Aspen Plus-FLUENT Integration Toolkit

The Aspen Plus-FLUENT Integration Toolkit developed by computational scientists and engineers at the Department of Energy's National Energy Technology Laboratory was recognized by R&D magazine as among the top 100 commercial products introduced this year.

This advanced process simulation technology provides for the first time the level of detail and accuracy needed for virtual power plant simulation. The powerful software enables design engineers to better understand and optimize the fluid mechanics that drive overall process plant performance and efficiency. NETL engineers are applying this technology to reduce the time, cost, and technical risk of developing high-efficiency, near-zero emissions power plants.

NETL on-site researchers developed the simulation technology with funding from the Power Systems Advanced Research Program, in partnership with Fluent Inc., Alstom Power, Aspen Technology, and West Virginia University.

The team named in the award includes Madhava Syamlal (Fluent Inc.) and Steven Zitney (NETL) as submitters, with Woodrow Fiveland (Alstom Power, Inc.), Randy Field (Aspen Technology, Inc.), William Rogers (NETL), Anthony Cugini (NETL), and Kurishinkal Cleetus (West Virginia University) listed as Joint Submitters.

The simulation technology is applicable to a variety of process industries.

The process industries manage some of the most sophisticated and expensive engineered systems in the world, spending on the order of $500 billion annually in plant design, operation, and maintenance. The process industries also face the unique challenge of designing the next generation of chemical, pharmaceutical, petroleum, oil and gas, and power plants to operate with unprecedented efficiency and near-zero emissions, while performing profitably amid cost fluctuations for raw materials, finished products, and energy.

To achieve such performance targets and at the same time reduce the number of costly pilot-scale and demonstration facilities, the designers of future plants must increasingly rely on high-fidelity computer simulations to design and evaluate *virtual plants.* This advanced process simulation product brings together, for the first time, the necessary resolution, speed and accuracy essential for *virtual plant* simulations.

Existing commercial simulation software products used in the process industries employ two main levels of model abstraction: models of the overall process (a forest-level description) and more detailed models of individual equipment items in the process (a tree-level description). To achieve the desired step change in plant efficiency and pollutant reduction, next-generation computer simulations must describe the entire forest without losing sight of the trees. The Aspen Plus–FLUENT Integration Toolkit is a commercial software product that offers breakthrough capability to combine process-level models with detailed equipment-level models.

Process plants typically consist of a large number of equipment items (reactors, turbomachinery, separation and mixing devices, heat exchangers, etc.) interconnected by a complex network of process streams – flows of solid (granular), liquid, and gaseous materials. Existing computational models describe either the entire plant as a network of simplified equipment models (process simulation model) or an isolated equipment item in great detail (equipment model). Over the last 20 years, several widely-used process simulators and equipment modeling software products have been developed and commercialized independently of one another. Today these simulation tools are widely used by the process industries and have radically changed the way that engineers design and optimize plants.

Process simulators perform material and energy balances, thermodynamic calculations, and chemical reaction computations for the entire plant. Such tools are used throughout the lifecycle of the plant for designing the overall plant configuration, evaluating plant economics, analyzing safety and environmental issues, and calculating plant-operating efficiency and performance under start up, shut down, and upset conditions. These tools offer libraries of simplified equipment models, which require input data that are not easily measured and that may change with operating conditions (e.g., pressure drop, heat transfer coefficient, and reactant conversion). Therefore, a plant design based on simplified equipment models may be suboptimal or may violate constraints imposed by a certain equipment item (e.g., local reactor catalyst temperature should not exceed the sintering temperature).

