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MODELING OF NONCATALYTIC GAS-SOLID REACTIONS THE REACTION ZONE THICKNESS

BY

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Abstract. A number of physical and mathematical models have been proposed for noncatalytic solid-gas reactions. In such a system, the reaction takes place in a part of the solid that can vary in large limits. Within this study, calculations with respect to the gaseous reactant, for simple isothermal first order reactions, have been carried out. The size of the specific reaction area is established and correlated with a mathematical model characterizing the chemical transformation that takes place. Depending on the specific thickness of the reaction zone, some well-known noncatalytic gas-solid reaction models such as: the shrinking core model (heterogeneous), the limited reaction zone model (general) and the total reaction zone model (homogeneous), have been re-established.

Keywords: gas-solid reaction models, specific thickness of the reaction zone, rectangular coordinates, spherical coordinates.

1. Introduction

In heterogeneous systems consisting of two phases, the chemical transformation is influenced by a large number of variables. The process

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mechanism is complex and the mathematical modeling necessitates numerous hypotheses. For liquid-liquid or gas-liquid heterogeneous systems, the chemical reaction takes place either at the phases interface, in a limited or the entire volume of the film, or inside the phase bulk (Levenspiel, 1999).

Solid-fluid reaction phenomenology is much more complex. For example, a reaction inside the solid-gas system takes place depending on the solid porosity and the chemical reaction rate, on a surface or a volume inside the solid bulk. The reaction zone thickness may vary in large limits and, in this case, the reaction takes place according to different models. One can establish what model can be used based on the calculation of the reaction zone thickness and the particle dimension.

Chemical and metallurgical industries operate frequently with systems consisting of solid, liquid or gas reactants. The chemical transformations in these systems take place, as stated before, according to extremely complex mechanisms. The chemical reaction can be accompanied by mass or/and heat transfer. One can mention the reduction of metallic oxides, the synthesis of calcium cyanamide or binitro-aniline, the combustion of solid fuels, the synthesis of copper ammonium derivates, the compound separation using ion exchange columns, the catalyst regeneration etc.

A noncatalytic solid-gas reaction can be written as:



which is a first order reaction with respect to the gaseous reactant and zero with respect to the solid reactant. In this case, the transformation rate is:

$$r_A = a r_B = a k_V c_{B_0} c_{A_r} \quad (2)$$

where k_V is the reaction rate constant with respect to the particle volume, c_{B_0} is the initial concentration of the solid reactant and c_{A_r} is the actual concentration of the gaseous reactant.

This paper discusses the reaction mechanism for a non-catalytic gas-solid system, the elementary processes and the dependence factors. A specific reaction zone thickness is defined, calculated and correlated with the global process model.

2. Theoretical considerations

2.1. The elementary processes

According to reaction (1), a solid porous material that contains the reactant B of concentration c_{B_0} is contacted to a gaseous phase that contains reactant A of concentration c_{A_0} . From this chemical transformation, a gaseous or a porous solid product can be obtained, within the solid inert of the particle, such that its dimension remains unchanged.

The chemical reaction takes place at the same time with the gaseous reactant diffusion inside the particle and in some cases, the resulting gaseous products diffuse from inside the particle towards its exterior. Thus, the global chemical transformation relies on few sequential elementary processes which depend on the solid structure (porous or non-porous), the gas properties, the operating conditions, the chemical kinetics etc.

The main elementary processes that may occur are:

- the gaseous A reactant diffusion through the solid particle external boundary layer;
- the gaseous component diffusion through the ash layer formed at the particle surface, where the chemical reaction has ended;
- the A reactant diffusion inside the reaction zone of the particle;
- the diffusion inside the non-reacted core pores of the particle;
- the chemical reaction;
- the reaction products diffusion through the solid particle pores and through the external boundary layer;
- the heat transfer through the external boundary layer and areas inside the particle depending on the operating conditions and chemical reaction thermal effect.

The elementary processes of diffusion and chemical transformation take place sequentially. One or two processes are taking place at a lower rate than the others and thus, these are process rate determining. Depending on the system properties and the working conditions, the proposed model will take into account the main elementary processes, especially, the restrictive ones.

