CADSIMulator

CADSIM Plus Process Simulation News

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Process Simulation of Integrated Forest Biorefineries

The following article was adapted from a paper by Tuhin Banerjee & Larry Wasik (Aurel Systems) and Mariya Marinova & Sakya Devy Sreng (École Polytechnique de Montréal)

CADSIM Plus has recently been selected as the process simulator of choice for a major Canadian research project focusing on the integration of biorefineries with existing pulp and paper mills. Aurel Systems has been working in collaboration with École Polytechnique de Montréal to develop new CADSIM Plus modules and thermodynamic prediction techniques for the successful process simulation of integrated forest biorefineries.

The Canadian pulp and paper industry is actively seeking solutions that could contribute to their long-term prosperity. One proposed solution is the implementation of Integrated Forest Biorefineries (IFBRs) into existing pulp and paper mills. Under-valued wood components such as hemicelluloses, lignin and extractives could be used to produce high-value biofuel products.

To successfully design and implement an IFBR both consultants and mill engineers will need new tools to assist them in designing the complete resources integration that is required for this task. There is a significant need for detailed energy and water optimization, economic, and environmental assessment studies. Modeling and simulation are important tools for performing detailed feasibility and integration studies. However, to date, little attention has been paid to modeling of bioproducts from wood feedstock.

Mill engineers will need new tools to help them understand how biorefineries will integrate into their existing processes.

Traditionally, chemical process simulators have specialized in modeling either hydrocarbon-based or water-based systems. Hydrocarbon-based simulators stand out for their ability to accurately model vapor-liquid equilibrium (VLE) along with performing flash and distillation calculations for systems where the stream chemistry can be clearly defined on a molar basis (such as for mixtures of ethanol and water). Water-based simulators are better at modeling complex water-based slurries and mixtures where the stream chemistry cannot be defined on a molar basis (chips, lignin, pulp).

The challenge in choosing a single simulator for modeling IFBRs is that, while the modeling of downstream purification and refining operations relies mainly on hydrocarbon-based VLE calculations, all of the upstream modeling of the pulp and paper mill is heavily dependent on the strengths of a predominantly water-based simulator. Therefore, a suitable process simulator for modeling IFBRs needs to be able to handle upstream water-based pulp and paper slurries, while being able to accurately predict the VLE behavior downstream.

CADSIM Plus's ability to accurately model process dynamics allows users to develop control strategies, study start-up and shut-down operations, and to troubleshoot problems within the plant. CAD-

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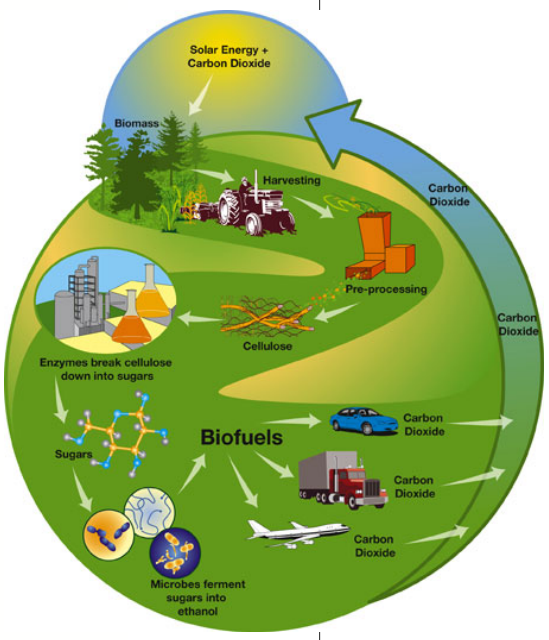

Source: DOE Joint Genome Institute, US Department of Energy www.jgi.doe.gov

(BioKrEn Project: continued from page 1)
SIM Plus can also be used to develop computer-based manuals for training, which can be linked with CADSIM Plus P&ID drawings. CADSIM Plus includes DDE, COM, and OPC capabilities for communication with Excel, DCS and mill information systems and has been successfully used for on-line applications such as Dynamic Data Reconciliation (DDR), process quality tracking, and predictive control.

