Stability simulations

New simulation programs are helping miners to gain stability in the fluctuating coal market.

The instability of the coal industry along with the constant search for alternative energy resources, has led many Australian coal miners to invest heavily in R&D to discover the optimal coal-to-liquid process (CTL). With CTL plants costing billions to establish it is critical to ensure the project is viable before proceeding. Sophisticated software simulation and process analysis tools have aided the reduction of costs during the feasibility phase and bring alternative, green energy to the market sooner.

Simulation software can aid miners in making the shift to coal to liquids processing.

Motivations for CTL

The volatility of coal prices and the unpredictability of coal demand are among the reasons many Australian coal miners are exploring new and complementary coal mining processes. Coal miners in, or considering, coal-to-liquid energy production need to make decisions on the most suitable liquefaction process, estimate the associated costs and predict the return-on-investment for the stakeholders during the current flux.

The coal-to-liquid process, in most instances, means that existing coal mines can convert coal into synthetic crude oil for further refining into diesel and other fuels, adding revenue and economic sustainability to the miner.

What is most crucial to the efficiency to all CTL processes and their variations is the gasification phase. One of the most common gasification designs is the Integrated Gasification Combined-Cycle (IGCC) plant. But since the plants represent investments of hundreds of millions of dollars it is essential to use the most advanced technology to identify the optimal process configurations. This will not only help to design equipment that will run reliably and safely, but also develops accurate cost estimates to ensure that the right decisions are made early in the design lifecycle.

The simulation solution

Decision makers need to consider the challenges of simulating IGCC and other large-scale integrated processes.

According to Steven Kratsis, director of area sales for AspenTech Australia "recent advances in engineering software and the relentless progress of Moore's law have made it possible to simulate large scale processes such as IGCC plants at increasingly higher levels of fidelity".

Simulators such as Aspen Plus allow users to break the process down into hierarchical sections ensuring each hierarchy captures an area in the plant, such as an air separation unit or the power island. The hierarchical sections are connected by the 'boundary streams', representing the material, heat, electricity, or shaft work flowing from one section of the plant to another.


As the coal price suffers globally, many miners are turning to new ways to harness their coal.

Hierarchical models can also be used as containers for complex equipment models. Gasifier models may be assembled from combinations of ideal reactor blocks, furnace models, mixers, and splitters. Building these reactor models in a hierarchy container allows the model developer to package the entire structure as a reusable template. The resulting templates can be inserted into a process model just like any of the built-in unit operation models.

Hierarchies improve the usability of these complex simulations by organsing the models into a sensible structure. In addition, hierarchies make the models easier to maintain since entire sections of a process can be updated by importing a single object into an existing simulation case.

Advances in design

The gasifier is the core of the IGCC plant. It is essential to design the gasifier properly to ensure high energy efficiency and good process economics. Engineers can apply computational fluid dynamics (CFD) tools which optimise equipment design to identify and eliminate dead zones, hot spots, and other potential operability problems.

These types of CFD models can also be used to characterise equipment performance over a range of operating conditions improving predictions of efficiency and performance under various scenarios.

Although CFD models are very powerful they have high computational requirements. As a result, the CFD models have been used primarily in isolation to design key equipment.

Recent work led by the Department of Energy National Engineering Technology Labs (DOE/NETL) show great promise for improvement. A number of organisations working together under the NETL-sponsored Advanced Power and Energy Co-Simulation (APECS) project are developing methods to convert rigorous models (including CFD models) to reduce order models (ROMs), which in turn can be used as integrated plant process simulation models. Advanced mathematical modelling techniques such as neural networks and principle component analysis (PCA) are used to perform data regression against simulation results from the high-order models. The models are fitted to complex equations which capture the essence of the equipment behaviour. The ROMs are much less computationally intensive than the original high-order models and can work inside simulators to help predict the global optimum operating conditions.

Since all mines have different grades of coal across their landscape the first step is to select the location of the optimum coal source. Using Aspen Plus, miners can enter the properties (moisture, carbon content etc) of a coal sample and then model the gasification process to determine both the gas output and the yield. This process is repeated until the best site is identified. The next step is design.

Detailed first-principle gasifier models have been developed using equation-oriented modelling tools such as Aspen Custom Modeller (ACM). These models, which capture rate-limited reactions, mass- and heat-transfer, can be used to optimise the steady-state operating conditions and the equipment designs.

Such models can also be used to study process dynamics, to test control schemes, and to identify the best start-up and shutdown procedures for these plants. These custom models can be plugged directly into the steady-state simulation environments (such as Aspen Plus) to examine the process as a whole.

Process simulation models can be used to predict the mass and energy balances and key equipment sizes for IGCC plants. These results can be used together with rigorous cost modelling software, such as Aspen Icarus Process Evaluator (IPE) and Aspen Process Economic Analyser (APEA), to carry out detailed economic evaluations of various process configurations and scenarios.

Rigorous cost modelling provides the accuracy needed to make the right investment decisions and to reduce the risks of cost overruns. Further, these tools allow estimators to carry out detailed economic analysis of various scenarios such as future escalation in coal production costs, and fuel price changes.