

### **573b Process Integration Analysis of Sustainable Production of a Fine Chemical Intermediate from Bioresources**

*Jeffrey R. Seay, Robert N. D'Alessandro, Mario R. Eden, and Christoph Weckbecker*

The purpose of this research is to assess the economic potential of a process to manufacture a widely used industrial chemical from renewable, bio-based feed stocks. The industrial chemical chosen as the subject of this research is an aldehyde which is used as an intermediate in the specialty chemical industry. The current industry standard for production of this intermediate is based on utilizing crude oil derived feed stocks as the primary raw material. Due to rising raw material costs, it is desired to utilize a more cost effective, renewable resource as the primary raw material. One potential raw material is Glycerin. Glycerin (or Glycerol) is a natural byproduct of the manufacture of soap from the hydrolysis of animal fats. More recently, Glycerin has been produced as a side product of the transesterification of vegetable oils to manufacture biodiesel. As the use of biodiesel increases, the cost of Glycerin could drop considerably leading to potential cost savings. The objective of this work is to develop a conceptual process design for the production of this fine chemical intermediate from the dehydration of Glycerin and evaluate the economic feasibility of the process. To meet these ends, a rigorous simulation model of the current crude oil based process has been developed. This simulation model has been used to evaluate the energy usage and by-product generation of the current industrial process. Using the standard process as a starting point, multiple candidate conceptual processes for converting the current process to one that utilizes biomass based Glycerin as a feedstock have been evaluated. Simulation models of these conceptual processes are then used to aid in the evaluation of the economic potential of a Glycerin based process. Costs trends of Glycerin and standard crude oil based feed stocks are also evaluated to analyze the profitability of the changeover to the biomass based process. Process integration and systems engineering approaches are utilized to optimize the candidate conceptual processes. Thermal pinch analysis methods are extensively utilized for this aspect of the evaluation. An integral part of this work is the determination of the reaction kinetics for the specific catalyst intended for this proposed process. In this work, a lab scale reactor has been designed for the purpose of determining the kinetic parameters of the Glycerin dehydration reaction and identifying possible side products. The preliminary results of the kinetic experiments will be used to enhance the process simulation models. In addition, the experimental apparatus will be utilized to determine the reaction conditions that will result in the most economical overall process. Once the final kinetic parameters have been established experimentally, a more rigorous process model will be developed. This contribution will illustrate the results of the process integration analysis along with preliminary evaluation of the potential economic and environmental benefits of replacing a fossil fuel based raw material with a biomass derived component. The results of this analysis provides an invaluable foundation for business decision-making regarding the possible transition to producing an important industrial chemical from renewable resources.