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Computational Research Challenges and Opportunities for the Optimization of Fossil Energy Power Generation Systems

Stephen E. Zitney
Director, Collaboratory for Process & Dynamic Systems
U.S. Department of Energy, National Energy Technology Laboratory
3610 Collins Ferry Road, Morgantown, WV 26507-0880
Email: stephen.zitney@netl.doe.gov

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ABSTRACT

Emerging fossil energy power generation systems must operate with unprecedented efficiency and near-zero emissions, while optimizing profitably amid cost fluctuations for raw materials, finished products, and energy. To help address these challenges, the fossil energy industry will have to rely increasingly on the use advanced computational tools for modeling and simulating complex process systems. In this paper, we present the computational research challenges and opportunities for the optimization of fossil energy power generation systems across the plant lifecycle from process synthesis and design to plant operations. We also look beyond the plant gates to discuss research challenges and opportunities for enterprise-wide optimization, including planning, scheduling, and supply chain technologies.

INTRODUCTION

The process and energy industries manage some of the most sophisticated, high-integrated, and expensive plants in the world, spending hundreds of billions of dollars annually in plant design, operation, and optimization. The fossil energy (FE) sector also faces the grand challenge of designing next-generation plants, including integrated gasification combined cycle (IGCC) power plants and poly-generation facilities, such as the zero-emission, coal-fired, gasification-based power and hydrogen production plant in the $1 billion, 10-year U.S. Department of Energy (DOE) FutureGen R&D Initiative (DOE, 2004). The 275-megawatt FutureGen plant will employ advanced coal gasification technology integrated with combined cycle electricity generation, hydrogen production, and capture and sequestration of carbon dioxide (CO_2). It will be the cleanest fossil fuel-fired power plant in the world, capturing and sequestering at least 90% of the CO_2 with potential for 100% sequestration.

To accelerate the development of next-generation power plants, the FE industry relies heavily on the use of computational process modeling and simulation across the plant lifecycle. Coupling this existing technology with high-fidelity modeling, advanced analysis, optimization, and high-performance computing will not only speed up technology development by reducing pilot/demo-scale facility design time and operating campaigns, but also lower the cost and technical risk in realizing high efficiency, near-zero emission power plants.

PROCESS SYNTHESIS

In the synthesis phase of the FE plant lifecycle, computational tools are used to systematically generate, from among a set of alternatives or superstructure (Figure 1), a sub-system network (e.g., reactor, separation, heat, water) or an overall plant flowsheet so as to meet certain objectives, for example, to maximize business potential. Once the conceptual design of a plant has been determined, a process simulator can be used for more comprehensive design work. Thus, process synthesis tools help ensure that the simulations in the process design phase of the plant lifecycle are performed on the best possible flowsheet. Recent efforts to integrate process synthesis and simulation tools have for the most part focused on enabling engineers to synthesize heat exchanger and distillation networks within a process simulator.

In the power and energy industries, the synthesis tools that see the most use are heat exchanger network design and pinch analysis. For the conceptual design of FE plants, synthesis technology will be important for generating candidate plant configurations from various technology modules. Synthesis tools will also be required to develop tightly integrated heat and water recovery networks.

Many recent approaches to process synthesis are based on rigorous mathematical programming algorithms, thereby avoiding the use of hierarchical decomposition and heuristics. These algorithmic approaches require considerable computational resources when used for plant-wide process synthesis.

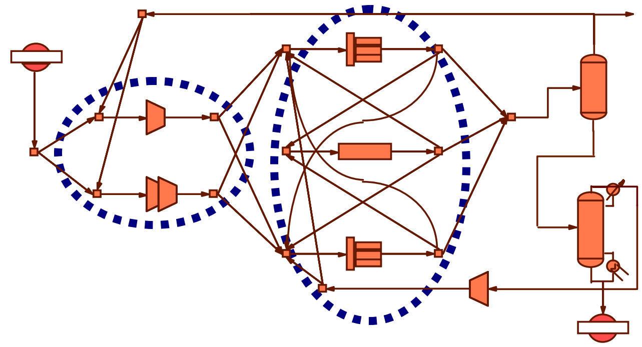


Figure 1. Process Synthesis – Superstructure with equipment assignment options (dashed circles)

Mixed integer nonlinear programming (MINLP) is the optimization technique of choice for systematically generating process/heat/water networks from a set of candidate technology options so as to meet certain objectives (e.g., Bruno *et al.*, 1998). MINLP involves the optimization of an objective function (e.g., cost) with respect to nonlinear equality constraints (e.g., mass and heat balances) and inequality constraints (e.g., specifications) and includes both continuous variables (e.g., state variables) and integer decision variables (e.g., equipment assignment). Common MINLP methods include branch and bound techniques which solve nonlinear programs (NLPs) at each node, outer-approximation (OA) methods, Generalized Benders Decomposition (GBD), and more recent logic-based methods (Grossmann and Biegler, 2004).

