ABSTRACT

CATALYSIS FOR FORMATION OF BIO-DERIVED ESTERS AS PRODUCTS AND AS INTERMEDIATES TO EPOXIDES

By

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The production of liquid fuels from renewable biomass resources will require multiple routes and feedstock sources beyond simple ethanol or biodiesel production. Esters are an important class of organic compounds that are used in several applications in the chemical industry as both end products and as intermediates to other value added products. Two reaction types have been studied in this dissertation that are very different in their chemistry, and thus their requirements, showing the range of processes involved in the design of bio-refineries. They are the liquid phase acid catalyzed parallel esterification reactions in batch reactor configurations, and vapor phase base catalyzed conversion of propylene glycol acetates to propylene oxide, a chemical with a fast growing global market, in a fixed bed reactor.

Four results should be highlighted in particular. The first is the development of a kinetic model for esterification that uses non ideal concentrations instead of conventional activity terms. The model enables the simulation of esterification occurring with feed streams of multiple alcohols and acids under a wide range of conditions. Second, a study of the structure-reactivity relationship of over eighty reactions from literature helps predict the rates for a number of simple esterification reactions with a number of catalysts.

Third, the reaction system involving esterification of propylene glycol with acetic acid has been successfully modeled to obtain rate constant parameters for esterification,
transesterification and hydrolysis using the non-ideal concentration model. Fourth, a detailed reaction and catalyst properties study that optimized selectivity to nearly 90%, and establishes the chemical nature of the catalyst under reaction conditions.

These findings improve our understanding of chemical systems involving organic esters in a wide range of physical and chemical conditions, and will be useful in the design of complex processes for the production of esters and their use as intermediates.