

Improvement of Lignocellulosic Biorefinery via Lumped Kinetic Model and Omics Analysis

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Biorefinery can provide an effective way for comprehensive utilization of lignocellulosic biomass (LB). Because of the complicated compositions and structure in LB, multiple inter-related reactions take place during lignocellulosic biorefinery operations. These reactions are closely related to the product formation and play a decisive role in the process economics by changing the product distribution. Optimization of the reaction conditions and increasing reaction selectivity are extremely important for the improvement of lignocellulosic biorefinery process economics. Because of the reaction complexity, traditional reaction engineering has difficulty in optimizing reaction conditions for lignocellulosic biorefinery processes. Lumped kinetic model and omics analysis are useful methods to address complicated reaction system kinetics and to optimize the reaction conditions. This editorial briefly discusses use of lumped kinetic model and omics analysis to improve biorefinery operations.

Keywords: lumped kinetic model; Omics analysis; Lignocellulosic biomass; Biorefinery

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Importance of Increasing Reaction Selectivity in Lignocellulosic Biorefinery

Lignocellulosic biomass (LB) is the most abundant and renewable natural resource in the world. With ever-increasing energy demands and environmental concerns, the comprehensive utilization of LB has drawn much attention in recent years. Lignocellulosic biorefinery is considered as an effective way for LB utilization. Different technical roadmaps for lignocellulosic biorefinery can be adopted, and its process economics is generally determined by its obtained products and its raw material consumption. Increase of the utilization efficiency of raw materials and the yield of targeted products is key to improve lignocellulosic biorefinery process economics. LB is known to have complicated compositions and structure. It mainly consists of carbohydrate polymers (cellulose, hemicellulose), and an aromatic polymer (lignin). These carbohydrate polymers contain different sugar monomers (six and five carbon sugars), and they are tightly bound to the lignin. The LB used for biorefinery also has a wide range of sources. From its sources, it can be broadly classified into three types: virgin biomass, waste biomass, and energy crops. Virgin biomass includes all naturally occurring terrestrial plants such as trees, bushes, and grass. Waste biomass is produced as a low-value byproduct of various industrial sectors such as agricultural (corn stover, sugarcane bagasse, straw, *etc.*), and forestry (saw mill and paper mill discards). Energy crops are crops with a high yield of LB produced to serve as a raw material to produce second-generation biofuels, examples of which include switch grass (*Panicum virgatum*) and elephant grass. Regardless of LB sources, multiple inter-related reactions will take

place during lignocellulosic biorefinery operations owing to the complicated compositions and structure of LB. These reactions are closely related to product formation and affect its product distribution. Improvement of reaction selectivity can play a decisive role in increasing LB utilization efficiency and the yield of targeted products, thus improving its process economics. Based on these analysis, it is clear that increasing reaction selectivity in lignocellulosic biorefinery is extremely important in improving its process economics.

Use of Lumped Kinetic Model and Omics Analysis to Improve Reaction Selectivity in Lignocellulosic Biorefinery

Traditional reaction engineering has been widely used in optimization of the reaction conditions to increase reaction selectivity for a relatively simple reaction system. Because of the reaction complexity, the established kinetic models for lignocellulosic biorefinery process using traditional reaction engineering methods are too complicated to be solved. Therefore, traditional reaction engineering is unsuitable for optimizing the reaction conditions for such complicated reaction systems as lignocellulosic biorefinery processes. In order to overcome the shortcomings of traditional reaction engineering used in complicated reaction systems and to render the established kinetic models capable of being resolved, some simplifications for the complicated reaction systems need to be adopted to establish relatively simple kinetic models. The lumped kinetic model is such a kind of simplified kinetic model. It is put together by using a few virtual components instead of the complicated components in practical reaction system and then establishing the chemical transformation of these virtual components by experiment. It was first used in the petroleum processing industry, and in recent years there have been some reports that it is used in such LB processing processes as gasification and liquefaction. These studies have shown that use of the lumped kinetic model has the potential to improve reaction selectivity in such a complex reaction system as a lignocellulosic biorefinery by optimizing its reaction conditions. The omics analysis is another method used to optimize the reaction conditions in such complicated reaction system as biochemical reactions to improve their reaction selectivity. There are lots of examples that use of omics analysis to optimize biological process, but there still have been no reports about its use in optimization of lignocellulosic biorefinery processes. In our lab, we combine the lumped kinetic model and the omics analysis together to optimize the reaction conditions in lignocellulosic biorefinery process. Our preliminary results have shown that the reaction selectivity can be effectively increased. At present, there are still only few examples of successfully using a lumped kinetic model and omics analysis to improve reaction selectivity in lignocellulosic biorefinery process. In summary, this approach provides a new technical means to optimize the lignocellulosic biorefinery process and improve its process economics.

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