2.2. Factors influencing the chemical transformation

The process mechanism and the model according to which a chemical transformation is taking place in a heterogeneous system are extremely complex and depend on a large number of factors. The mathematical model has to take into account the particle form and size. In many cases, the particle has not a regular shape. The solid particles have usually small sizes such that the reaction takes place within acceptable time limits.

Particle size and shape can modify or remain constant as a result of the chemical transformation taking place. The dimensional stability is reached if the particle contains a rigid inert or if one of the reaction products is solid, with a density close to the particle density and with a certain porosity to facilitate the gaseous reactant access towards the particle inner region. Thus, the aggregation state of the reaction products and their structure, if solid, influence the global process kinetics.

The particle initial structure, its porosity and the degree of homogeneity, is essential to the chemical transformation evolution mechanism and to the eventual occurrence of some instability phenomena. The solid particle porosity

allows for the gaseous reactant diffusion towards its interior, the chemical reaction can take place in areas of different sizes. The heterogeneities can lead to instability with respect to the increase or the delay of the advancing reaction front rate and to the mass transfer area modification.

The chemical reaction type – simple or multiple – as well as its reversibility or irreversibility, are factors that affect the global process mechanism. The simple reaction model is characterized by the occurrence inside the particle of a simple reaction zone. When multiple reactions are taking place, for example, in the case of iron oxide reduction Fe_3O_4 to iron, characterized by three consecutive reactions, the reaction zone number is equal to the number of reactions taking place (Ramachandran and Doraiswamy, 1982).

The chemical processes are described by complex models characterized by transformation zones, partially overlapped, that interfere. In this case, the theoretical consideration is far from being completely clarified.

The reversible reactions are, in some cases, limited by the diffusion of the gas or liquid reaction products through the particle pores and the external boundary layer. The elementary processes related to the reaction products removal can be neglected in the case of the irreversible reactions.

An extremely important factor is the ratio between the elementary processes rates, indicating the limitative elementary process and suggesting the global process mechanism. This type of information facilitates the mathematical consideration of the process and leads to the equations establishing the degree of conversion and the reaction time.

The reaction thermal effect, the reaction rate and order are also important factors that influence the chemical conversion. A transformation with kinetics strongly influenced by the temperature increase, indicates that the chemical reaction is process controlling.

The altering of the elementary process rates during the transformation leads to an instability characterized by the modification of the global process mechanism.

The hydrodynamical conditions of the fluid phase, the solid distribution and the manner in which the phases are contacted influence the global process mechanism. In most of the cases, the solid layers have small resistances to the external gaseous A reactant diffusion. The multidispersed solids will contain particles in different development stages of the chemical process. The retention time in reactor depends on the particles having the largest sizes.

A detailed analysis of the influence factors and the literature data (Yagi and Kunii, 1955; Ishida and Wen, 1968; Tudose, 1970; Bozga and Muntean, 2001; Zaikov and Kozlovski, 2010) shows that non-catalytic heterogeneous gas-solid reactions can take place on the particle surface, in a limited or the entire particle volume. This is equivalent to different values of the ratio between the specific size of the reaction zone δ_r^* , the particle size L and its porosity (Fig. 1a).

Chronologically three models have been proposed:

– the model with non-reacted core or heterogeneous model, specific to nonporous particles and to porous particles characterized by a large chemical reaction rate (Yagi and Kunii, 1955). The reaction takes place on a surface of thickness $\delta_r^* = 0$, formed at the external part of the particle and moving towards its interior. The process is taking place in one stage, characterized by the reaction zone movement.

– the homogeneous model characterized by a reaction zone extending inside the entire particle, $\delta_r = R$. It has been proposed by Ausman and Watson (Ausman and Watson, 1962) for the catalysts regeneration and modified, in a more complex manner, later (Ishida and Wen, 1968), for relatively slow reactions.

– the limited reaction zone model or the model with diffused reaction zone, characterized by $0 < \delta_r < R$ (Tudose, 1970). It is considered more general compared to previous models since for certain simplifications, *i.e.* for $\delta_r = R$ and, respectively, $\delta_r^* = 0$, the first two mentioned models are obtained.

