Kinetic Model Development for Heterogeneous Catalysis

Jason Yang
Chemical Engineers Organization
Email: journal@cheeng.org
Website: www.cheeng.org

Reviews and Reports in Chemical Engineers Organization, 2017, 2 (12), pp 235-240

Abstract:
Both experimental and mathematical model can be used in investigations on the influence of mass transfer between the external surface of a catalyst particle and the reaction mixture bulk. To carry out an intrinsic kinetic study, one must exclude both external and internal mass transfer effects.

1 Introduction

Chemical kinetics, also known as reaction kinetics, is the study of rates of chemical processes. Chemical kinetics includes investigations of how different experimental conditions can influence the speed of a chemical reaction and yield information about the reaction’s mechanism and transition states, as well as the construction of mathematical models that can describe the characteristics of a chemical reaction. [1]

Diffusion is the net movement of molecules or atoms from a region of high concentration with high chemical potential to a region of low concentration with low chemical potential. This is also referred to as the movement of a substance down a concentration gradient. A gradient is the change in the value of a quantity e.g. concentration, pressure, or temperature with the change in another variable, usually distance. A change in concentration over a distance is called a concentration gradient, a change in pressure over a distance is called a pressure gradient, and a change in temperature over a distance is called a temperature gradient. [2, 3]

Without diffusion effect, the reaction rate (rate of reaction) or speed of reaction for a reactant or product in a particular reaction is intuitively defined as how quickly or slowly a reaction takes place. For example, the oxidative rusting of iron under Earth’s atmosphere is a slow reaction that can take many years, but the combustion of cellulose in a fire is a reaction that takes place in fractions of a second. Chemical kinetics is the part of physical chemistry that studies reaction rates. The concepts of chemical kinetics are applied in many disciplines, such as chemical engineering, enzymology and environmental engineering. [4] In this paper we will discuss how to experimentally and mathematically carry out a catalytic study for given reaction systems.
2 Experimental

In a given reactor section, consecutive tests are carried out by increasing both reactant flow rate (volume of reactant per unit time, F) and catalyst volume (V), while keeping constant their ratio (LHSV). The conversion of reactant will change until interphase limitations (external diffusion) are present. [5, 6, 7] An useful diagnostic test to check for the presence of intraphase concentration gradient consists of determining the isothermal conversion for particles of different size at constant space velocity. If the conversion varies by decreasing the particle size, intraphase mass transfer is limiting, whereas a constant conversion indicates that the system is under chemical kinetic control. [8, 9]

3 Mathematical

Instead of conducting experimental kinetic measurements, using well known procedures, the plug flow condition can be confirmed by satisfying the criteria proposed previously [10]. Specifically, the reactor diameter is more than 10 times the catalyst particle diameter, while the catalyst bed height is more than 50 times the catalyst particle diameter. [11, 12] Further, the criteria by Weisz and Prater [13] \( \left( \frac{d_{tp}^2}{C_{1}D_{eff}} < 1 \right) \) and Mears [14] \( \left( \frac{r_{i}\Delta H_{p}d_{p}E_{ai}}{nRT^2} < 0.15 \right) \) should be both satisfied as well, confirming the absence of mass and heat transfer effects in all measurements. [15, 16]

4 Concluding Remarks

In the present work, both experimental and mathematical model are shown to be used in investigations on the influence of mass transfer between the external surface of a catalyst particle and the reaction mixture bulk, which are required before conducting a intrinsic kinetic study.[17]

5 Acknowledgments

This work was supported Chemical Engineers Organization (www.cheeng.org).

References


Figure 1: Influence of flow rate on conversion at a constant space velocity
Figure 2: Experimental test to evaluate the influence of catalyst particle diameter on the conversion
Chemical Engineers Organization

Chemical engineering is a branch of engineering that applies physical sciences (physics and chemistry), life sciences (microbiology and biochemistry), together with applied mathematics and economics to produce, transform, transport, and properly use chemicals, materials and energy. A chemical engineer designs large-scale processes that convert chemicals, raw materials, living cells, microorganisms and energy into useful forms and products. Chemical engineers are involved in many aspects of plant design and operation, including safety and hazard assessments, process design and analysis, control engineering, chemical reaction engineering, construction specification and operating instructions.

Other Catalogs:

Unit Operation  
Thermodynamics  
Kinetics  
Process Engineering

See discussions, stats, and author profiles for this publication at www.cheeng.org