A key research challenge in process synthesis is to develop computationally reliable and efficient MINLP methods and solvers to optimize the large process flowsheet superstructures arising from the synthesis of complex FE power generation systems with integrated heat and water management networks. Continued advances in rigorous algorithmic approaches to process synthesis will enable FE process design engineers to consider more process alternatives in a shorter time. Parallel computing also provides opportunity to reduce greatly the solution times for these combinatorial problems.

PROCESS DESIGN AND OPTIMIZATION

In the process design phase of the plant lifecycle, process simulators are the computational technology workhorses. These tools typically consist of unit operation models, thermodynamic calculation models, reaction models, and physical property databanks. The unit operation models are typically lumped-parameter models that perform mass and energy balances. A 2D graphical layout of the process flowsheet is created by dragging and dropping icons from the unit operations model library and connecting them with process streams. Large flowsheets that contain hundreds of unit operations and streams, as well as a large number of chemical species, may involve solving tens of thousands of equations. The user interface generally provides plotting capabilities for viewing simulation results. Engineers use process simulators to quickly predict the steady-state and dynamic behavior of entire plants, as well as to perform equipment costing and sizing calculations.

Steady-State Design and Optimization

Process analysis, design, and optimization for continuous processes are typically done using steady-state process simulators. Most steady-state simulators use the sequential-modular (SM) approach, in which the process flowsheet consists of unit operation models, all recycle streams are torn, each unit operation is solved separately, the flowsheet is worked through sequentially, and iterative solution is continued until the entire flowsheet is converged.

Another way to solve a steady-state process model is to use the equation-oriented (EO) approach, where all of the process equations are solved simultaneously. The EO approach offers speed and flexibility for steady-state calculations, especially when dealing with highly interconnected flowsheets with many recycle streams and design specifications. It also is an excellent approach for performing process optimization and dynamic simulations, as discussed below. These potential benefits are generally recognized today, and there is increasing industrial interest in this approach. EO process simulation requires the solution of a large sparse system of nonlinear algebraic equations (NLAE). While initial work in EO simulation typically involved solution by tearing to reduce the number of variables iterated on, today the solution is almost always by simultaneous linearization. In this case all the equations are linearized and all the variables iterated on simultaneously using a Newton-type method.

For power and energy applications, the commercial steady-state simulator, Aspen Plus® (Aspen Technology, 2007), is often used by the DOE, industry, and other researchers. Aspen Plus offers solids handling capabilities important for coal combustion and gasification modeling; comprehensive physical properties, thermodynamics, phase and chemical equilibrium relations, and reaction kinetics for gas cleanup modeling; and an extensive library of heat exchange and rotating equipment models for simulating combined cycles. Aspen Plus also provides both the SM and EO solution approaches

Steady-state process optimization gives rise to nonlinear programming problems (NLP) with constraints (equality or inequality). Many commercial process simulators provide a sequential quadratic programming (SQP) method for continuous variable optimization. SQP solvers allow the creation of a number of NLP algorithms based on Newton steps. Moreover, these solvers have been shown to require the fewest function evaluations and they can be tailored to a broad range of process optimization problems with different structure. Large-scale optimization algorithms for NLPs with several thousand variables may be needed to augment the current SQP optimization methods in process simulators which are equipped to handle only up to 100 variables or so. One potential alternative for solving much larger models is the new class of interior point methods (Wächter and Biegler, 2006). Finally, considerable opportunity exists for additional research on global optimization methods (Sahinidis, 1996), since nonconvexities in the design problems are likely to yield suboptimal solutions since the corresponding bounds for the variables are rather loose in these problems. Global optimizers find the "best optimum" when multiple local solutions exist, for example in applications such as the consumption of freshwater in integrated process water systems (Karuppiah and Grossmann, 2006).

