## 2.16 Modeling and Simulation of Processes


Presented below are a variety of simulation and modeling software categories and a partial list of their suppliers.

<table>
<thead>
<tr>
<th>Category</th>
<th>Software</th>
<th>Supplier</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steady State to Design Complex Chemical Processes:</td>
<td>ASPEN plus</td>
<td>Aspen Technology, Inc. /www.aspentech.com/</td>
</tr>
<tr>
<td></td>
<td>CHEMCAD</td>
<td>Chemstations, Inc. /www.chemstations.net/</td>
</tr>
<tr>
<td></td>
<td>Design II</td>
<td>WinSim Inc. /www.winsim.com/</td>
</tr>
<tr>
<td></td>
<td>gPROMS</td>
<td>Process Systems Enterprise Ltd. /www.psenterprise.com/</td>
</tr>
<tr>
<td></td>
<td>HYSYS</td>
<td>Hyprotech, Ltd. /www.hyprotech.com/</td>
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<tr>
<td></td>
<td>PEGS</td>
<td>CADcentre Ltd. /www.energyweb.net/OSO/</td>
</tr>
<tr>
<td></td>
<td>Pro II</td>
<td>SIMSCI-ESSCO division of Invensys /www.simsci.com/</td>
</tr>
<tr>
<td></td>
<td>ProChem</td>
<td>OLI Systems, Inc. /www.olisystems.com/</td>
</tr>
<tr>
<td></td>
<td>SIMSMART</td>
<td>Simsmart Inc. /www.ahtco.com/</td>
</tr>
<tr>
<td></td>
<td>VisualModeler</td>
<td>Omega Simulation Co, Ltd. /www.omegasim.co.jp/</td>
</tr>
<tr>
<td></td>
<td>HYSYS RTO</td>
<td>Hyprotech, Ltd. /www.hyprotech.com/</td>
</tr>
<tr>
<td></td>
<td>cc-Dynamics</td>
<td>Chemstations, Inc. /www.chemstations.net/</td>
</tr>
<tr>
<td></td>
<td>DynaChem</td>
<td>OLI Systems, Inc. /www.olisystems.com/</td>
</tr>
<tr>
<td></td>
<td>DYNSIM</td>
<td>SIMSCI-ESSCO division of Invensys /www.simsci.com/</td>
</tr>
<tr>
<td></td>
<td>gPROMS</td>
<td>Process Systems Enterprise Ltd. /www.psenterprise.com/</td>
</tr>
<tr>
<td></td>
<td>HYSYS Dynamics</td>
<td>Hyprotech, Ltd. /www.hyprotech.com/</td>
</tr>
<tr>
<td></td>
<td>VisualModeler</td>
<td>Omega Simulation Co, Ltd. /www.omegasim.co.jp/</td>
</tr>
<tr>
<td>Dynamic to Design Specific Unit Operations in Batch Processes:</td>
<td>cc-Batch</td>
<td>Chemstations, Inc. /www.chemstations.net/</td>
</tr>
<tr>
<td></td>
<td>BatchCAD</td>
<td>Hyprotech, Ltd. /www.hyprotech.com/</td>
</tr>
<tr>
<td>Dynamic for Custom Simulation:</td>
<td>acsXtreme</td>
<td>AEGis Technologies Group Inc. /www.acsxtreme.com/</td>
</tr>
<tr>
<td></td>
<td>ANSYS Multiphysics</td>
<td>ANSYS Inc. /www.ansys.com/</td>
</tr>
<tr>
<td></td>
<td>Custom Modeler</td>
<td>Aspen Technology, Inc. /www.aspentech.com/</td>
</tr>
<tr>
<td></td>
<td>MatLab-SimuLink</td>
<td>MathWorks Inc. /www.mathworks.com/</td>
</tr>
<tr>
<td>Real Time for DCS Configuration Checkout and Operator Training Systems:</td>
<td>Autodynamics</td>
<td>Trident Computer Resources Inc. /www.tridentusa.com/</td>
</tr>
<tr>
<td></td>
<td>DYNSIM</td>
<td>SIMSCI-ESSCO division of Invensys /www.simsci.com/</td>
</tr>
<tr>
<td></td>
<td>MIMIC</td>
<td>MYNAH Technologies division of Experitec, Inc. /www.mynah.com/</td>
</tr>
<tr>
<td></td>
<td>XANALOG NL-SIM</td>
<td>Xanalog Corporation /www.xanalog.com/</td>
</tr>
<tr>
<td>Dynamic to Optimize and Estimate Parameters for Continuous Systems:</td>
<td>ACSL optimize</td>
<td>AEGis Technologies Group Inc. /www.acsxtreme.com/</td>
</tr>
<tr>
<td></td>
<td>SIMUSOLVE</td>
<td>Dow Chemical Co.</td>
</tr>
<tr>
<td>Dynamic to Optimize and Estimate Schedules for Discrete Systems:</td>
<td>GPSS/H</td>
<td>Wolverine Software Corp. /www.wolverinesoftware.com/</td>
</tr>
<tr>
<td></td>
<td>SLAM</td>
<td>Advanced Planning &amp; Scheduling division of Frontstep /www.pritsker.com/</td>
</tr>
</tbody>
</table>
Some of the benefits of simulation are listed in Table 2.16a. Simulation has an expanding role in many aspects of industrial production, including research, design, operations, maintenance, and regulatory compliance.