As a leading simulator in the pulp and paper industry, CADSIM Plus has been used by pulp mills and consulting engineers across the globe. Its pulp and paper-specific module libraries and its ability to accurately model slurries and mixtures makes it great for handling the up-stream non-molecular pulp and paper side of the biorefining process. The optional CADSIM plus Hydrocarbon Processing Library includes features typically found in most hydrocarbon-based simulators, including an extensive physical properties database, a choice of several thermodynamic methods and accurate VLE modeling of flash and distillation calculations for down-stream purification steps.

A distillation column module is required to properly simulate the integrated forest biorefinery. CADSIM Plus includes a more complex DC that allows the specification of the number of trays, etc. However, as part of the BioKrEn Project, development has begun on a simpler distillation column module for CADSIM Plus that is based on the Fenske-Underwood-Gilliland (FUG) method, commonly referred to as the "shortcut method". The FUG method, is widely used in industry for making preliminary designs and optimization of simple distillation.

The need to dehydrate aqueous solutions of ethanol and water was identified, and these are known to exhibit azeotropic behavior. Unlike pure components, when solutions flash, their resulting vapor and liquid phases have different compositions. This allows solutions to be separated by distillation. When azeotropes form, solutions start behaving like pure components and it becomes impossible to separate them beyond their azeotropic composition by simple distillation alone. Therefore, in the simulation of IFBRs, it is important for a process simulator to have the thermodynamic capabilities necessary to anticipate azeotropic behavior and to model it accurately.

Simulators capable of modeling VLE need a selection of thermodynamic property methods that are used to perform flash calculations. Common thermodynamic prediction routines include equations of state-based methods such as Soave-Redlich-Kwong (SRK) and Peng-Robinson (PR). These methods are useful when working with non-polar compounds and can also be used to predict azeotropic formations in non-polar hydrocarbon systems.

If mixtures containing polar substances are to be modeled, however, equation of state methods are no longer sufficient. This can be illustrated by looking at the T-x-y phase-diagrams. Figure-1 was obtained using experimental data for ethanol and toluene mixtures.

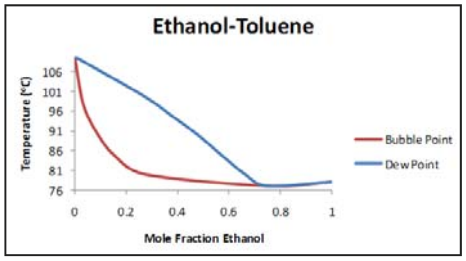

Figure-1: Phase Diagram Using Experimental Data

Figure-2 was constructed using an equation of state-based property method, which does not produce good results.

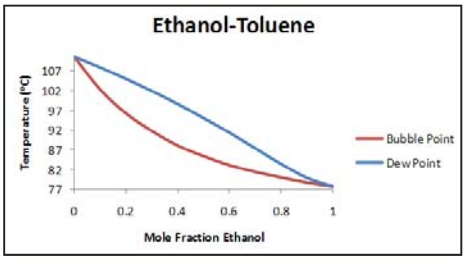

Figure-2: Phase Diagram Using Peng-Robinsion Equation

An azeotrope can be spotted on a T-x-y diagram as the point at which the dew and bubble point curves meet (for mole fraction values other than 0 or 1). Looking at Figure-1, the presence of an azeotrope is visible. From Figure-2, however, it is obvious that using an equation of state method alone does not model this polar ethanol-toluene mixture well as it fails to predict the formation of the azeotrope.

Highly non-ideal mixtures involving polar compounds such as alcohols and water are best represented by an activity coefficients model. Activity coefficients models use binary interaction parameters (BIPs) that have been fitted to experimental data. The BIPs are used to calculate activity-coefficients, and these coefficients can be used to model non-ideality of mixtures. Common activity coefficients methods include Wilson, and Non-random Two Liquid (NRTL) equations.

As ethanol is a key end product to an essentially water-based process, a robust activity coefficients method has been developed for the accurate thermodynamic modeling of alcohol-water systems. Both Wilson and NRTL equations are capable of predicting vapor-liquid equilibrium conditions for non-ideal systems.

However, if liquid-liquid extraction is to be modeled anywhere in the biorefining process, it is important that the thermodynamic model of choice be able to model liquid-liquid equilibrium (LLE). The Wilson equation can only handle single liquid phases and therefore is not suitable for modeling LLE. The activity coefficients from the NRTL equation however, can be used to predict LLE conditions well. Therefore, the NRTL equation has been selected for this development.

The VLE calculation capabilities of the NRTL activity coefficients method have been developed and tested in CADSIM Plus. The results show that the simulated values are in good agreement with experimental data.