High-Fidelity Co-Simulation

To improve the accuracy of FE system design, steady-state equipment models evolve in complexity from lumped-parameter to spatially distributed representations based on partial differential equations (PDEs) in multiple dimensions. Due to the need for accurate spatial discretizations for fluid flow, heat and mass transfer, and reacting systems, optimization problems involving PDE formulations are often orders of magnitude larger than typical optimization applications. In addition, the integration of high-fidelity PDE-based equipment models (such as computational fluid dynamics (CFD) models) with overall process models leads to the creation of very large models for process optimization.

The Advanced Process Engineering Co-Simulator (APECS) developed at the DOE's National Energy Technology Laboratory (NETL) provides process/equipment co-simulation capabilities (Zitney *et al*., 2006). The hierarchy of equipment models ranges from high-fidelity CFD models to custom engineering models (CEMs) to fast reduced-order models (ROMs) based on pre-computed CEM or CFD results. At NETL, system analysts typically use APECS to run power plant co-simulations coupling the steady-state process simulator, Aspen Plus, with CFD models based on FLUENT® (ANSYS/Fluent, 2006), a leading software package for comprehensive flow analysis. As shown in Figure 2, the APECS integration framework uses the process industry-standard CAPE-OPEN (www.colan.org) software interfaces to provide plug-and-play interoperability between process simulation and equipment simulations (Zitney, 2004a).

The APECS process/CFD co-simulation technology enables process design engineers to analyze and optimize power plant performance with respect to fluid flow in key equipment items, such as combustors, gasifiers, syngas coolers, steam and gas turbines, heat recovery steam generators, and fuel cells. At NETL, system analysts, oftentimes in collaboration with R&D partners (e.g., ALSTOM Power), are applying APECS to a wide variety of advanced power generation systems, ranging from small fuel cell systems to commercial-scale power plants (Figure 3).

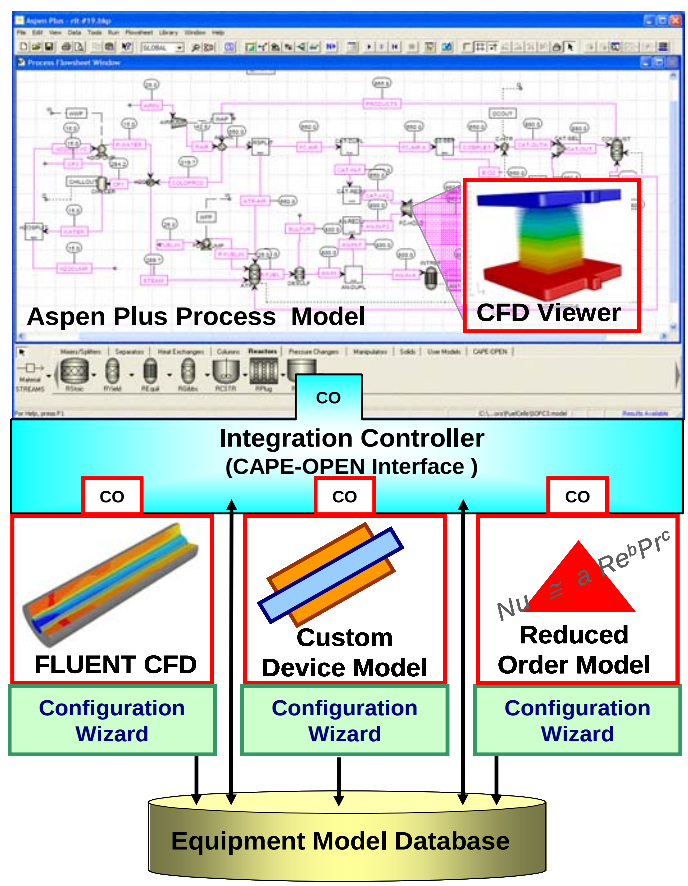
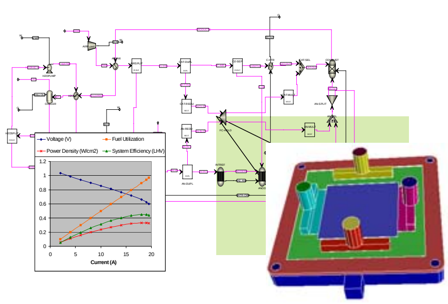