Equipment models, like trees, are diverse. Some custom equipment models are developed by companies to encapsulate the experience from many years of designing and operating the equipment. Many are built using commercially available computational fluid dynamics (CFD) software. Engineers use CFD software to describe the detailed geometry of the equipment and the physiochemical processes that occur in the equipment with rigorous equations. Representative examples include the atomization and drying of a solution injected through a complex arrangement of nozzles in a spray dryer, the reaction between hydrogen and oxygen in the membrane electrode assembly of a fuel cell, the mixing of chemicals as they flow around the moving blades in a mixing tank, the transformations of coal particles in a furnace as they are entrained by air through the combustion chamber and through the boiler tube banks. Equipment models allow designers to optimize specific parameters (e.g., spray nozzle geometry, blade pitch, baffle arrangement, impeller speed, etc.). However, equipment models do not directly consider the effect of the other equipment items in the plant (e.g., the effect of a recycle loop). Therefore, optimizing the performance of an isolated equipment item does not guarantee that a global optimum for the process will be achieved.

Over the years, these two levels of modeling developed as separate activities with little interaction; two different groups of software vendors offer commercial process simulators and CFD packages; two different groups of engineers (process engineers and CFD engineers) use the software, often working in separate departments of companies within process industries. The knowledge generated by one group is at best transmitted manually (and often not at all) to the other group. Questions such as how local fluid flow in a particular equipment item affects other parts of the plant or whether an equipment item will operate within its design limits are answered only in a labor-intensive, iterative, manner, which is highly inefficient.

Differences in "domain knowledge," data sources, and practices for the two levels of modeling have thus created a barrier that has limited the effectiveness and value of simulation. The segregated analysis approach worked satisfactorily in the past because some degree of over design was acceptable. But the stringent new requirement for high-efficiency, reconfigurable, near-zero emission plants calls for a dramatic change in how design and analysis are conducted. There is a growing recognition that a combined holistic and high fidelity approach to plant simulation is essential, which is the challenge we address with our integrated software toolkit.

To ensure immediate and widespread adoption of this software solution, the developers focused on seamlessly integrating two widely-used commercial software products: Aspen Plus® for process simulation and FLUENT® for equipment simulation. Each is the market and technology leader in its respective field. The toolkit was also designed to facilitate the integration of additional simulation tools, such as custom equipment models based on legacy proprietary software (also known as "in-house codes"). Using this powerful combination to incorporate detail exactly where it is most needed, designers can conduct process simulations to a level of detail and

accuracy never before possible. Figure 1 shows how the integration toolkit couples Aspen Plus process simulations, with various equipment models including CFD models (e.g., FLUENT), custom equipment models, and fast reduced-order models (ROMs) based on previously-computed CFD results.

The Aspen Plus – FLUENT Integration Toolkit overcomes the principal barrier to combining process and equipment models: the significant time and effort required to carry out the integration. Since established commercial software was not written with the expectation that the models at different levels of abstraction would be combined, in the past only engineers that understood the two types of models and were adept at computer programming could combine process models with detailed equipment models. In the rare instances when such coupling was attempted two or more months of work was required to couple a CFD model into a process model