During a chemical reaction, one can establish three stages: the occurrence of a reaction zone of limited thickness near the particle surface, $0 < \delta_r^* < R$, the movement of the reaction zone and finally, the disappearance of the reaction zone. During the second stage, one can distinguish three zones inside the particle: the ash zone of δ_c thickness, the reaction zone δ_r^* and the non-reacted core of δ_m thickness. Summing them up gives the particle radius:

$$\delta_c + \delta_r^* + \delta_m = R \quad (3)$$

Dividing the last expression to the particle radius R and denoting the ratios by λ , one obtains:

$$\lambda_c + \lambda_r^* + \lambda_m = 1 \quad (4)$$

Several models for non-catalytic gas-solid reactions have been proposed (Ramachandran and Doraiswamy, 1982). One worth mentioning is the particle-pellet or grain model. The solid pellet is visualized as consisting of a number of small particles (microparticles). The pellet has either macro-pores through which the gas has to diffuse to reach the various grains or micro-pores pertaining to the microparticles. Each micro-particle reacts according to the non-reacted core model. Micro-particle reaction initiates in a layer at the pellet exterior and moves gradually towards its center. The micro-particles react according to the non-reacted core model and the pellet, according to the limited reaction zone model, such that one can say that this model has mixed features.

3. Results and discussions

3.1. The reaction zone thickness-rectangular coordinates

A porous rectangular particle of large thickness, L , in the l -direction is considered in Fig. 1a. The solid contains an inert material and a reactant B of concentration c_{Bo} , uniformly distributed.

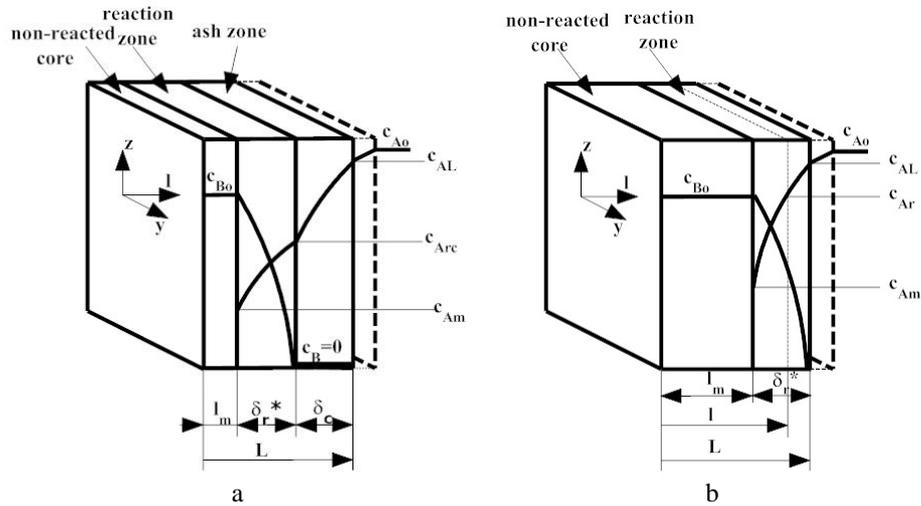


Fig. 1 a, b – Concentration profiles during the first two stages of a noncatalytic gas solid reaction–rectangular coordinates.

One side of the particle is immersed in a gaseous mixture containing the A component that reacts with the B component from the solid phase, according to Eq. (1).

The gaseous reactant A, of concentration c_{A0} diffuses through the outer boundary layer of the particle. The chemical reaction is initiated on the particle surface and as the reactant A diffuses through the particle pores, a reaction zone of continuously increasing δ_r thickness is formed. The reactant concentration decreases from the particle surface towards inside. The B reactant is consumed as the reaction zone extends. The reactant consumption rates depend on their concentration and also on the reaction order according to the Eq. (2). The initial particle and the solid reaction product porosities play also an important role.

The reaction zone thickness δ_r increases as the A reactant diffuses inside the particle. After a certain period of time, the solid reactant B from the particle surface is entirely consumed, $c_B = 0$ and a new zone named ash-zone has formed. The inert component from the initial particle or the reaction product, if solid, ensures the dimensional stability of the particle and a certain porosity of the new zone formed at the surface as indicated in Fig. 1b.

The gaseous reactant diffuses through the external boundary layer and through the ash zone towards the reaction zone. The ash zone thickness increases and the reaction zone moves towards the particle inner part.