Figure 2. APECS Co-Simulator

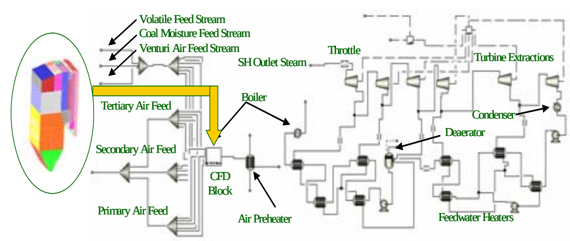
Using APECS, the overall performance of solid oxide fuel cell (SOFC) auxiliary power units (APUs) modeled using Aspen Plus are optimized with respect to the local fluid flow, heat and mass transfer, electrochemical reactions, current transport, and potential field in the SOFC simulated using detailed, three-dimensional, steady-state FLUENT CFD models (Zitney *et al.*, 2004). The process/CFD co-simulations are performed over a range of fuel cell currents to generate a voltage-current curve and analyze the effect of current on fuel utilization, power density, and overall system efficiency.

In collaboration with cycle engineers at ALSTOM Power, APECS co-simulations have been developed for a conventional 30 MWe pulverized coal-fired (PC) steam plant for municipal electricity generation and an advanced 250 MW, natural gas-fired, combined cycle (NGCC) power plant. In the PC co-simulation, an Aspen Plus process design specification is used to adjust a FLUENT CFD model parameter for the boiler damper position (bypass resistance) to maintain a specified steam temperature over a range of loads, from the load at the maximum continuous rating to a control load, below which the boiler cannot sustain the required turbine inlet temperatures (Sloan *et al.*, 2004). For the NGCC co-simulation, an Aspen Plus process design specification is used to manipulate designated control parameters for the FLUENT CFD model of the heat recovery steam generator (HRSG) so that a specified superheat steam temperature is maintained for various load points over the range from 100% to 50% gas turbine load (Sloan *et al.*, 2005).

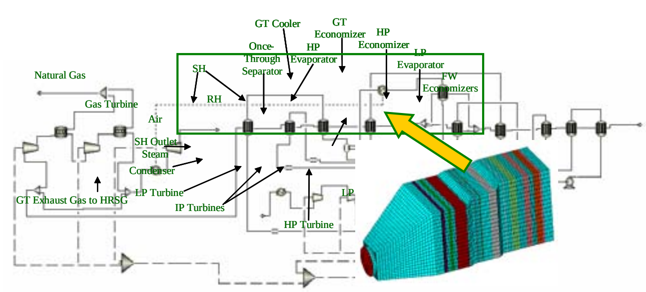
At NETL, research engineers are also developing APECS co-simulations to analyze potential FutureGen plant configurations (Zitney *et al.*, 2006). In a recent demonstration case, the FutureGen co-simulation combines a plant-wide Aspen Plus simulation with two FLUENT CFD-based equipment models, one for the entrained-flow gasifier where fluid dynamics strongly affect syngas quality and carbon conversion and one for the gas turbine combustor where the blending of air and fuel is at the heart of gas turbine combustor performance and efficiency. Using APECS, Aspen Plus controls the co-simulation and automatically executes the gasifier and combustor CFD models as needed to converge the tail gas recycle loop and a design specification on the gas turbine inlet temperature. The design specification is met by manipulating the synthesis gas split between power production and hydrogen production.



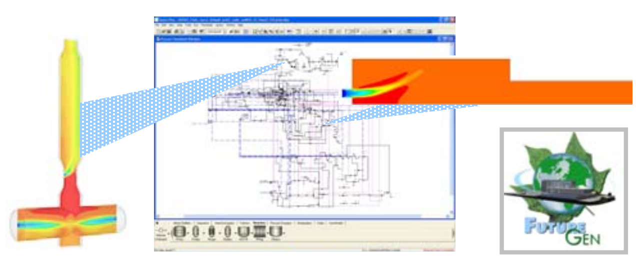
Fuel Cell Auxiliary Power Unit (APU) with 3D CFD SOFC