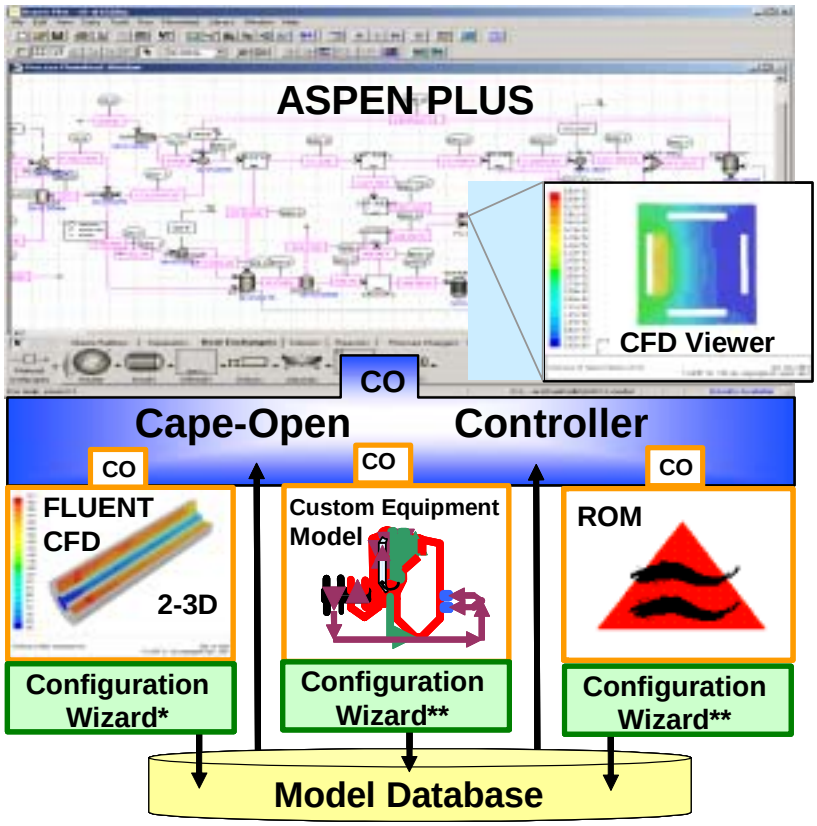

Fig. 1 Aspen Plus – FLUENT Integration Toolkit

using a tailored, one-off approach. Using process-industry open standard interfaces and advanced user aids, the new toolkit reduces the integration time to less than two hours – more than two orders of magnitude improvement!

The Aspen Plus –FLUENT integration toolkit is based on the CAPE-OPEN (CO)[1] standard for interfacing process modeling software components for use in the simulation, design, and operation of processing plants. The toolkit exploits three major classes of CO interfaces—unit operations, physical properties, and reaction kinetics. The CO unit operation interface enables the seamless use (e.g., create, edit, solve) of FLUENT equipment models in the Aspen Plus process flowsheet. This interface also facilitates the bi-directional exchange of stream information (flow rate, temperature, pressure and compositions) between Aspen Plus and FLUENT. The multi-dimensional CFD boundary conditions are mapped automatically to Aspen Plus streams and vice versa. The CO physical property interface is used to transfer constant or temperature-dependent physical properties (e.g., density, viscosity, heat capacity, thermal conductivity, molecular weight) from Aspen Plus to FLUENT. The CO reaction kinetics interface facilitates the automatic transfer of reaction stoichiometry and power-law parameters from Aspen Plus to FLUENT. Use of the CO standard also ensures that any CFD model or proprietary custom model that uses CO interfaces can be linked to the software framework. NETL provides an easy-to-use template for wrapping legacy models as CO-compliant models that can be used in Aspen Plus.

Osawe et al. (2002) presented the details of the integrated software architecture shown in Fig. 1. They also described the use of the CO interfaces for exchanging information between CFD models and process simulation. A recent review of industrial applications of the CO standard, including a brief discussion of the integrated Aspen Plus and FLUENT solution described here, can be found in Pons (2003).

The integration toolkit includes *Configuration Wizards* to help the CFD engineer prepare the various equipment models for use by the process engineer in Aspen Plus. The wizards are used primarily to specify which CFD model parameters (e.g., current and voltage for a fuel cell) and zones (i.e., boundaries) to make available as variables and stream ports, respectively, in Aspen Plus. The configured equipment models are then stored in the *Model Database*.

The integration toolkit has three main graphical user interfaces (GUIs), which are typically accessed by the process engineer in the following order as part of the integrated workflow: 1) *Model Selection GUI*, 2) *Model Edit GUI*, and 3) *CFD Viewer*.

After placing the detailed equipment model icon on the process flowsheet, the process engineer uses the *Model Selection GUI* to browse and select a suitable equipment model from the *Model Database*. Upon selection, the corresponding ports and parameters are automatically associated with the equipment model instantiated on the flowsheet. The process engineer can then connect the appropriate number of input and output streams to the equipment model icon.

The *Model Edit GUI* enables the process engineer to modify parameters for the equipment model. Examples of equipment parameters include the current and voltage for a fuel cell or the impeller speed for a stirred tank reactor. The initial parameter values correspond to those set in the *Configuration Wizard*.

