GAS-SOLID NON CATALYTIC REACTIONS: A MATHEMATICAL MODEL BASED ON HEAT TRANSFER ANALYSIS

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***Abstract*— The analysis of temperature profiles in spherical samples under chemical reaction is presented here as an adequate tool to identify if a gas-solid reaction system belongs to the unreacted core model or to the progressive conversion one. This analysis has been applied to the thermal decomposition of natural carbonates (dolostone, limestone and travertine from San Juan, Argentina and limestone from Neuquén, Argentina). The mathematical model based on heat transfer combined with chemical reaction presented here, allows to predict temperature profiles in spherical samples of natural carbonates under thermal decomposition. Reaction times obtained from thermogravimetric studies of thermal decomposition of dolostones, and those predicted by the calculation procedure presented here, disagree in less than 12%.**

***Keywords*: Mathematical Modeling; Transport Processes; Heat Transfer; Kinetics; Reaction Engineering.**

I. INTRODUCTION

The study of an heterogeneous solid–gas reaction system usually involves heat and mass transport, and reaction kinetics, in order to predict its evolution under the chemical reactor operating conditions. Doraiswamy and Sharma (1984) presented a summary of mathematical models for heterogeneous gas-solid non-catalyzed chemical reactions, which include parameters characterizing mass and energy transport, and the chemical reaction rate.

There are many works on mathematical modeling of gas-solid non-catalyzed reactions, having a wide range of mathematical complexity. Some of them are developed without application to a particular reaction system, that is, the authors assume the reaction kinetics, and the mass and heat transfer coefficients values (Seggiani *et al*., 2000; Uhde and Hoffmann, 1997; Fatehi and Kaviany, 1997; Villa *et al*., 1992; Villa and Quiroga, 1990). In other works, the results predicted by the models are compared with experimental data obtained for a particular reaction system, whose reaction kinetics, and mass and energy transport coefficients are known (Patisson *et al*., 1998; Mutasher *et al*., 1989; Bowen *et al*, 1989; Ulkutan *et al*., 1982, Narsimhan, 1961).

In addition to mathematical complexity, another important feature to be considered is the calculation of the above mentioned parameters. An incorrect prediction can result in wrong conclusions when these models are used to describe real systems. We agree with Levenspiel opinion (1987) that "It is of little use to select a model which very closely mirrors reality but which is so complicated that we cannot do anything with it. Unfortunately, this all too often happens". Due to this, it seems advisable to use simple models, with a minimum of those parameters, when they are going to be applied to engineering problems.

The rate of some gas-solid non-catalyzed chemical reactions can be followed analyzing the structural changes that take place in the solid during the reaction. One of the properties that can show these changes is the diffusivity of reactants and products through the solid structure, although it is very difficult, and almost impossible, to measure variations in the diffusion rate of chemical species through the porous structure.

The use of properties characterizing heat transport in porous solids (e.g. effective thermal conductivity) to follow chemical reactions has some advantages over those describing mass transfer. For example, the determination of the thermal conductivity of a solid requires relatively simple experimental equipment, compared with that necessary to determine the effective diffusivity.

This work proposes an experimental method to determine if a gas-solid reaction system belongs to the unreacted core model or to the progressive conversion one, based in the measurement of temperature gradients between two isothermal surfaces, when heat flows constantly through a spherical sample. The analysis of the temperature profile, and its variations with time, allows to identify the material located between two isothermal surfaces, provided that the thermal conductivity of solid reactants and products is known. To detect changes in the temperature profile, the thermal conductivity of the solid reactant has to be different from that of the solid product.

Two calculation procedures, based on heat transfer combined with the chemical reaction, are developed to

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