Fractal-Based Research Approach for Lignocellulose-to-Ethanol Conversion

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The microstructure of porous lignocellulose has irregularity, which represents self-similarity within the scope of a certain scale, and the conversion process of lignocellulose to bioethanol is complex. The fractal theory appears to be well suited to be an effective tool for describing and studying such irregularity and complexity. Why not introduce the fractal theory as a potentially efficient and effective way to describe the process? Here in this paper, the research development of fractal theory and its potential application in lignocellulose microstructure and enzymatic hydrolysis kinetics are discussed.

Keywords: Fractal theory; Lignocellulose; Bioethanol; Ultrastructure

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Can Fractal Theory Be Used in Lignocellulose-to-Ethanol Conversion?

The concept of fractals is derived from the research on coastline measurement by Mandelbrot in the 1970's. This was an important achievement in nonlinear science research. Fractals can describe complex and regular phenomena in nature that are difficult to describe using traditional Euclidean geometry (Mandelbrot 1977, 1982; Mandelbrot *et al*. 1984). In the last 20 years, fractal theory has been widely used in various disciplines, such as physics, chemistry, biology, material science, computer graphics, economics, and philosophy. Actually, striking similarities have been found in different disciplines, and it appears that fractal theory is likely to become the latitude line for connecting various subjects.

Self-similarity and scale invariance are the two basic properties of fractals (Falconer 1990). The characteristics of fractals can be described by fractal dimension, which is the basic concept in geometry and space theory. In the Euclidean space, Euclidean dimension is the number of independent coordinates needed for determining one specific point. Generally, it is integer, such as one dimension for a line, two dimension for a plane, and three dimension for a cube. However, the fractal dimension can be a fraction, indicating the complexity of a fractal object. The bigger the fractal dimension, the more complex the fractal object is.

Lignocellulose is one of the most abundant biomass resources on the earth, and it has the potential to be converted to bioethanol. It is a porous material with complex structure, and the porosity tends to become more distinct after certain pretreatment and enzymatic hydrolysis processes. Furthermore, as a heterogeneous reaction, the kinetics of enzymatic hydrolysis is difficult to study. Therefore, it is proposed that the fractal theory can be used in the lignocellulose-to-ethanol conversion to simplify the research process.

Fractal Study in Lignocellulose Microstructure

As is well known, lignocellulose is a porous material. The pores within the cell wall have two sources: the porous structure of native lignocellulose, and the further development of an irregular porous structure after pretreatment and subsequent process. The BET method (low-temperature nitrogen adsorption method) can be used for analyzing the porous structure parameters, such as pore size and pore volume. Electron microscopy and atomic force microscopy can be used for describing the surface and interior structure. There is potential to employ a fractal approach to describe this complexity in an efficient and effective way.

Li *et al.* (2007) investigated the calculation of fractal dimensions of fibrils based on the distorted scheme of a fiber. They found that the bigger the warping fractal dimension is, the more complex the structure is, and the more rigid it is. Luo *et al*. (2011) calculated the fractal dimension based on the determined microfibril angle of spruce. They further explored the radial and tangential variation rule of fiber fractal structure. The results show that the fractal dimension is the largest for heart wood.

Fractal Kinetics of Enzymatic Hydrolysis

Generally, enzymatic saccharification involves reactions taking place in two different phase locations. One step involves solid-phase reactions, with the adsorption of exoglucanase and endoglucanase on the cellulosic substrate surface to degrade into cellobiose. The other step is a liquid-phase reaction, the hydrolysis of cellobiose into glucose by β-glucosidase. The product of the former reaction is the substrate of the latter, and the whole reaction is controlled by the lower reaction rate.

The quasi-steady-state theory fails in the heterogeneous reaction, and the rate constant decreases all the time. The enzymatic hydrolysis takes place on the lignocellulose surface, a space that inherently has fewer than three dimensions. The enzyme clusters in the fiber pore, a situation that conforms with the features of fractal kinetics. As a consequence, there is potential to use fractal theory as a substitute for the traditional Michaelis-Menten equation to describe the enzymatic hydrolysis kinetics.

The concept of fractal kinetics was first put forward by Kopelman (1988). In recent years, some researchers have worked on the modeling and optimization of fractal kinetics, consistent with the foregoing discussion. Wang *et al.* (2010) proposed a model for studying the fractal kinetics of enzymatic hydrolysis. They found that the lignin contributes to the fractal dimension, which results in a decrease of enzymatic hydrolysis efficiency. Furthermore, the glucose yield decreases with the increase of fractal dimension (Wang *et al*. 2011).

Conclusion and Perspectives

As an effective research approach, fractal theory has been widely used in various fields and there has been success in dealing with challenging issues. Fractal approaches will provide new views, new ideas, and new thoughts for scientists and researchers. Therefore, applying fractal theory in the lignocellulose-to-ethanol conversion will simplify the research process and further clarify the mechanism. With the rapid development of analytical method and fractal theory, its potential applications are promising, and more innovative achievements will likely emerge in the future.

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