solid surface and in the core (experimental data results) [2]

The dolomite decomposition rate decreases progressively after the oxide layer formation because of the increased heat transfer resistance through the already formed calcium and magnesium oxide layer. The time evolutions for the reaction front velocity and dolomite granule radius are shown in figure 5 and figure 6.

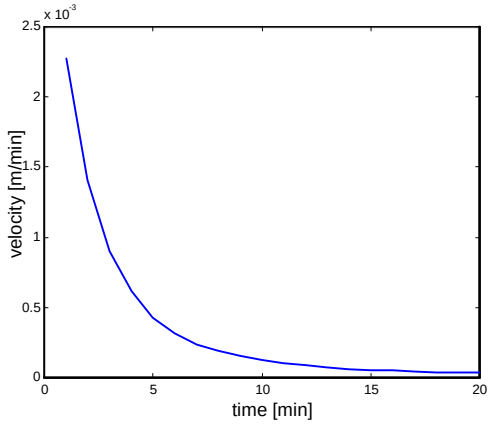

Fig. 5 Dolomite reaction front velocity vs time

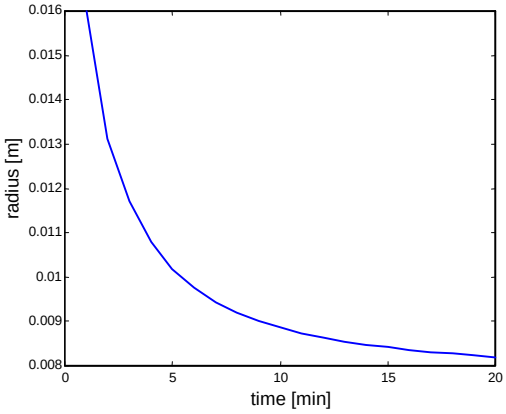

Fig. 6 Dolomite granule radius vs time

The good agreement between the process simulation results and the experimental data results is pointing out that the unreacted core model for dolomite thermal decomposition may be successfully used to describe the dolomite thermal decomposition and to investigate the decomposition process at temperatures between 900 – 1200^{o}C.

Conclusions

The paper presents the modelling and simulation results of the dolomite thermal decomposition. The model offers the possibility to estimate the time and space distribution of the obtained over heated oxide and the unreacted dolomite core, under different conditions of the granule size and temperature of the gaseous phase.

The involved PDEs have been solved using a special developed recursive algorithm based on the parabolic equation solver of FEMLAB, working with the Finite Element Method.

The mathematical model of the dolomite thermal decomposition may be also used to study the behaviour of the process in changing operating conditions and the influence of different impurities on the thermal decomposition of dolomite.

The process simulation results are useful to establish the optimal operation conditions but also for the control system design of the commercial plant.

The dynamic simulations of the dolomite granule with moving boundary reaction geometry allows the investigation of the dolomite decomposition process offering, at the same time, a general framework for the study of gas-solid reaction systems fitted to the unreacted core model description.

Nomenclature

a - thermal diffusion (m^2/h)
T - temperature (^oC)
r - distance from the centre of the granule (m)
t - time (h)
λ - thermal conductivity ($W/m\ ^oC$)
c_p - heat capacity ($J/kg\ ^oC$)
M - molecular mass (kg/kmol)
ρ - density (kg/m^3)
T_G - gaseous phase temperature (^oC)
K_T - heat transfer coefficient (W/m^2 h grd)
V_S - dolomite granules velocity (m/h)
S_v - specific surface (m^2/m^3)
W_G - thermal capacity of the gaseous stream (W/m^2 h grd)
T_{sp} - temperature on the external surface (^oC)

Indices:
1 - porous oxide product from product zone
2 - dolomite (unreacted zone)
m - core
d - decomposition

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