Fundamental Understanding Of The Biochemical Conversion Of *Buddleja Davidii* To Fermentable Sugars (2011)

Bioethanol is becoming one of the leading substitutes for fossil fuel and is being commercially produced from corn and sugarcane. Lignocellulosic bioethanol is currently being explored as an alternative to corn/sugarcane ethanol because the former is not involved with the —fuel or food‖ issue. Many biomass sources are being examined but the importance is to find those with attractive agro-energy features. Thus, there is always a necessity to broaden the bioresource base. In addition, cellulosic ethanol production is more challenging than corn/sugarcane ethanol production because biomass is resistant to chemical and biological degradation. To reduce the recalcitrant nature of biomass, a pretreatment stage is required but it is the most intensive operating/operating cost component of cellulosic ethanol production. Therefore, research is heavily focused on understanding the effect of pretreatment technologies on the fundamental characteristics of lignocellulosic biomass.

The first study in the thesis investigates *Buddleja davidii* as a potential biomass source for bioethanol production. The work focuses on the determination of ash, extractives, lignin, hemicellulose, and cellulose content in this plant, as well as detailed elucidation of the chemical structures of both lignin and cellulose by NMR spectroscopy. *B. davidii* has several unique agro-energy features ranging from its distribution and wide range of growth habitat to aspects of its composition (cellulose DP of 100), as well as some undesired characteristics such as, relatively high lignin (30%) and hemicellulose (34%) contents, low cellulose content (35%), and a high cellulose crystallinity index (0.55). To determine the balance between these positive and negative factors on potential glucose yields, evaluation and enzymatic hydrolysis behavior of *B. davidii* was needed. The second study presents research on the ethanol organosolv pretreatment of *B. davidii* and its ability to produce enzymatically hydrolysable substrates. Furthermore, the study explored the fundamental characteristics of pretreated *B. davidii* in the context of developing an efficient bioconversion of cellulose to glucose. The presence of high lignin and hemicellulose contents in *B. davidii* wood was not found to be a negative factor since these biopolymers were easily removed during ethanol organosolv pretreatment (EOP). It was also concluded that the removal of hemicellulose, delignification, reduction in DP of cellulose, and the conversion of crystalline cellulose dimorphs (I_α/I_β) to the easily degradable *para*-crystalline and amorphous celluloses were the characteristics accounted for efficient enzymatic deconstruction of *B. davidii* after EOP.

The third study provides a detailed elucidation of the chemical structure of ethanol organosolv lignin (EOL) of *B. davidii* by NMR spectroscopy and compares the data to that of the native (untreated) lignin. Such research was needed to understand the pretreatment mechanism in the context of delignification and alteration of the lignin structure. Future applications of the resulted EOL will be valuable for industrially viable bioethanol production process. EOP mainly cleaved *β-O*-4' interlinkages via homolysis, decreased the DP of lignin, and increased the degree of condensation of lignin. EOL had low oxygen content, molecular weight, and aliphatic OH as well as high phenolic OH, which are qualities that make it suitable for different co-product applications. The last study provides information on the anatomical characteristics of pretreated *B. davidii* biomass after EOP. The importance of this research was to further understand the alterations that occur to the cellular structure of the biomass which can then be correlated with its enzymatic digestibility. The results

concluded that the physical distribution of lignin within the biomass matrix after pretreatment, and the partial removal of middle lamella lignin were key factors influencing enzymatic hydrolysis.