ALSTOM Conventional Steam Plant (250MWe) with 3D CFD Boiler



ALSTOM NGCC (250MWe) with 3D CFD HRSG



FutureGen Plant (250MWe) with 3D CFD Gasifier and 2D CFD Turbine Combustor

Figure 3. APECS Power Generation Applications

To improve co-simulation turnaround time, APECS provides options on both ends of the performance spectrum, including the use of fast ROMs and parallel execution of the CFD models on high-performance computers. ROMs are a class of equipment models that are based on pre-computed CFD solutions over a range of parameter values, but are much faster than CFD models. For example, the APECS system currently provides for the automatic generation and use of ROMs based on multiple linear regression (Syamlal and Osawe, 2004) and artificial neural networks (Osawe *et al*., 2006). Future ROM solvers will include non-linear regression, principal component analysis (PCA) and proper orthogonal decomposition (POD). For parallel execution, the APECS CAPE-OPEN integration controller allows process simulations running under the Windows operating system to use equipment models running locally/remotely and serially/in parallel on Linux clusters and/or supercomputers (Zitney, 2004b).

The APECS system also provides a wide variety of powerful computational analysis tools for optimizing overall power plant performance (Zitney, 2004b). Design specifications are used to calculate operating conditions or equipment parameters to meet specified performance targets. Case studies are used to run multiple simulations with different input for comparison and study. Sensitivity analysis shows how process performance varies with changes to selected equipment specifications and operating conditions. Optimization is used for maximizing an objective function, including plant efficiency, energy production, and process economics. For process optimization in the face of multiple and some time conflicting objectives, APECS offers stochastic modeling (Figure 4) and multi-objective optimization capabilities developed to comply with the CAPE-OPEN software standard (Subramanyan *et al*., 2005).

Several key computational research challenges and opportunity areas for high-fidelity co-simulation include:

- Reduced-order modeling strategies
- Parallel solution strategies for co-simulations with multiple embedded CFD models
- Optimization strategies for large-scale process/CFD co-simulation
- Computational strategies for dynamic co-simulation
- Data management, analysis, and virtual engineering

Stochastic Simulation

The FE industry can benefit from a systematic approach for characterizing the impact of process uncertainties on economics, safety, and environment. Failure to account for the uncertainty of key parameters (e.g., technical coefficients, product demands) has the drawback that the solution of deterministic models can lead to non-optimal or infeasible decisions. Unlike sensitivity analysis which varies only one or two parameters at a time, a stochastic analysis handles many uncertainties simultaneously and provides insight as to the likelihood of different outcomes.

For optimizing power plant performance under uncertainty, stochastic optimization methods are required. The typical approaches can be classified in two broad classes: (i) deterministic, in which the parameter uncertainty is typically described through bounds of expected deviations, and (ii) stochastic, that describes the uncertainty through a probability distribution function (Sahinidis, 2004). The latter approach to uncertainty analysis is considered here and typically consists of four main steps: (1) characterization and quantification of uncertainty in terms of probability distributions, (2) sampling from these distributions, (3) propagation through the modeling framework, (4) analysis of results (e.g., Diwekar *et al*., 1997).

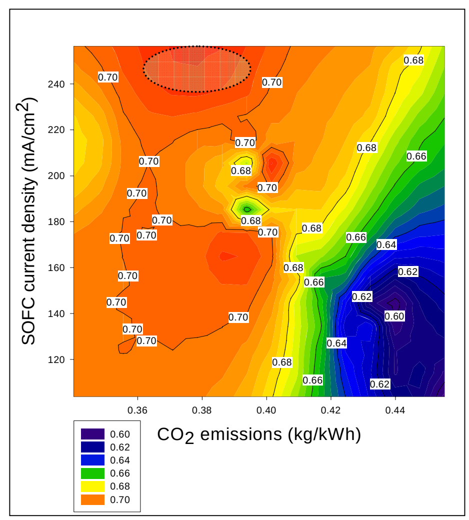


Figure 4. APECS Stochastic Simulation Results

Computational research challenges and opportunities in stochastic analysis include the development of more efficient sampling techniques to minimize the number of repeated process simulations required for plant design and single objective optimization problems needed for stochastic multi-objective plant optimization. It is also clear that computational approaches to stochastic simulation are inherently parallel since the samples (process simulations) are independent and can be performed simultaneously. Therefore, stochastic process simulation applications would benefit significantly from the use of parallel computers, especially for cases involving complex flowsheets for coarse-grain parallelism. Continued progress on stochastic simulation technology will enable system analysts to optimize fossil energy applications with respect to risk and uncertainty, as well as plant safety and operational flexibility.