### TYPES OF SIMULATIONS

Dynamic simulations are employed to obtain test results more rapidly, less expensively, and in a more controlled environment than through laboratory experimentation. Simulations can model both chemical and biological systems. They can be used to significantly narrow the range and detail of the types of experiments needed in chemical and biochemical research. Custom simulations typically numerically integrate the differential equations that were set by the user.

### Steady-State Simulation

Steady-state simulations are extensively used for process design and optimization and provide data for process flow sheets in terms of material and energy balances. They are also used to design process equipment such as heat exchangers, reactors, and distillation columns. These simulations usually consist of blocks of unit operations interconnected by the user and of physical property data for the chemical components of input streams specified by the user.

### Dynamic Simulations

*Dynamic discrete simulations* are run to optimize schedules to maximize throughput and minimize equipment requirements for batch processes, inventory management, and parts manufacturing and assembly. These simulations sequence an event list detailed by the user, provide random numbers for stochastic models, and accumulate statistics. *Dynamic continuous simulations* enable users to improve control system design strategies to reduce control-loop errors, reduce startup time, and improve on-stream time. These simulations are similar in construction to those used for experimental design except that they provide a library of functional blocks or subroutines to model the more common types of process equipment and instrumentation. Consequently, iteration of the dynamic solution is usually unnecessary.

### Real-Time Simulations

*Real-time simulations* are run to debug configurations and train personnel in the use of distributed control systems (DCS) and programmable logic controllers (PLC). These simulations are essential to smooth commissioning, continuing operation, and maintenance of the systems. They were first extensively used in utility power plants. Their benefits are realized not only in improved process and control system performance but also in greater safety.

Operations, maintenance, and control system responses to various scenarios of disturbances or to equipment and instrument failures can be examined quickly and repetitively. Simulation can be used to reduce safety interlock trips through human factors engineering. Simple or small-scale simulations have been configured into various DCS software packages to eliminate the need for an external computer, its associated interface, and wiring or serial communication. Expansion of simulations to develop the detailed response of large complex processes demanded the use of dedicated external computers and either the emulation of the controls or the development of serial communication with them. The increased power of personal computers and workstations has

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**TABLE 2.16a**

<table>
<thead>
<tr>
<th>Function</th>
<th>Type</th>
<th>Benefits</th>
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<tbody>
<tr>
<td>Experiment design</td>
<td>Dynamic iterative</td>
<td>Better, fewer experiments and faster research</td>
</tr>
<tr>
<td>Process design</td>
<td>Steady state</td>
<td>Faster design and better process performance</td>
</tr>
<tr>
<td>Equipment design</td>
<td>Steady state</td>
<td>Faster design and better equipment performance</td>
</tr>
<tr>
<td>Event optimization</td>
<td>Dynamic discrete</td>
<td>Better utilization, less equipment, more capacity</td>
</tr>
<tr>
<td>Controls design</td>
<td>Dynamic continuous</td>
<td>Faster design and better control-loop performance</td>
</tr>
<tr>
<td>Controls test</td>
<td>Dynamic real time</td>
<td>Safer and faster startup and greater onstream time</td>
</tr>
<tr>
<td>Sequence test</td>
<td>Dynamic real time</td>
<td>Safer and faster startup and greater onstream time</td>
</tr>
<tr>
<td>Interlock test</td>
<td>Dynamic real time</td>
<td>Safer and faster startup and greater onstream time</td>
</tr>
<tr>
<td>Operator training</td>
<td>Dynamic real time, custom or generic</td>
<td>Safer and faster startup and greater onstream time</td>
</tr>
</tbody>
</table>
facilitated the migration of simulation applications to PCs from
general-purpose computers. Whatever computing hardware is
used, the benefits are significant. It has been found that it is
20 times faster to correct a program error on a simulator than
to correct an error in the field.9

