Case Study 4 – Biomass Pulping Process Model

To better understand the synergies between the cellulosic ethanol and wood pulping processes, a client had hired this consultant to develop a preliminary Aspen Plus® component slate and property model for a kraft pulping process applied to eucalyptus feedstock. The objective of this evaluation is to create a comprehensive, accurate Aspen Plus® component slate, and select the proper physical property model(s) for the different sections of a kraft pulping plant. The kraft process applies a variety of chemistries for the sole purpose of dissolving or otherwise removing lignin from a woody biomass without destroying or losing significant amounts of cellulose fiber for paper production. Varying degrees of delignification are necessary to achieve certain paper qualities. This evaluation first identified all the steps necessary to achieve high quality pulp for paper manufacturing, recovering and recycling pulping chemicals while generating plant steam and power:

- Biomass handling
- Pulp digestion (kraft process, sodium hydroxide/sodium sulfide digestion liquor)
- Pulp washing
- Pulp bleaching
- Black liquor evaporation
- Green liquor recovery
- Steam/power generation

The first challenge was to identify representative components to characterize the biomass feedstock. Fortunately, the National Renewable Energy Laboratory (NREL) provides a basis for this representation in Aspen Plus®, making available the necessary biomass component property data online. Since the pulping and bleaching processes are basically defined as delignification processes (generating and solubilizing lignin fragments), identifying model compounds representing various lignin fragments was necessary for property model development. Compounds like vanillyl alcohol and its sulfided derivatives have been used in past studies to represent lignin fragments generated in the kraft pulping process. Because many of the fragment compounds do not exist in the Aspen Plus® database, this consultant used molecular group association techniques embedded in Aspen Plus® to estimate the pure component and interaction properties of the model compounds. Other compounds, like trans-3,5 dimethylstilbene, were used to represent fragment forms from oxygen delignification (primary bleaching). Vanillyl alcohol, as identified above, can act as a suitable model compound for fragments generated in chlorine dioxide bleaching (secondary bleaching). Abietic and linoleic acids (organic acids) are used to represent the 'tall oil' portion of the biomass.

The next challenge for the simulator is to represent the highly electrolytic environment of a kraft digester accurately. Fortunately, Aspen Plus® is well suited to handle electrolyte chemistry, having much of the ionic reaction equilibrium data necessary to accurately describe the kraft pulping environment already archived in the simulator.

The entire component list for the property model totals 90 compounds (including all ionic species and possible salt formation compounds). The electrolyte predictions were validated against literature data over the entire possible pH range with great success. Even though this consultation opportunity did not include a process simulation of the kraft process, it provided a sound starting point for future pulping process simulation activities.