LLE plays an important role in the biorefining process. In order to simulate this, a reliable thermodynamics

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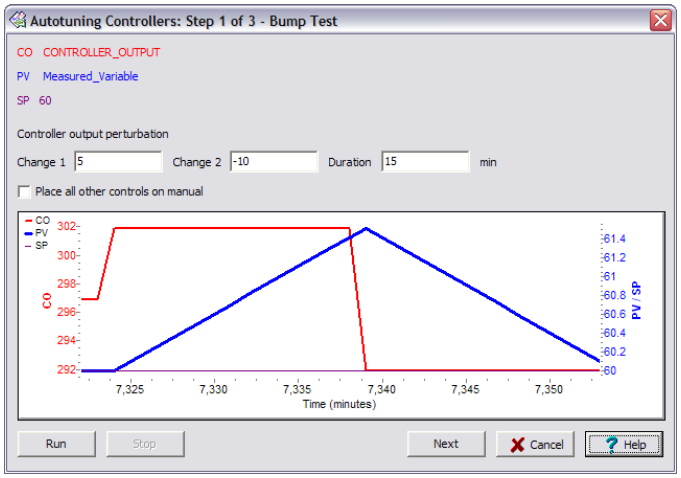
Tech Corner: Controller tuning with Autotune

A controller turning wizard called Autotune was introduced with CADSIM Plus v2.5. Autotune utilizes the Lambda tuning method, which was first documented in a book published by TAPPI PRESS titled *Process Control Fundamentals for the Pulp & Paper Industry* by Nancy J. Sell, Frederick Y. Thomasson et al. This method allows proportional constant, integral reset time and differential time to be estimated using PID controller tuning equations.

Autotune automates the Lambda tuning method by breaking the process down into three steps.

Step 1: Bump Test

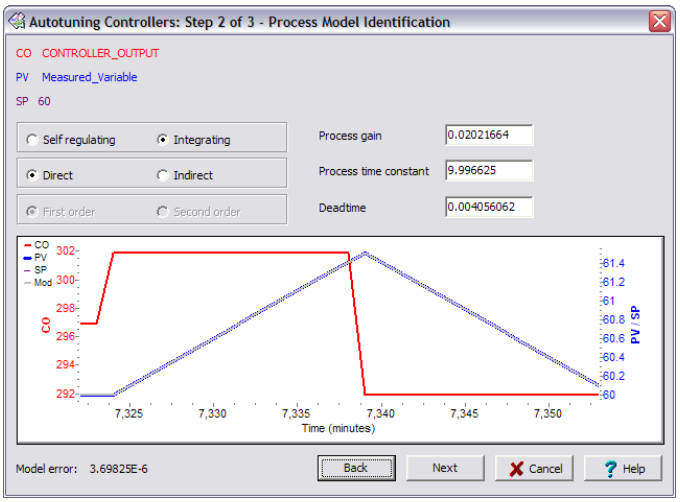
The bump test consists of two step changes in the Controller Output (CO) while tracking the changes in the measured Process Variable (PV). The Autotune wizard analyzes the results of the bump test, attempts to do a process identification, and then compares those results to the response from the actual process model.



Step 2: Process Model Identification

For the purposes of controller tuning, processes generally fall into one of the following categories: first order, second order, first order plus delay and integrating. These process groups are further broken into two types: self-regulating vs. integrating. A step change (or bump) in the CO of a self-regulating process will cause a change in the measured PV that will eventually settle out. A step change in the CO of an integrating process will cause the PV to continue to ramp.

