Gasification Process Modeling

An Industry White Paper

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About AspenTech

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Introduction

High energy prices, the desire for greater energy independence, and environmental concerns are all creating the 'perfect storm' for next-generation gasification technologies. Hundreds of companies and government organizations around the world are investing in the development of a wide variety of processes, utilizing various feedstock materials and gasifier designs in an attempt to capture part of this critical market. However, given the technical challenges, fluctuating economic cycles and strong competition, it is likely that only a handful of these processes will prove to be viable. Since gasification plants represent investments of hundreds of millions of dollars, it is essential to leverage advanced technology to identify optimal process configurations, design equipment that will run reliably and safely, and develop very accurate cost estimates to ensure that the right decisions are made early in the design lifecycle.

Technology Advances in Gasification Process Modeling

Fortunately, recent advances in engineering software and the relentless progress of Moore's law have made it possible to simulate large scale processes such as Integrated Gasification Combined-Cycle (IGCC) plants at increasingly higher levels of fidelity.

Consider the challenges of simulating IGCC and other large-scale integrated processes. Today's simulators, such as *Aspen Plus*®, allow users to break the process down into hierarchical sections. 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 section. Hierarchical models can also be used as containers for complex equipment models. For example, 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 organizing the models into a sensible structure. In addition, hierarchies make the models easier to maintain since an entire section of a process can be updated by importing a single object into an existing simulation case.

Improvements in computer hardware and software have allowed process engineers to significantly increase the scope of the process included inside a single simulation case. Specifically, equation-oriented and hybrid (mixed EO-SM) simulation allows users to carry out wide-scale process optimizations of entire plants. Simulating and optimizing the whole process using an integrated plant model allows process engineers to avoid time-consuming manual work reconciling designs spread across multiple case files. More importantly, optimizing a process using an integrated model ensures that the resulting designs capture the true global optimum instead of a local optimum.

The gasifier is the core of 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 to optimize 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 characterize equipment performance over a range of operating conditions to improve predictions of efficiency and performance under various scenarios.

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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) shows great promise for improving this situation. A number of organizations working together under the NETL-sponsored Advanced Power and Energy Co-Simulation (APECS) project are developing methods of converting rigorous models (including CFD models) to reduced order models (ROMs), which in turn can be used in the context of an integrated plant process simulation model. Advanced mathematical modeling 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 behavior. The ROMs are much less computationally intensive than the original high-order models, so they can work inside simulators to help predict the global optimum operating conditions.

Detailed first-principle gasifier models have also been developed using equation-oriented modeling tools such as *Aspen Custom Modeler®*. These models, which capture rate-limited reactions, mass- and heat-transfer, can be used to optimize 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 startup 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.

In many regions, CO_2 credits will make carbon capture economically viable. Absorber-stripper loops, using amines or other types of solvents, are commonly used to extract CO_2 from syngas and fuel gas generated in the process. Simulating these types of absorber-stripper loops is technically challenging for several reasons. The process involves rate-limited and equilibrium electrolytic reactions. The absorber and scrubber are mass-transfer rate limited; apparent tray efficiencies can be less than 20%. Further, the flow rate of solvent flowing in a loop between the absorber and stripper is much higher than the gas flux through the process.

Several recent advances in process simulation technology have made it easier to accurately predict the performance of the CO_2 scrubbing systems. Second-generation rate-based distillation models, such as *Aspen Rate-Based Distillation*, reliably predict the mass-transfer limits inside the columns using new discretization methods to account for concentration profiles across the vapor-liquid interface. With the 2006 release of *Aspen Plus*, these rate-based column models can work in equation-oriented mode. This allows process engineers to apply equation-oriented solution methods which can handle the high recycle flow rates typical in these types of processes. The resulting models can be used to find operating conditions or identify the best solvents to minimize the recycle loop flow rate, which can reduce operating and capital costs associated with the process by reducing the required size of the process heat exchangers and the required column diameters.

AspenTech, in conjunction with the University of Texas at Austin, is actively researching these processes to establish next-generation thermophysical and transport property models to further enhance the reliability of these models. New types of semi-predictive activity coefficient models are being designed. We expect these models to do a better job of characterizing new types of industrial solvents and solvent mixtures using a minimal amount of measured data.

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 modeling software, such as *Aspen Icarus Process Evaluator*, to carry out detailed economic evaluations of various process configurations and scenarios. Rigorous cost modeling 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 raw material and energy costs.

Summary

There are a number of excellent technologies available today to help guide decision-making with respect to process selection, feedstock selection, process configuration, and detailed equipment design. Companies who leverage these technologies most effectively to develop the most economical and reliable IGCC plants will emerge as the winners in this competitive race.

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