PROCESS OPERATIONS

Dynamic Simulation and Process Control

Interest in dynamic simulation and optimization of FE power generation systems is increasingly significantly. Dynamic simulation tools provide a continuous view of a process in action by calculating the transient behavior of the plant over time. Typical applications include plant startup, upset, shutdown and transient analysis, and the evaluation of control schemes. Dynamic simulation is also utilized for operability analysis, environmental and safety studies, and training applications requiring real-time or faster simulation.

Plant-wide dynamic simulation is used in an off-line mode to evaluate alternative control strategies without the expense and, perhaps, without the unexpected hazards of plant experimentation. Engineers can manipulate various control variables in a dynamic model to establish the best control strategies together with the most effective controller settings. This capability is essential when dealing with complex processes or with new processes for which little or no operating experience is available.

For gasification-based power plants, such as IGCC systems and the DOE's FutureGen plant, dynamic simulation is required to determine key equipment response times and to investigate interactions between major plant sections, including the air separation unit, gasifier, gas cleanup system, combined cycle, and heat recovery steam generator. Dynamic simulation is also essential for predicting the transient behavior of the fossil energy plants during startup and shutdown, as well as subsequent to planned (e.g., loading, unloading) or unplanned (e.g., gasifier trip, gas turbine trip, steam turbine trip) disturbances of the steady-state operation. At NETL, process researchers are applying dynamic simulation to hybrid fuel cell gas turbine systems (Shelton *et al*., 2005) and plant-wide IGCC systems (Zitney *et al*., 2007), as shown in Figure 5.

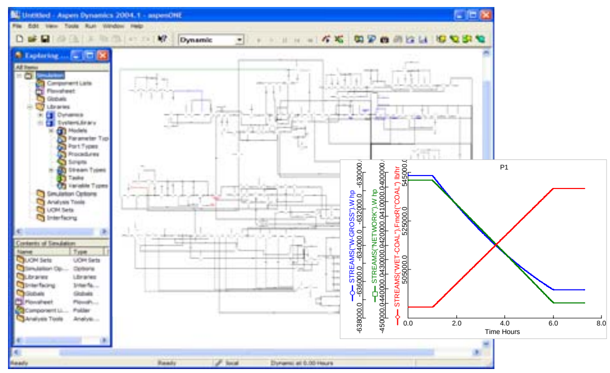


Figure 5. Plantwide IGCC Dynamic Simulation

Well-known commercial dynamic simulators include Aspen HYSYS Dynamics® (Aspen Technology Inc.) and the EO-based packages, Aspen Dynamics® (Aspen Technology Inc.) and gPROMS® (Process Systems Enterprise Ltd.). HYSYS Dynamics uses a simultaneous-modular approach, combining the EO approach for solving pressure-flow equations and the SM approach for solving energy and composition balances. These dynamic simulators are tightly coupled with their steady-state counterparts. Such integration enables engineers to start with an existing steady-state solution and quickly move to a running dynamic simulation complete with an automatically generated default control scheme. This capability also allows companies to fully leverage their existing investments in steady-state models and ensures the consistency of steady-state and dynamic simulation results. While these popular commercial dynamic simulators are most heavily used in the chemical process industries, they are seeing some increased use in power and energy applications.

Dynamic process simulation is typically more computationally intensive than steady-state simulation. The EO approach to dynamic simulation requires the solution of large, sparse differential-algebraic equation (DAE) systems, consisting of differential equations that describe the dynamic behavior of the system, such as mass and energy balances, and algebraic equations that ensure physical and thermodynamic relations. These DAE systems typically contain ordinary differential equations and algebraic equations. PDEs occur in dynamic models that are distributed spatially, but even these models can be converted to DAE form by using the well-known methods of lines to approximate the spatial derivatives using finite differences or orthogonal collocation on finite elements.

The majority of dynamic simulators use difference approximation schemes to solve the DAE systems. In the context of process simulation, the backward difference formulation method of Gear has emerged as a reliable method. Other popular dynamic integrators include Euler's method, fixed- and variable-step implicit Euler, and Runge Kutta. Given a set of consistent initial conditions, the DAE system is reduced to a NLAE system to be solved at various time steps. The NLAE system is solved using a Newton method so that the solution of a large, sparse system of linear equations is at the core of the dynamic simulator. The linear system is solved several times for each nonlinear solution, while the NLAE-solving step is executed for each time step in the simulation. For large industrial simulations, the linear equation solver is usually a direct sparse matrix solver (e.g., Harwell's MA48) and may be the dominant computational step.