Following these stages, a third phase starts at the moment when the non-reacted core region disappears, $\lambda_m = 0$. The reaction zone continuously decreases until it disappears as shown in Fig. 1c.

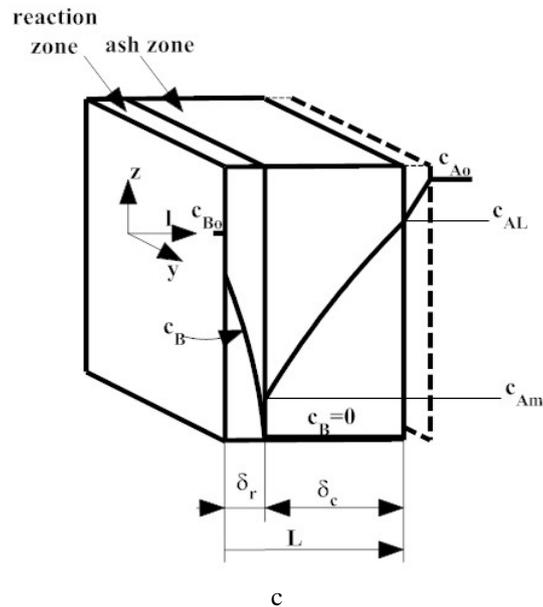


Fig. 1c – Concentration profiles during the third stage of a noncatalytic gas-solid reaction – rectangular coordinates.

At every stage, one or two elementary processes can be controlling or rate decisive for the global process. For a given system, one can inquire how large the reaction region is and according to what model the global process of chemical transformation is taking place.

The noncatalytic gas-solid reactions take place on a moving surface, in a limited moving volume or inside the entire particle volume. As above mentioned, the global process mechanism depends on the system properties. Diffusion takes place along the l -direction. A specific thickness of the reaction zone δ_r^* is defined and used to establish the reaction mechanism. It represents the maximum value of the region thickness, from the beginning of the first stage during which the B solid reactant concentration varies from c_{Bo} inside the particle to 0 on the external surface of the particle, according to Fig. 1a. The reaction region moves towards the particle interior and the ash region is formed on the particle surface, as seen in Fig. 1b.

To calculate the reaction region thickness, one can consider a surface inside the particle, located at a distance l from the particle surface, as shown in Fig. 1a. The gaseous reactant A flux that diffuses through this surface is equal to the reactant flux that is consumed in the chemical reaction in the volume region placed at the rear side of this surface:

$$D_{Ar} \frac{dc_{Ar}}{dl} A_s = r_A V \quad (5)$$

where D_{Ar} is the effective diffusion coefficient of the A component, A_s is the diffusion surface- constant in this coordinate system, r_A is the reaction rate given by the Eq. (2) and V is the considered volume:

$$V = A_s(l - l_m) \quad (6)$$

The volume, the transfer surface and the reaction rate expressions are substituted in Eq. (5) and one obtains:

$$\int_{l_m}^L (l - l_m) dl = \frac{D_{Ar}}{ak_v c_{Bo}} \int_{c_{Am}}^{c_{Al}} \frac{dc_{Ar}}{c_{Ar}} \quad (7)$$

$$(L - l_m)^2 = \frac{2D_{Ar}}{ak_v c_{Bo}} \ln \frac{c_{Al}}{c_{Am}} \quad (8)$$

Thiele modulus for the reaction zone has the expression:

$$Ti_r = L \sqrt{\frac{ak_v c_{Bo}}{D_{Ar}}} \quad (9)$$

and the difference $L - l_m = \delta_r^*$ represents the specific thickness of the reaction zone. After substitution in Eq. (8), it results:

$$\delta_r^* = \frac{L}{Ti_r} \sqrt{2 \ln \frac{c_{Al}}{c_{Am}}} \quad (10)$$

When resistance for diffusion through the gaseous boundary layer is negligible, $c_{AL} = c_{Ao}$ and the last equation becomes:

$$\delta_r^* = \frac{L}{Ti_r} \sqrt{2 \ln \frac{c_{Ao}}{c_{Am}}} \quad (11)$$

For a sufficiently large ratio $\frac{c_{AL}}{c_{Am}}$, the specific thickness of the reaction zone depends on the Thiele modulus. According to the Eq. (11), the dependence of the specific thickness δ_r^* on the particle size L is not valid. The particle size can influence only the type of reaction model, but it cannot influence the δ_r^* value. The specific thickness of the reaction zone, according to the Eq. (11) and the Thiele modulus expression is given by a function of the following form:

$$\delta_r^* = f \left(\frac{D_{Ar}}{k_v} \right)^{1/2} \quad (12)$$

which indicates a dependence on the internal diffusion represented by D_{Ar} and on the chemical reaction rate given by k_v .

In Fig. 2, the specific thickness of the reaction region as a function of the ratio Ti_r/L indicated by the Eq. (11) has been represented.

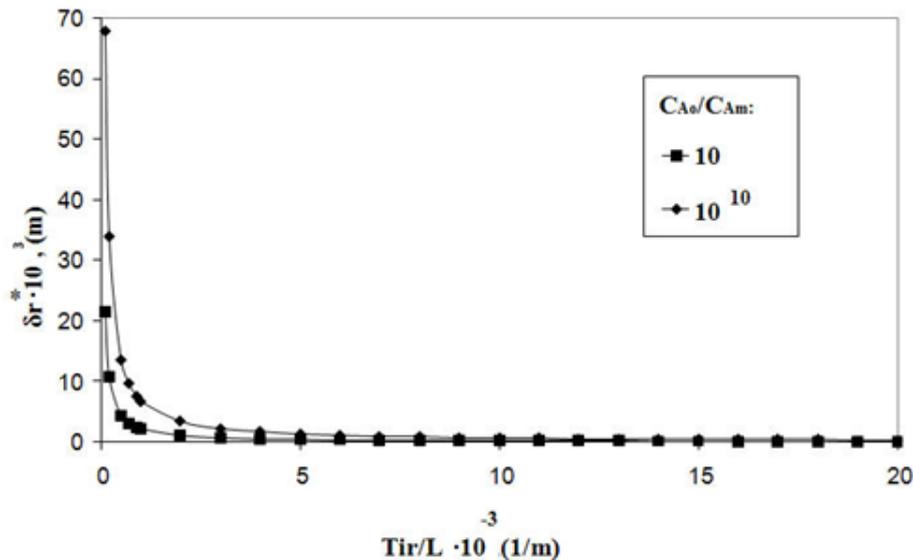


Fig. 2 – Dependence of the specific thickness of the reaction region and the ratio Thiele modulus/particle size (Ti_r/L).

The graph reveals the existence of three regions depending on the values of δ_r^* . At small δ_r^* values, for non-porous particles, *i.e.* $D_{Ar} = 0$ or for porous particles with a high rate of the chemical reaction, *i.e.* k_v very large, the specific thickness of the reaction zone δ_r^* becomes independent of the ratio $(Ti_r/L)^{1/2}$ and equal to zero. In porous particles, the diffusion coefficient D_{Ar} has relatively large values and if the reaction rate is enough small, the relative thickness of the reaction zone increases significantly. In this case, the reaction is taking place in the entire particle volume according to the homogeneous model. In between these two extremes, in the maximum curvature region of the graph represented in Fig. 2, the variation of the ratio $(D_{Ar}/k_v)^{1/2}$ induces changes of the same order of magnitude with those of the specific thickness of the reaction zone δ_r^* . It is an instability region where the model with a limited reaction zone can evolve towards another model. Depending on the ratio between the two elementary process rates – the internal diffusion and the chemical reaction - the specific thickness of the reaction zone can vary within large limits.

The first order chemical reactions, with negligible thermal effects, can take place according to different models as a function of the region size δ_r^* where the process is taking place. The specific reaction zone thickness dependence on the particle size L is represented in Fig. 3.