New packages are emerging to systematically screen all
possible discrete input and output combinations for valid
patterns or exceptions and search for common mode failures
in safety shutdown systems, as well as to provide dynamic
simulation of plant operation. These packages detect both
supplier and user software errors to provide a comprehensive
verification of software integrity and reliability.

Although software cannot be proven to be bug-free, sim-
ulations can go a long way toward reducing software errors
to a safe level and ensuring compliance with environmental
and safety regulations.

The implications of the management of change dictated
by the Occupational Safety Health Act’s (OSHA) Process
Safety Management Center are greater than realized by most
participants in the process industry. The documentation
requirements of the initial design are just the tip of the ice-
berg, as illustrated by Figure 2.16b. The identification and
incorporation of changes in existing and new plants require
a very large effort that will demand new tools, such as the
integration of simulation and computer-aided design with
DCS or PLC configurations.

Part of the attractiveness of DCS and PLC is their ability
to readily accommodate changes to improve plant operations.
Although heaviest during the test and commissioning of the
system, the ongoing effort to improve the configuration
increases as we proceed with more and more automation. The
number of configuration parameters, which can be adjusted
manually and automatically, rises exponentially as systems
move toward the “Horizon” plant concept. In this system,
routine operator actions have been eliminated and the opera-
tor’s role is elevated to the higher technical role of process
optimization.10 The motivation for the “Horizon” plant is not
manpower reduction but a step improvement in product quality,
on-stream time, yield, and safety. Simulation is a key prereq-
usite for such a plant.

**Generic Real-Time Simulations**

Generic real-time simulations are used to train operators for processes such as ammonia
production. Packages have been developed for many of the
more common hydrocarbon processes. The packages can be
modified to include the user’s instrument tag numbers, scales,
and control system. For those systems that emulate the control
system, the user’s interface is also mimicked by the package.
The emphasis is not on addressing the peculiarities of the
plant or control system for an individual application but is
more on the familiarization of operators with general process
behavior.

These models represent years of process knowledge, sim-
ulation development, and improvement. The benefits are sig-
ificant and have led to such statements as, “Two days on a
simulation is worth several years of training in a control
room.”11 Such models usually provide more realistic process
interactions and simulation control options than do custom-
built simulations.12–14 An effective plant training center uses
a variety of generic and project-specific simulations.15

**STEADY-STATE SIMULATIONS**

Steady-state simulations for process design are much more
rigorous in the employment of chemistry and chemical engi-
neering principles than are dynamic custom simulations writ-
ten in software such as ACSL and MatLab, which are based
on setting up and numerically integrating differential equa-
tions. Most of the newer steady-state simulation software pack-
ages now allow the user to graphically configure the model as
a process flow diagram (PFD).

A new class of PFD-based dynamic simulation software,
such as Aspen Dynamics, DYNSIM, CC-Dynamics, gPROMS,
HYSYS Dynamics, and Visual Modeler, has also emerged that
has a process fidelity as good as that of the steady-state models
used to design processes. However, real-time simulations for
configuration checkout and operator training and to optimize
business decisions and scheduling generally lack the sophis-
tication of physical property database integration found in
the PFD simulators. Some exceptions are HYSYS OTS16 and
RTO17, which are extensions of HYSYS Dynamics.

Steady-state simulators, while primarily for process
design, can accurately estimate the steady-state process
gain, which is important for control-loop analysis and tun-
ing. Multiple runs are made to show changes in the con-
trolled variable in response to changes in the manipulated
variable. Since most processes exhibit nonlinearities in their
operating points and direction, the simulation runs are made
for changes in both directions around the projected set
point.