The following is a list of some of the key computational research challenges and opportunity areas for dynamic simulation:

- High-index DAE systems
- Model consistency
    - Degrees of freedom (DOF) and dynamic degrees of freedom (DDOF)
    - Structural non-singularities
    - Consistent initial conditions
- Faster DAE solvers with discontinuity and bounds handling
- Direct and iterative sparse matrix methods
- Real-time performance for training applications
- Parallel dynamic simulation for large-scale plant-wide or multiple plant problems
    - Parallel-modular iterative approach, waveform relaxation

Dynamic optimization becomes increasingly important to enhance operation of FE processes during transient phases such as grade transitions, start-up or shut-down, as well as real-time applications for optimization-based monitoring and optimal control on receding horizons. The general differential–algebraic optimization problem (DAOP) is solved either by the variational approach or by applying some level of discretization that converts the original continuous time problem into a discrete problem (Grossmann and Biegler, 2004). Full discretization of state and control profiles is typically handled using multiple shooting or collocation methods (large NLP), while partial discretization of control profiles is done using control vector parameterization (Iterative Dynamic Programming (IDP) or NLP/DAE).

For gasification-based power plants, rigorous dynamic simulations are also needed to support development and evaluation of advanced process control (APC) methodologies based on model predictive control (MPC). At the core of MPC technology is a mathematical model of the process that is used to predict future process behavior. Using this predictive model the controller is able to calculate an optimum set of process control moves which minimize the error between actual and desired process behavior subject to process constraints. Since the late 1970s, MPC technology has performed reliably in the petrochemical and refining industries because of its ability to account for process interactions and constraints, thereby reducing process variability and driving the process closer to its limits.

Current research efforts are focused on novel and emerging developments in MPC technology for use in IGCC power plant applications. MPC areas of interest include, but are not limited to dynamic matrix control, nonlinear advanced control, and real-time adaptive control. Additional work is required to develop and evaluate strategies for applying MPC solutions to various IGCC operating control modes. For the power production control, MPC strategies are required for driving the gasifier to satisfy load demands while meeting IGCC plant integration, performance, and environmental objectives. Considerable research challenges and opportunities exist in the development of advanced MPC strategies for IGCC-based polygeneration plants that must simultaneously satisfy power, hydrogen, chemical, and steam demands.

Real-Time Dynamic Simulation

A common use of real-time dynamic simulation is operator training. Plant personnel can be trained to operate complex processes and to deal with dangerous procedures such as commissioning, start-up, changeovers, emergency handling, and shut-downs. By interfacing a dynamic simulator to a distributed control system, a realistic environment for hands-on training can be provided without the complications, risks, and costs arising from operating the real plant. The combination of a rigorous dynamic model with the plant control system also has major applications in process monitoring and control. The operating conditions of many plants must be adjusted periodically to optimize plant performance given economic, environmental, and safety constraints. By using on-line, dynamic models either as a guide to operators for process monitoring, or directly for rigorous nonlinear model-predictive control, it is possible to generate significant increases in operating profit.

Figure 6. IGCC DS&R Center at WVU's NRCCE

To meet growing demand for education and experience with the analysis, operation, and control of IGCC plants, NETL has launched a collaborative R&D project to develop a generic, full-scope, IGCC dynamic simulator (Zitney and Erbes, 2006). The IGCC simulator will combine a process/gasification simulator and a power/combined-cycle simulator together in a single dynamic simulation framework for use in research and development as well as engineering studies. The key features of the IGCC simulator will include:

- High-fidelity, real-time dynamic model of process-side (gasification) and power-side (combined cycle) for a generic, commercial-scale IGCC plant based on slurry-fed entrained-flow gasification technology
- Full-scope dynamic simulator capabilities including plant startup, shutdown, load following and shedding, response to fuel and ambient variations, control strategy analysis (turbine and gasifier lead), malfunctions/trips, alarms, scenarios, trending, snapshots, data historian, and trainee performance monitoring
- Extendable to incorporate additional gasification and gas turbine technologies, as well as new, advanced technologies such as fuel cells and membrane separation systems

The IGCC dynamic simulator will be used to establish a world-class R&D center at West Virginia University's (WVU) National Research Center for Coal and Energy (NRCCE) (Figure 6). The IGCC Dynamic Simulator & Research (DS&R) Center will be established under the auspices of the Collaboratory for Process & Dynamic Systems Research (CPDSR) organized between NETL, WVU, the University of Pittsburgh, and Carnegie Mellon University. The DS&R Center will offer much-needed plant operation and control demonstrations, onsite training courses, and computer-based training.