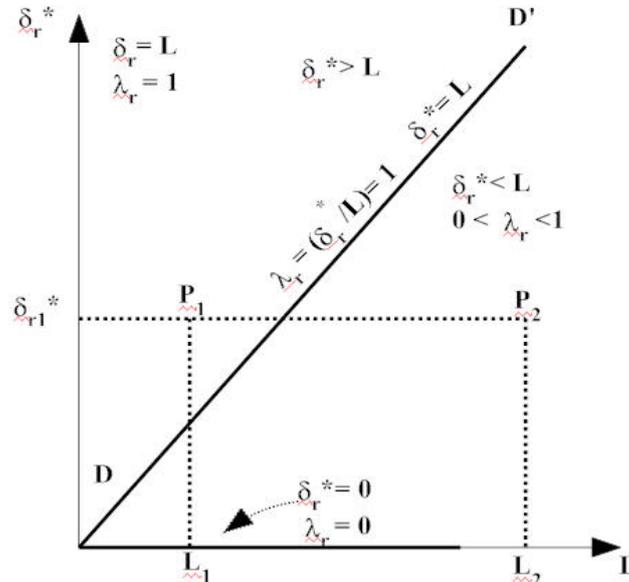


Fig. 3 – Different models in the δ_r^* - L space.

The DD' line corresponds to the equality condition between the specific reaction zone thickness and the particle size. The area between the abscissa and the DD' line corresponds to $\delta_r^* < L$, respectively to the non-dimensional thickness of the reaction zone $\lambda_r = \delta_r^*/L$ varying between 0 and 1 ($0 < \lambda_r < 1$). This case (Tudose, 1970) has been considered according to a general model since for the extreme values $\lambda_r = 0$ (for $\delta_r^* = 0$) one can recover the non-reacted core model or the heterogeneous model proposed by Yagi and Kunii (Yagi and Kunii, 1955), and for $\lambda_r = 1$, respectively for $\delta_r^* \geq L$, the homogeneous model is retrieved. Thus, for any L -value any point on the x-coordinate represents the case of the non-reacted core model ($\delta_r^* = 0$). Between the abscissa and the DD' line one can find the general model or the limited reaction zone model ($\delta_r^* < L$ or $0 < \lambda_r < 1$).

All the points between the y-coordinate and the DD' line refer to the model with a specific reaction zone thickness δ_r^* larger than the particle size L ($\delta_r^* > L$). Practically speaking such a dependence is not possible. The real thickness of the reaction region can be at most equal to the particle size. As a result, if theoretically $\delta_r > L$, then practically $\delta_r = L$ and $\lambda_r = 1$.

A solid-gas system with a specific thickness of the reaction region δ_r^* is considered in Fig. 3. The particle size depends on the solid milling degree. For a porous particle of size L_1 , the reaction takes place according to the homogeneous model corresponding to point P_1 . The larger particles, of thickness L_2 will react according to the general model or the model with a limited reaction region corresponding to point P_2 . For $\delta_r^* = 0$, the model for the chemical transformation

becomes independent on the particle size. The reaction takes place according to the model with a non-reacted core.

3.2. The reaction zone thickness-spherical coordinates

In spherical particles, as the reaction zone front moves from the surface towards the interior, the reaction zone thickness possibly modifies and consequently, the process mechanism does too. An instability state is occurring. In such cases, characteristic to the spherical particles, the diffusion surface is continuously decreasing as in Fig. 4.

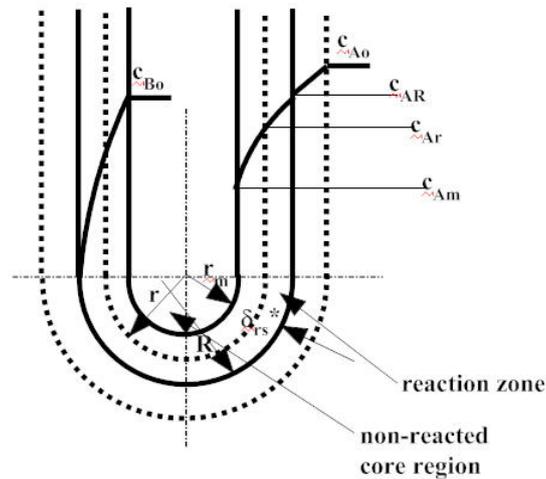


Fig. 4 – Concentration profiles for a noncatalytic gas-solid reaction – spherical coordinates.