For distillation column control, these runs are used to
select the best location of the control tray for temperature
control. The selected tray is the one that shows the largest
and most symmetrical change in temperature for a change in
distillate-to-feed ratio. For pH control, these runs are used to
generate a titration curve (a plot of pH versus the ratio of
reagent to influent flow). The titration curve is critical for assessment of system difficulty, control valve selection, signal linearization, set point selection, and controller tuning (for further discussion of pH control, see Chapter 8).

For column temperature control, the point with the highest process gain (sensitivity) is sought because the measurement sensitivity is normally low, and the temperature measurement error can translate to a significant composition error. For pH control, the point with the lowest process gain is sought because near neutrality the measurement sensitivity is normally extremely high, and large oscillations in pH can result from imperceptible fluctuations in reagent or influent flow or composition. The process gains are computed by taking the change in temperature and pH at set point and dividing these by the change in distillate and reagent flow, respectively.

Software Packages

The steady-state process flow diagram (PFD) simulators have integrated extensive physical property packages and/or provided links to the American Institute of Chemical Engineering (AIChE) DIPPR, the British PPDS, and the German DEHEMA data compilations. Some also provide the ability to model polymer and electrolyte systems.

ProChem extensively and rigorously models the equilibrium of ionic species in aqueous solutions (electrolyte systems). It is useful for accurately modeling the compositions and pH of waste streams to meet environmental regulations for surface discharges and deep wells. It is not well known that dissociation constants significantly change with temperature and are expressed in terms of activities and not concentrations.

ProChem can compute the change in dissociation constants with temperature and the change in activity from ionic interaction (data that is usually not available). Thus, ProChem can generate titration curves that include the effects of temperature and ionic strength for complex mixtures and are extremely useful for pH control system design.

ProChem is actually a package of programs such as ElectroChem (single-stage electrolyte model), DynaChem (dynamic model), FraChem (multistage electrolyte and reaction model), ReaChem (single-stage nonelectrolyte continuous stirred reactor model), ScaleChem (scale formation tendency model), TransChem (chemical upsets to natural geological formation model), and DataChem (data bank manager). Environmental Protection Agency (EPA) and international lists of chemicals of environmental concern and a process analysis section have been added to create an Environmental Simulation Program (ESP).

Dynamic Simulations

Dynamic simulations are used to model systems that are in transition to or from a steady state or that are in a state of flux and consequently never reach a steady state. Thus, they are used to investigate biological systems, upsets, failures, and startup/shutdown conditions for continuous processes, batch process conditions and scheduling, discrete manufacturing, fiber-spinning viscoelastic effects, and control system behavior.

The art of dynamic simulation is related to the need for economy. Since custom dynamic simulations numerically integrate and normally require significant original effort, the process detail must be less than that used in steady-state simulations. Similarly, the details of instrumentation and control system dynamics also need to be reduced.

The new class of PFD-based dynamic simulations and the virtual plant have as much or more process detail than do the steady-state simulations used to design the process and can be interfaced to the actual control system configuration. However, these are generally lumped models with perfectly mixed volumes, which means that transportation and mixing delays must be added.

The art is to know, a priori, what is and is not important to include. Since loop performance heavily depends on total loop dead time, it is critical to seek out all the major dead-time contributors. The tendency is to concentrate on the dead-time contributions from process equipment and neglect the potentially larger sources of dead time shown in the block diagram for a pH loop in Figure 2.16c. For example, the dead time from reagent piping transportation delay and control valve dead band and stick-slip are significantly larger than the dead time from mixer turnover time for well-designed neutralizers (see the section on pH control in Chapter 8).

Differential equations set up for dynamic simulations are based on the principle of conservation of mass, energy, momentum, spin, and charge (the conversion of mass to energy for nuclear reactions will not be addressed). The net accumulation of these quantities at any point in the process is the integral of the net difference between the input and output, as shown in Figure 2.16d. For steady-state simulations, the output equals the input, so the accumulation and hence the process variable is constant.

There may be multiple inputs and outputs in various forms or phases. These need to be converted to common dimensions and summed. For example, inputs and outputs for a mass balance would be mass flow (e.g., pounds per hour) and would include vaporization, condensing, reaction, precipitation, and crystal growth rates besides stream flows.