ENTERPRISE-WIDE OPTIMIZATION

Enterprise-wide optimization (EWO) is a promising research frontier that combines process systems engineering and operations research, and has become a major target in the process and energy industries due to the mounting pressures for strengthening competitiveness in the worldwide marketplace (Grossmann, 2005). EWO involves optimizing the operations of supply, production, and distribution activities of an enterprise to reduce expenditures, waste, lead times, and inventories. A major challenge in EWO is the optimal operation of production plants, which often requires the use of nonlinear process models. Key operational considerations include planning, scheduling, real-time optimization, and inventory control. One of the key features of EWO is integration of the information and the decision-making among the various functions that comprise the supply chain of the enterprise.

EWO problems are typically formulated as linear problems, linear programming (LP) and mixed integer linear programming (MILP), for planning, scheduling, and supply chain. These optimization problems can be computationally expensive to solve since in the worst case complexity increases exponentially with problem size. However, recent progress in algorithms and hardware has resulted in significant performance improvements in MILP solvers such as CPLEX (from ILOG) and Xpress (from dash optimization).

For companies in the process and energy industry to remain competitive and economically viable, it appears that EWO is likely to emerge as major research challenge area over the next decade. Several examples of potential applications in the FE sector include:

- Power generation capacity expansion planning with uncertain load forecasts (Stochastic programming)
- Cost minimization of combined fossil energy co-production facilities and CO2/H2 pipeline networks (Co-optimization)
- Supply chain model for optimal planning of the production and distribution of liquid fuels with uncertainties in demands and supplies, as well as supply disruptions (Multi-period MILP with stochastic programming)

CONCLUDING REMARKS

Future FE power generation systems will consist of plants that individually represent complex, tightly integrated, multipurpose designs. All allowable technologies will be required to meet aggressive engineering goals (such as producing near-zero emissions); even so, system planners will need to choose among a wide range of potential plant configurations with differing design, operability, and control characteristics. Issues to be considered include not only technical requirements but also the need to operate profitably amid cost fluctuations for raw materials, finished products, and energy.

FE systems are described by a variety of computational structures and problems that arise across the plant lifecycle from synthesis (e.g., superstructure optimization) to design (e.g., steady-state and dynamic simulation, high-fidelity process/equipment co-simulation) to operations (e.g., dynamic simulation, process control, real-time applications). In addition, enterprise-wide problems at the highest levels need to be addressed to enable system-wide planning of capacity expansion, production, and distribution.

The FE industry has already invested to excellent effect in R&D on process modeling, simulation, and advanced optimization methods, but many challenges remain. Significant nonlinearities as well as a mixture of continuous and discrete variables can be found in realistic models of plant planning, scheduling, operations, supply, and process synthesis and design. Here a future trend will be increased use of MINLP optimization models where there have been applications in power generation systems, and significant progress is being made for solving larger problems. However, there is little mathematical theory about existence and uniqueness of solutions for general mixed-integer nonlinear optimization problems.

An additional set of computational challenges and opportunities arise because of the non-convex formulations that occur in current FE system models, which result in the possibility of non-unique solutions. Despite progress within the past decade on global optimization methods, current techniques and solvers are often unacceptably expensive for large commercial-scale problems. Finally, an obvious consideration in FE applications is the presence of significant levels of both uncertainty and risk which can be handled using stochastic simulation technology.

To improve the accuracy of FE system design calculations, process simulation can be combined with high-fidelity equipment simulations such as those based on distributed-parameter CFD and custom PDE-based engineering models. The key computational research challenges and opportunity areas for high-fidelity process/equipment co-simulation include reduced-order modeling, parallel co-simulation techniques, and computational strategies for co-simulation optimization and dynamics.

Plug-and-play interoperability of numerical solvers and optimizers in process systems engineering software is facilitated by the process-industry CAPE-OPEN software standards (www.colan.org). Future developments for large-scale FE system optimization will be driven by rapid advances in scientific computing research, both in parallel/distributed computing hardware and in parallel optimization algorithm and software development.

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