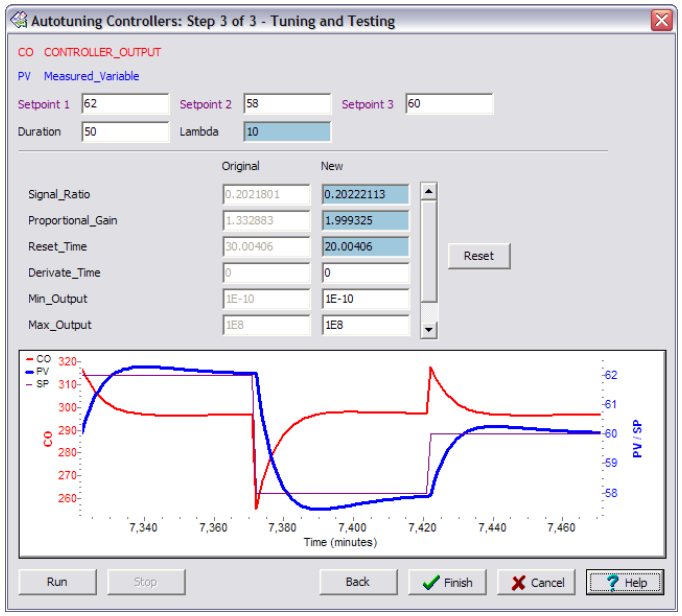
The tuning approach differs between integrating and self-regulating processes. That is why the process model identification step is important. The Autotune wizard makes an attempt to identify the process model type based on its response to the bump test. This step gives the user the opportunity to review those automatic choices, change parameters and compare the resulting model response with the CO response (integrating model shown superimposed on PV, below).



Step 3: Tune and Test

When the 3rd step is reached, Autotune has suggested a new set of tuning parameters for the controller. The user may compare these new tuning parameters with the original values. The user may also edit any of the parameters and then run additional tests to see the results. Each test consists of two step changes (bumps) to the Setpoint (SP).

The user can adjust the automated tuning suggestions by changing the Lambda value (in minutes) which makes calculated adjustments to the other fields automatically. Increasing the value in the Lambda field provides the controller with a slower response and stabilizes an unstable process. Decreasing the Lambda value provides a faster response.



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CADSIMPLUS

Did you know...?

You have made changes to a running simulation and now it doesn't seem to be running correctly. Before you made the latest changes, you saved a good start file. Load that start file when you start the simulation running, then click on a stream or unit to see the current calculated values. Now click the checkbox named "Show Startup Values" in the information dialog box. You can now quickly compare the saved stream or unit values against your current calculated values to locate problems.

(BioKrEn Project: continued from page 2)

property method, which supports LLE, is going to be required.

The validation of the NRTL model in its ability to perform VLE calculations has been of great significance to the next phase of development. The same activity coefficients that are calculated to model VLE can also be used to predict LLE conditions. As simulated VLE results have been in good agreement with experimental data, it has indicated that the activity coefficients being calculated by the current NRTL model are accurate and can be trusted. The next phase in the thermodynamic prediction methods development is going to focus on adding to the NRTL model in order to model LLE in CADSIM Plus.

École Polytechnique de Montréal has been working on developing an algorithm to be used for the thermodynamic modeling of LLE. Once an algorithm has been validated, the method will be integrated with the NRTL properties method that currently exists in CADSIM Plus, allowing users to simulate LLE and the presence of multiple liquid phases.

We will also be developing and improving several modules for CADSIM Plus. For hemicelluloses biorefinery, fermentation, a liquid-liquid separator and a distillation column for aqueous azeotropic multicomponent mixtures must be developed. For lignin biorefinery, a reactor for complex systems not defined by molecular formulas will be created. For gasification, a reactor for complex systems not defined by molecular formulas and enhanced gas turbines. For these modules, heat loads, temperatures, pressures, compositions and phase have to be calculated.

Through collaboration between members of industry, researchers, and suppliers, it is planned to form a collection of key performance data for biorefining unit operations. The overall goal of having this data is to provide engineers and researchers with a good reference point for the design and simulation of various integrated biorefining processes.

Based on the criteria required for successful process simulation, CADSIM Plus by Aurel Systems has been selected as the chemical process simulator of choice for the modeling of IFBRs for the BioKrEn project. Aurel Systems and École Polytechnique de Montréal have successfully developed new unit modules and thermodynamic prediction techniques for CADSIM Plus in order to simulate IFBR processes. Future steps in development include the addition of new IFBR-specific modules and thermodynamic models, along with forming a collection of key performance data to assist scientists and engineers in their simulation and design efforts.

Aurel Systems is pleased to announce two new additions to our professional services staff:

Uma Ati (Ati) joined Aurel following completion of a Master of Applied Science degree (specializing in **advanced process control**) at McMaster University. Ati is heading up development of our **new on-line optimization services**.

Tuhin Banerjee joined us full time following two successful co-op work terms at Aurel while completing his chemical engineering degree at UBC. Tuhin's duties include continuing development of our **hydrocarbon processing library** and expanding our **simulation modeling consulting services**.