Aspen Plus Process Modeling of NARA Biorefinery Departments

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Introduction

Process modeling as a tool is able to provide an improved estimate of the mass and energy balance in a process. In this work, the NARA biorefinery departments were modeled using Aspen Plus v8.2 using inputs provided by the various teams, as well as adapted from existing literature and the 2011 and 2013 National Renewable Energy Laboratory (NREL) reports. The first stage of this model was developed on a department level. This means that each larger subunit of the model is separately modeled. In the future, after all the department models are complete and verified, they will be assembled into a larger, integrated model.

The current departments that are completed are:

1. Feedstock milling
2. Mild bisulfite pretreatment
3. Enzymatic Hydrolysis (Saccharification)
4. Co-products (Spent Sulfite Liquor to Lignosulfonate and Fermentation Residual to Activated Carbon.

This Aspen model has also been used to provide process inputs to the Gevo Aspen model for the fermentation and upgrading processes. Two of the department models for the NARA biorefinery, pretreatment and enzymatic hydrolysis, are shown below.

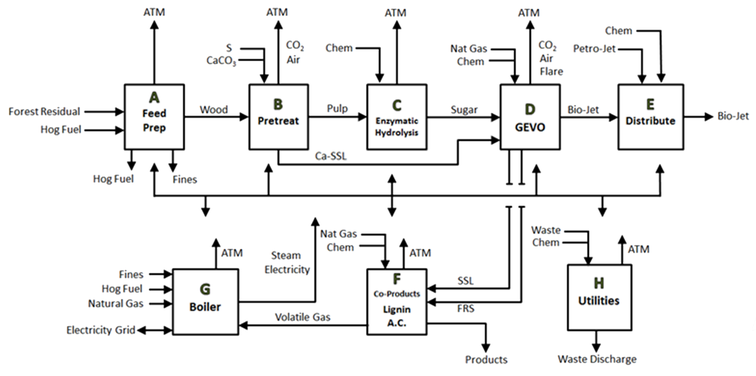


Figure: Slash to Fuel Diagram for NARA Biorefinery

Methods

Assumptions: The development of an Aspen model requires accurate physico-chemical parameters for the chemicals and materials used. In several cases, the Aspen database did not contain chemical properties for the operations that we wished to model. In these cases, the NREL model was used as a base point for comparison. The NREL model gave specific chemical property parameters which were used in this model. In addition, some assumptions that were used in the NREL model were also incorporated into this model. For example:

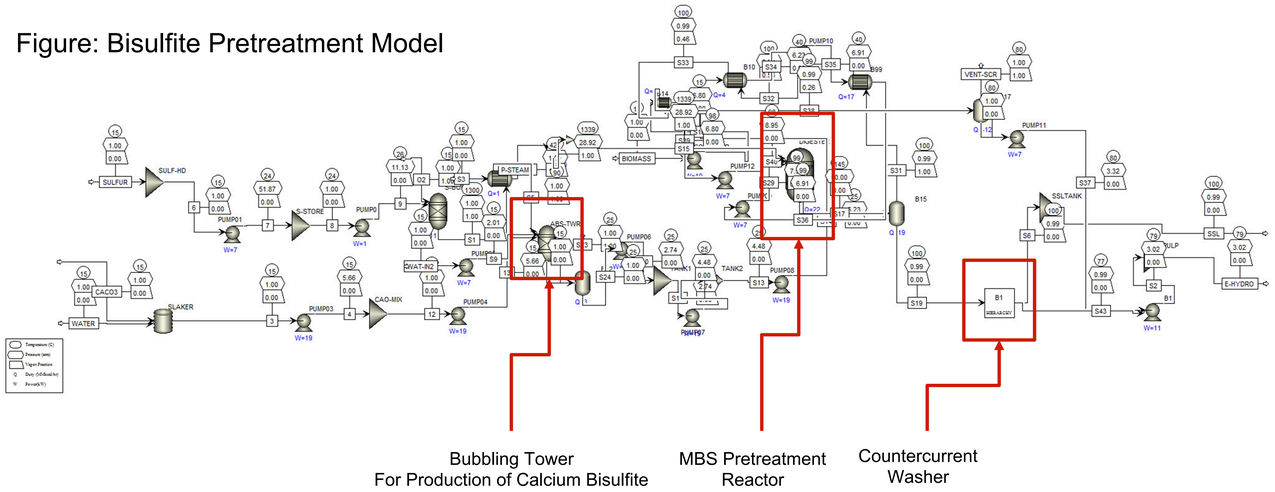
- Vanillin was assumed to have similar chemical properties as lignin
- Xylan, arabinose, and galactose were assumed to have similar structures and properties, and were all modeled after xylan

Modeling: The process model was built using an iterative process, where Aspen output was checked after each rendition of the model for its closeness to predicted data.

Additionally, as more information became available from the pretreatment teams and co-products teams, the new data was added to the model, which allowed us to look at process benefits from changed parameters.

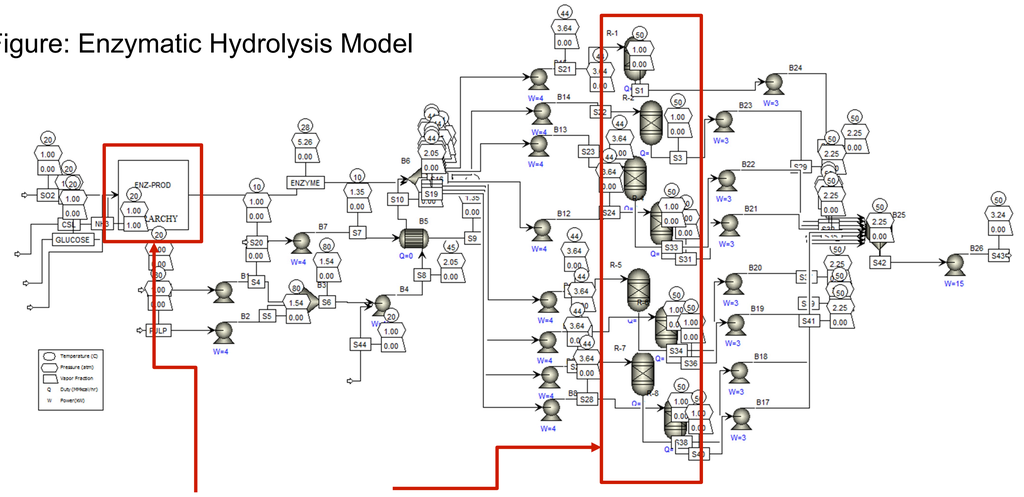
The two models below show the detailed schematic view of the MBS pretreatment process (left) and enzymatic hydrolysis (right). The Aspen software produces an estimate of energy usage (heat and electricity) and has also been used to estimate capital costs.

Figure: Bisulfite Pretreatment Model



- The MBS process utilizes a mixture of calcium carbonate, water, and sulfur dioxide to form the calcium bisulfite pretreatment liquor
- The pretreatment liquor is loaded into the reactor with the biomass and cooked for 4 hours.
- The biomass is separated into two fractions. The spent sulfite liquor is sent directly to fermentation, and the pretreated pulp is sent to saccharification.

Figure: Enzymatic Hydrolysis Model



- In the current model, cellulase enzyme is produced from corn dextrose in the biorefinery, which is significantly cheaper than purchasing enzyme directly.
- The pretreated pulp is neutralized to pH 4.8 for the hydrolysis, and placed in the saccharification reactors for 72 hours.

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