In Aspen Plus, the process engineer interactively runs and monitors the combined simulation which involves an iterative sequential-modular solution process. Aspen Plus controls the integrated simulation and automatically executes the detailed equipment model (e.g., FLUENT) at each flowsheet iteration. The CFD results are saved at each Aspen Plus iteration so that subsequent FLUENT simulations converge more quickly. Stream information, physical properties,

[1] The CAPE-OPEN standard represents over five years of international collaborative work involving more than thirty of the leading process-industry companies, academic institutions, and software vendors in Europe, Asia, and North America. Today the CAPE-OPEN Laboratories Network (CO-LaN, www.colan.org) is the internationally recognized, user-driven organization for the management, exploitation, and dissemination of the CO standard.

and reaction kinetic data are transferred automatically from Aspen Plus to FLUENT by the *Controller* software component. Using the CFD parameter values specified in Aspen Plus, FLUENT computes the flow pattern and chemical species distribution. The weighted averages of the stream variables at each equipment outlet are then sent back to Aspen Plus. This direct coupling of FLUENT and Aspen Plus avoids the time-consuming, error-prone, manual back-and-forth calculations required when a CFD model is embedded in a process recycle loop or heat integration loop.

Upon completion of the integrated simulation, the process engineer reviews the results for streams, blocks (including CFD-based equipment items), and overall convergence in Aspen Plus. The *CFD Viewer* then allows the process engineer to display, within the process simulator, the results of a CFD simulation conducted as a part of an integrated simulation. Typical CFD results include contours of velocity, temperature, pressure, and species mass fractions for a specified surface inside the equipment.

Another significant problem that the Toolkit overcomes is that high-fidelity CFD models take much more computational time than the process simulations based on simplified models. The process engineer often needs to run many simulations in a short period of time; detailed equipment models could lead to unacceptable turnaround times. Developers addressed this barrier by developing a framework for *reduced order models* and *solution strategy*. The *reduced order models* are built automatically from the results of detailed CFD simulations, but are much faster than the detailed model. For example, a simple *reduced order model* is a multi-linear interpolator based on CFD data. Using the *Model Edit GUI*, the process engineer can define a flexible *solution strategy* that uses a hierarchy of simple to complex models to describe an equipment item. For example, one common solution strategy is to have the initial flowsheet iterations use a fast ROM and the final iterations use a high-fidelity CFD model. In addition, FLUENT's parallel solver enables process engineers to compute a CFD solution using multiple processors that may be executed on the same computer, or on different computers in a network.

Table 1 highlights six integrated Aspen Plus and FLUENT applications, including two industrial power generation applications from ALSTOM Power. In a chemical process application, Zitney and Syamlal (2002) coupled a two-dimensional FLUENT CFD model of a stirred tank reactor model into a reaction-separation-recycle flowsheet in Aspen Plus. The integrated simulations are used to determine an optimum shaft speed (CFD model parameter) for maximizing the rate of production of one of the products.

In a fuel cell application, Zitney et al. (2003) recently coupled CFD and process simulations to analyze high-temperature, auxiliary power units (APUs) based on solid oxide fuel cells (SOFCs). A 3D CFD model is used to simulate the fluid flow, heat and mass transfer, electrochemistry, and current distribution in the SOFC. Process simulations are used to perform overall material and energy balances on the tightly integrated APU flowsheet consisting of equipment items such as a reformer, desulfurizer, fuel cell stack, combustor, and various heat exchange and rotating equipment items. Using the FLUENT and Aspen Plus integration toolkit, coupled CFD and process simulations are performed over the current range to generate a voltage-current curve and analyze the effect of current on fuel utilization, current density, power density, and overall process efficiency.

Syamlal et al. (2003) also presented several applications of the integrated process simulation environment to model fuel cell systems. In one example a solid oxide fuel cell (SOFC) is modeled with a CFD-based SOFC model. The Aspen Plus process flowsheet consists of a

reformer, SOFC, post-stack combustor, and heat exchangers. The SOFC model considers the detailed fluid flow, electrochemistry, and current distribution in the fuel cell.