The diffusion rate of A component that traverses an area A_s of radius r , located within the reaction region is equal to the chemical transformation rate within the volume V located at the rear side of this surface.

$$D_{Ar} \frac{dc_{Ar}}{dr} A_s = r_A V \quad (13)$$

The ratio between the reaction volume and the diffusion surface is:

$$\frac{V}{A_s} = \frac{4}{3} \pi (r^3 - r_m^3) \frac{1}{\pi r^2} = \frac{4}{3} \left(r - \frac{r_m^3}{r^2} \right) \quad (14)$$

Substitution of the Eq. (14) in the Eq. (13) and separation of the variables renders:

$$\int_{r_m}^R \left(r - \frac{r_m^3}{r^2} \right) dr = \frac{3}{4} \frac{D_{Ar}}{ak_V c_{B0}} \int_{c_{Am}}^{c_{Ar}} \frac{dc_{Ar}}{c_{Ar}} \quad (15)$$

The integrals are solved and the following notations are used: $\lambda_m = r_m/R$ the non-dimensional thickness of the non-reacted core, $\delta_{rs}^* = R - r_m$ the specific thickness of the reaction zone and $Ti_r = R(ak_v c_{b0}/D_{Ar})^{1/2}$ the Thiele modulus. In this case, one obtains:

$$\delta_{rs}^* = \frac{R}{Ti_r} \sqrt{\frac{3}{2} \cdot \frac{1}{1+2\lambda_m} \cdot \ln \frac{c_{Ar}}{c_{Am}}} \quad (16)$$

The diffusion resistance of the external boundary layer can be neglected such that $c_{AR} = c_{Ao}$ and the last equation becomes:

$$\delta_{rs}^* = \frac{R}{Ti_r} \sqrt{\frac{3}{2} \cdot \frac{1}{1+2\lambda_m} \cdot \ln \frac{c_{Ao}}{c_{Am}}} \quad (17)$$

The last equation suggests that the specific thickness of the reaction zone is also dependent on the nondimensional thickness of the non-reacted core region. As the reaction takes place, λ_m value decreases continuously from 1 to 0 which indicates an increase of the specific thickness of the reaction zone δ_{rs}^* as shown in Fig. 5.

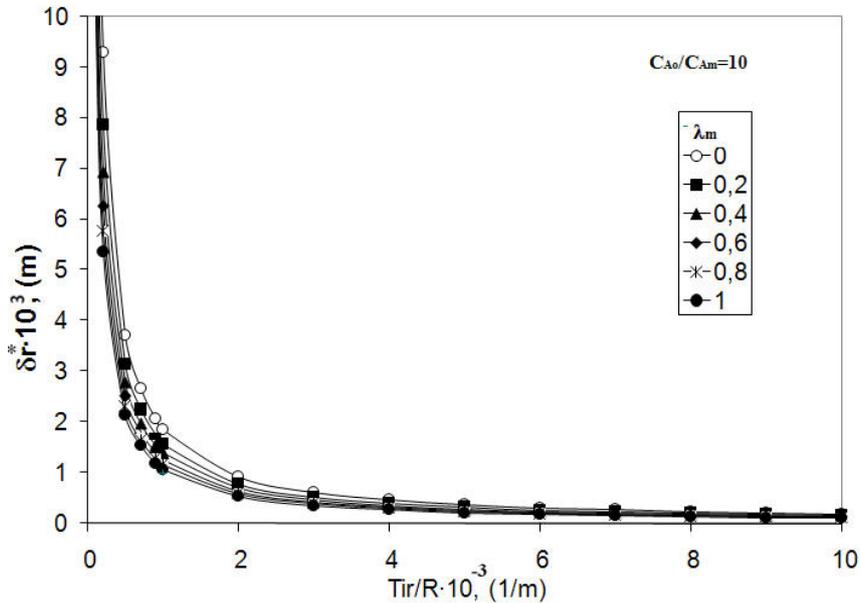


Fig. 5 – Dependence of the specific thickness of the reaction region and the ratio Thiele modulus/particle size (Ti_r/R).

The smaller the ratio $(D_{Ar}/k_v)^{1/2}$ is or the more the diffusion coefficient D_{Ar} value decreases as a function of the distance from the particle surface, the

more significant the increase of δ_{rs}^* is. Thus, a particle that initially reacts according to the non-reacted core model, can react towards the end according to the limited reaction zone model.

