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Research Interest: Mechanistic Kinetic Modeling for Optimal Design of Cellulose Hydrolysis by Cellulases

Recent advances in biochemical engineering have made lignocellulosic biofuels a feasible fossil fuel alternative, but there are major production and processing burdens that must be overcome to make them economically viable. In particular, cellulase enzymes, which convert lignocellulose to glucose, are slow acting and expensive. If the stability, yield, and specific activities of these enzymes could be engineered for maximum cellulytic efficiency, the cost of biofuels production could be dramatically reduced (1). AI intend to develop a mechanistic kinetic model for cellulose hydrolysis that can be used for optimizing cellulase performance through enzyme design.

Through a quantitative and qualitative study of reaction and binding kinetics, I will create a model for cellulose hydrolysis based on cellulase species likely to be useful in biofuels production. My work will be based upon the key proteins involved in converting lignocellulosic materials to glucose monomers.

Previous modeling attempts have failed to utilize a single set of kinetic parameters that can be used for various enzymes, substrates, and operating factors. Considering the diversity of lignocellulose sources and processing conditions, truly comprehensive models are needed for scenario-specific cellulase development.

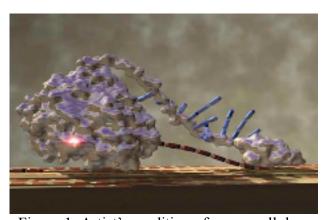


Figure 1: Artist's rendition of an exocellulase

I will be working with mesophilic and thermophilic species that grow over desirable ranges in pH and temperature. Experimental determination of kinetic constants and parameters for targeted cellulases under different microbial environment conditions will hopefully allow me to specify optimal enzyme characteristics for particular processing setups.

I will also attempt to design novel chemical techniques to study the active sight structure of cellulases and gain insight into their mechanisms of action.

A comprehensive kinetic model, based on the aforementioned investigations, will be used to optimize hydrolysis rates as a function of cellulase composition and substrate properties over a range of conditions.

In the end, predicted hydrolysis rates for various enzyme mixtures on different substrates will be compared with experimental measurements. Components of the model that cannot be experimentally verified will be adjusted and reanalyzed. In this way, I will create a comprehensive kinetic model that will allow researchers to design scenario-specific enzymes and mixtures of enzymes for maximal overall cellulase effectiveness. The resulting highly productive cellulase formulations will make biofuels more competitive, helping to jump-start a burgeoning renewable energy industry.

1. Knauf, Michael and Mohammed Moniruzzaman. Intern. Sugar. 106, 1263 (2004).