In a second system, a natural gas-based, proton exchange membrane (PEM) fuel cell system is considered. The Aspen Plus flowsheet used for the coupled simulations consists of a reformer, shift converter, fuel cell, anode exhaust combustor, and heat exchangers. The reformer is modeled with a CFD model that calculates the 3D distribution of the flow field, temperature, pressure and concentration in the reactor. When the reformer model is executed from within the fuel cell flowsheet, the CFD model benefits from the ability to account for the effect of recycle streams. The fuel gas is heated with the products of combustion from the anode exhaust burner. The conversion in the reformer is limited by the energy available from the hot gas, which in turn depends upon the conversion in the reformer. Furthermore the feed stream to the reformer is preheated with the outlet stream from the shift converter and the shell outlet gas. The CFD model accounts for the radial variation in the temperature in the catalyst bed (in the tube) and predicts conversions that account for the limitations imposed by the heat transfer to the bed. Another advantage of the coupled CFD model is that the detailed calculations provide the process engineer with information that is important for the overall system design, although it may not be required for the process simulation. In the case of the reformer model, the detailed temperature distribution in the catalyst bed is useful to ensure that the temperature anywhere in the catalyst bed does not exceed the sintering temperature.

Representing industrial power plant applications, ALSTOM Power modeled a conventional 30 MWe coal-fired steam plant for municipal electricity generation and an advanced 250 MW, natural gas-fired, combined cycle (NGCC) power plant (Sloan et al., 2002, 2003). In the conventional steam plant, a FLUENT 3D CFD model represents the gas-side and steam-side of the boiler. An Aspen Plus design specification is used to adjust a FLUENT model parameter, namely the damper position, to control the steam temperature at 763 K. In the NGCC plant, a FLUENT 3D CFD model is used for the heat recovery steam generator (HRSG), which consists of several nested heat exchangers and pollutant control devices. An Aspen Plus design specification is used to adjust the high-pressure pump feed rate to achieve steam temperature of 838 K.

At NETL, work is under way to couple CFD models for key equipment items (see Table 1) into Aspen Plus process simulations of potential FutureGen power plant configurations. The Department of Energy's $1 billion, 10-year demonstration FutureGen project is aimed at creating the world's first coal-based, near zero emissions electricity and hydrogen production power plant.

Table 1. Commercial and Research Applications of Aspen Plus–FLUENT Integration Toolkit

Application Area	Aspen Plus Model	FLUENT CFD Model	Objective	Organization(s)	Reference
Chemical Process	Reaction-Separation-Recycle Flowsheet	Reactor	Optimize overall product purity and yield with respect to impeller speed in CFD reactor	AspenTech; Fluent	Zitney and Syamlal (2002)
Power	Fuel Cell System	Reformer; Solid Oxide Fuel Cell	Analyze system performance and heat integration	AspenTech; Fluent	Syamlal et al. (2003)
Power	Fuel Cell System	Reformer; Proton Exchange Membrane Fuel Cell	Analyze system performance and heat integration	AspenTech; Fluent	Syamlal et al. (2003)
Power	Fuel Cell Auxiliary Power Unit	Solid-Oxide Fuel Cell	Optimize overall process efficiency with respect to fuel cell current	National Energy Technology Laboratory; Fluent	Zitney et al. (2003)
Power	30 MW Coal-Fired Power Plant	Boiler	System analysis; Use Aspen Plus design spec to adjust FLUENT CFD model parameter damper position (bypass resistance) to control steam temperature	Alstom Power	Sloan et al. (2002, 2004)
Power	250 MW Natural Gas Combined Cycle Plant	Heat Recovery Steam Generator	System analysis; Use Aspen Plus design spec to adjust high-pressure pump feed rate to achieve desired steam temperature	Alstom Power	Sloan et al. (2002, 2004)
Power	FutureGen Power Plant (IGCC with CO2 Capture)	Gasifier; Gas Turbine Combustor; Heat Recovery Steam	Analyze system performance	National Energy Technology Laboratory	Work in progress

		Generator			