The ratio of the specific thicknesses of the reaction zone δ_{rs}^*/δ_r^* according to the Eqs. (11) and (17) gives:

$$\frac{\delta_{rs}^*}{\delta_r^*} = \frac{1}{2} \sqrt{\frac{3}{1+2\lambda_m}} \quad (18)$$

The last equation indicates the variation of the specific thickness of the reaction zone δ_{rs}^* for the spherical particles compared to the flat particles as a function of the non-reacted core thickness, λ_m , decreasing from 1 to 0.

4. Conclusions

The solid-gas noncatalytic reactions are of a great complexity due to the interactions between solid and fluid phases having different properties and also, the simultaneous occurrence of chemical and physical processes. The theoretical approach of these reactions generated a number of physical and mathematical models. According to these models, the reaction takes place in a solid region of variable size. A specific parameter, namely the specific thickness of the reaction zone, has been defined and calculated. The specific thickness may be zero in nonporous particles and also, in porous particles with a very high chemical reaction rate. In all other cases the specific thickness corresponds to that part of the particle thickness for which in the initial reaction stage, the solid reactant concentration varies from the initial value to zero. Thus, the reaction zone extends only over a part or the entire particle volume. It has been demonstrated that in flat particles, the specific thickness depends on the effective diffusion coefficient and the chemical reaction rate constant. In spherical particles, a dependence on the non-reacted core thickness also occurs.

The calculations within this study refer to simple isothermal first order reactions. Depending on the specific thickness of the reaction zone, the authors have confirmed some of the noncatalytic gas-solid reaction models such as: the shrinking core model (heterogeneous), the limited reaction zone model (general) and the total reaction zone model (homogeneous).

Notations

a – stoichiometric coefficient, nondimensional

A_s – surface, m²

c_{Ao}, c_{Bo} – initial A and respectively B concentrations, mol/m³

c_{AL}, c_{AR}, c_{Ar} – A component concentrations at the particle surface and respectively, in the reaction zone

D_{Ar} – the effective diffusion coefficient in the reaction zone, m²/s

- k_v – the chemical reaction rate constant with respect to the particle volume, $\text{m}^3/\text{mol}\cdot\text{s}$
 l – coordinate, m
 l_c, l_m – the coordinates of the ash zone and respectively of the nonreacted core, m
 L – the particle thickness, m
 r – the radial coordinate, m
 r – the nonreacted core radius, m
 r_A – A component reaction rate
 R – the particle radius, m
 $Ti_r = R\sqrt{\frac{ak_v c_{Bo}}{D_{Ar}}}$ or $Ti_r = L\sqrt{\frac{ak_v c_{Bo}}{D_{Ar}}}$, Thiele modulus, nondimensional
 V – volume, m^3
 δ_r^* – the specific reaction zone thickness, m
 δ_r – the reaction zone thickness, m
 δ_{rs}^* – the specific reaction zone thickness in spherical coordinates, m
 δ_c, δ_m – the ash zone thickness, the non-reacted core thickness, m
 $\lambda_c = \delta_c/R, \lambda_m = \delta_m/R, \lambda_r = \delta_r/R$ – nondimensional thicknesses of the ash zone, the non-reacted core zone and respectively, of the reaction zone

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MODELAREA REACȚIILOR NECATALITICE GAZ-SOLID. GROSIMEA ZONEI DE REACȚIE

(Rezumat)

O serie de modele fizice și matematice pentru reacțiile solid-gaz necatalitice au fost propuse în literatura de specialitate. Reacția într-un astfel de sistem are loc într-o parte a solidului care poate varia în limite mari. În cadrul acestui studiu, au fost efectuate

o serie de calcule raportate la reactantul gazos, pentru reacții izoterme simple de ordinul întâi. Mărimea ariei specifice de reacție se stabilește și se corelează cu un model matematic care caracterizează transformarea chimică ce are loc. În funcție de grosimea specifică a zonei de reacție, unele modele de reacție gaz-solid necatalitice bine-cunoscute, cum ar fi: modelul miezului în contracție (eterogen), modelul zonei de reacție limitate (general) și modelul zonei de reacție totală (omogen), au fost restabilite.