Case Study 2 – Acetone, Butanol, and Ethanol Recovery Process

The technology to produce acetone, butanol, and ethanol from a sugar source via fermentation has existed for more than one hundred years. However, the cost of product recovery has been prohibitive to commercialization due to high energy consumption. To address the energy efficiency issue, novel product recovery technologies, like hybrid extraction/distillation, have been proposed by others. A client dedicated to the development of biomass conversion has requested this consultant identify the most promising recovery technology and evaluate potential efficiency improvements and capital cost reduction using available Aspen Engineering Suite simulation tools.

Using purchased literature to provide the most accurate source of process and property data, the physical properties of the hybrid system (acetone, butanol, ethanol, water, and extraction solvent) were extracted from available databases within Aspen Plus® and compared to the literature data. Because of the unique nature of the chosen recovery system, much of the data needed to evaluate the process did not exist in Aspen Plus®. To specifically match the measured data found in the literature for this unique system, this consultant first had to regenerate a material balance based on the literature component distributions and selectivities to reflect the extraction experiments. The consultant subsequently used the material balance to back-calculate stream compositions. Once the stream compositions were determined, the stream data were regressed in Aspen Plus® to determine the specific adjustments to the liquid/liquid equilibria (LLE) predictive capability within the process simulator, i.e, generating new Renon coefficients for the fugacity, enthalpy, entropy, and Gibbs free energy calculations of this highly non-ideal mixture. As a result of the regression, a dedicated set of Renon coefficients for combinations of acetone, butanol, ethanol, and water with the extraction solvents were made available to the process simulator. Because the system is unique, vapor/liquid equilibria (VLE) data were also estimated, not by regression (due to lack of literature data), but by UNIFAC, a group association method embedded in Aspen Plus®.

Once the component physical properties were validated, this consultant used a distillation column shortcut method (Winn-Underwood-Gilliland) to approximate the tradeoff between reflux ratio and theoretical stages for each product recovery step. This information was then transferred to a rigorous distillation technique, allowing the consultant to use column targeting techniques (exergy analysis, column pinch analyses using composite temperature/enthalpy and composite stage/enthalpy diagrams) to minimize energy consumption. Once optimized, this consultant used flowsheet pinch analysis by applying the Aspen Energy Analyzer® (a rigorous process pinch analysis tool) to provide pathways to theoretical minimum energy, operating cost, and capital cost scenarios.

Finally, this consultant determined the overall project capital cost by applying the Aspen Process Economic Analyzer (based on the ICARUS cost estimating environment), providing the most accurate capital cost estimate for this phase of the design. Provided in a thorough, proprietary report, the client will use the estimated operating and capital cost data to determine the overall economic feasibility of this process based on their own assessment of feedstock costs and product values.