DIFFUSION TOWARDS A HETEROGENEOUS CATALYST: AN APPROACH FROM THE INFORMAL TO THE FORMAL

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1   Introducction

In this article, I will address the problem of the diffusion of a chemical species A towards the surface of a spherical catalyst particle, where a second-order reaction occurs. The following approach will be followed to make a more informal and easy-to-understand approach. First, an informal and intuitive approach will be presented. Second, a formal approach will be made containing some hints of key concepts such as second-order kinetics or heterogeneous catalysts.

2   Problem Statement

We propose the case in which a spherical catalyst particle is immersed in a solution containing a reactive chemical species A. The catalyst facilitates the transformation of A into products, but the reaction only occurs on its surface. Since the particle is impermeable to A, the species must travel from the surrounding medium to the surface of the particle by diffusion. Upon reaching the surface, A is consumed by a second-order reaction.

2.1   Key Concepts

I will start by recalling a few concepts. First, diffusion is the process of transporting molecules from a region of high concentration to a region of low concentration due to the random movement of the molecules. Particularly, in the spherical catalyst in suspension, diffusion describes how the molecules of the chemical species A move through the liquid medium to the surface of the catalyst. In this case, the particle is impermeable to A. That is, the chemical species A cannot penetrate the catalyst material. A must reach the catalyst surface from the surrounding medium by diffusion.

Since the catalyst is spherical and the surrounding medium remains static, diffusion occurs radially from the surrounding medium to the surface of the catalyst particle. Molecules of A move through the liquid due to concentration differences between the environment and the catalyst surface.

When referring to a heterogeneous catalyst, we mean that the catalyst is in a different phase from the reactive species A. Specifically, it is in a solid state, while A is in solution. Furthermore, a catalyst is a substance that accelerates a reaction without being consumed in the process.

When I mention second-order kinetics, I mean that in a second-order reaction, the consumption rate of a reactant is proportional to the square of its concentration. In particular, the reaction rate at the catalyst surface is proportional to $[c_A(R)]^2$, where $c_A(R)$ is the concentration of A at the particle surface.

3 Informal approach

We will begin to model the diffusion of a chemical species A towards the surface of a spherical catalytic particle of radius R. In this, a second-order chemical reaction occurs at the surface. The concentration of A varies radially as a function of r, which is the distance from the center of the particle.

In the case statement, it has been described that A is transported towards the surface only by diffusion. Therefore, the flux of A can be described by Fick's Law. The flux of A towards the surface of the particle in $(r = R)$ is equal to the diffusion of A due to a concentration gradient. According to Fick's Law, the flux of a substance is proportional to the concentration gradient. The flux of A towards the surface of the particle is described as:

$$J_A = -D\frac{dc_A}{dr} \tag{1}$$

This equation contains the term D which is the diffusion coefficient of A and $\frac{dc_A}{dr}$ is the concentration gradient in the radial direction r.

The diffusive flux of A at the particle surface must be equal to the amount of A that is consumed in the second-order reaction. The consumption rate of A at the surface is:

$$R_S = -k_S[c_A(R)]^2 \tag{2}$$

The term k_S is the rate constant for the second-order reaction. R_S is the rate at which A is consumed at the particle surface. The flux of A reaching the particle surface due to diffusion must equal the consumption of A due to the reaction at the surface. Therefore, equating the diffusive flux with the reaction rate gives the boundary condition for diffusion:

$$-D\left.\frac{dc_A}{dr}\right|_{r=R} = -k_S\left[c_A(R)\right]^2 \tag{3}$$

Rearranging the terms describing the diffusive transport of A and its consumption at the catalytic surface, we obtain:

$$D\frac{dc_A}{dr}(R) = k_S[c_A(R)]^2 \tag{4}$$

the intuitive solution to the problem.

4 Formal Approach

We are going to tackle the same problem, except that now, it will be done in a more formal and rigorous way. To do so, we will start with the interfacial balance and the

differential equations that describe the transport of the species A and its consumption at the catalyst surface.

The interfacial balance describes how the flow of a species crosses an interface that separates two regions. In particular, we will consider the interface between the catalyst solid, where A reacts (region 1), and the aqueous solution, which is where A diffuses (region 2).

The interfacial balance equation is described by:

$$\hat{n}(F_2 - F_1) = R_S \tag{5}$$

Where $\hat{n}$ is the normalized vector. F is the flux of A regarding region 1 or 2, or in other words, regarding the solution or the solid. R_S is the consumption rate of A at the catalyst surface. For this specific case, since the solid is impermeable to A it is considered zero. Reducing the interfacial balance to:

$$\hat{r} \cdot F_2 = R_S \tag{6}$$

Fick's Law can be expressed for the flux A in an aqueous solution as:

$$F_2 = -D\nabla c_A \tag{7}$$

However, since we are working on a spherical system, only the radial component of the flow is considered. Expressing the diffusivity (D) of A in the solution and the radial concentration gradient:

$$F_2 = -D\frac{dc_A}{dr}\hat{r} \tag{8}$$

The consumption rate of A at the surface of the catalyst particle follows the second order kinetics given by equation 2. Combining the flux at the surface with the reaction rate, we arrive at the boundary condition as before in equation 3 and, rearranging, we conclude with the same equation 4 as in the intuitive process. Where the nonlinear boundary condition that describes the relationship between the diffusion of A to the surface and its consumption in the catalytic reaction is described.

5   Conclusions

This article belongs to the analysis of transport phenomena. Specifically, to the branch of mass transfer because it is analyzing how a chemical species A diffuses through a medium to reach a surface where a chemical reaction occurs. In addition, concepts of chemical kinetics have appeared.

In this analysis of diffusion towards a heterogeneous catalyst, topics of mass transfer have been dealt with, as related to transport phenomena; chemical kinetics because

it has been considered how a chemical species reacts when reaching a catalytic surface; chemical engineering, where transport phenomena and chemical kinetics are essential for the design of industrial processes, particularly the design of heterogeneous reactors and catalytic systems.

This type of analysis is applied in areas such as hydrocarbon refining (catalysts in oil refining), production of fine chemicals, or catalytic industrial processes. Since these areas require maximizing reaction efficiency by controlling how the chemical species moves toward the catalytic surface and how the conversion of the reactant into products is optimized.