Inputs and outputs for an energy balance would consider the energy flow (e.g., BTUs per hour), and the simulation model would include heat transfers, heats of reaction multiplied by reaction rates, heats of dilution and neutralization multiplied by reagent flows, heats of vaporization multiplied by vapor flows, and heats of condensation multiplied by condensing rates, plus the sensible heats of streams multiplied by flow rates. The various heat terms are functions of temperature.
Temperature and Vaporization

Temperature processes are simulated by the segmentation of the equipment into volumes, each described by an individual differential equation for an energy balance. The temperature is the energy accumulation divided by the product of the mass and heat capacity of the contents. The smaller the volume, the greater the accuracy. The division into volumes should be greatest where the temperature changes are the largest.

For example, a heat exchanger would be split into volumes for the tube side fluid, the tube wall metal, and the shell side fluid. For counterflow exchangers, either the initial coolant temperature profile must be known or an iterative search should be done for the exit coolant temperature that gives the right inlet coolant temperature. For boiling mixtures, the boiling point as a function of pressure and composition is computed. When the temperature rises to the boiling point, vaporization starts in proportion to the net heat input (BTUs per hour) from streams and heat transfer surface areas divided by heat of vaporization (BTUs per pound).

Vaporization also occurs due to humidification. For scrubbers and textile air washers, the outlet air can be assumed to be saturated. The mole fraction water content of the exiting air can be estimated by dividing the partial pressure of water as a function of pressure and composition is computed. When the temperature rises to the boiling point, vaporization starts in proportion to the net heat input (BTUs per hour) from streams and heat transfer surface areas divided by heat of vaporization (BTUs per pound).

Pressure and Water Hammer

Gas pressure processes are simulated by segmentation of the system into volumes, each with an individual differential equation for a mass balance. The pressure is computed from the mass accumulation via the ideal gas law and hence depends on the compressibility factor, molecular weight, temperature, and volume of the gas. For vapor spaces above solids and liquids, the gas volume changes with level. For furnace pressures of a few inches of water column, a temperature change can cause the measurement to go off scale, because the interaction between the energy and material balances is significant.

Liquid pressure processes are simulated by the use of pump curves and profiles of pressure drops through the system. The pump discharge pressure is computed from the curve for changes in speed or control valve position. The new pressure drops are proportional to the new flow rate squared, divided by the initial flow rate squared, and that ratio multiplied by the initial pressure drop. The new pressure drop determines a new intersection point of the system drop with the pump curve for variable speed pumps or a new pressure drop for a throttling control valve.

An algebraic loop is created, which is typically broken by the addition of a filter to simulate the gradual response due to impeller inertia, fluid inertia, and/or control valve actuator characteristics. Algebraic loops occur in a model when differential equations are omitted, and they create numerical instability unless a filter is added.

The simulation of water hammer, shock waves (i.e., pressure waves that travel at the speed of sound through the fluid), compressor surge, and the viscoelastic effect of fiber spinning requires the use of a momentum balance. The dynamics are extremely fast and require small integration step sizes. Momentum balances often create stiff systems (i.e., systems
with relatively fast and slow dynamics) that require special variable order and step size integration methods to prevent excessively long run times.

**pH and Solubility**

The simulation of pH requires a component mass balance for each ionic species and for the solvent. The solvent and component concentrations and dissociation constants are substituted into an equation for a charge balance, and interval halving is used to search for the pH value that gives a net charge of zero for the volume. For greater accuracy, activities instead of concentrations should be used, the dissociation constants should be made a function of temperature, and electrode alkalinity and acid error should be included in the measurement response.

Precipitation processes require a solubility calculation based on temperature and concentrations in the liquid phase. Thus, they necessitate energy and component balances. When the solute concentration goes above or below the solubility limit, the precipitation and dissolution rate, respectively, proceed as fast as permitted for numerical stability.

**Sensors, Transmitters, and Final Control Elements**

The response of a variable speed drive or the stroke of a control valve is simulated by a velocity-limited filter. For the control valve there is also a prestroke dead time associated with the filling and exhausting of air from the actuator, and a dead time caused by dead band. The prestroke dead time is usually negligible, except for large actuators with accessories (e.g., air sets, solenoid valves, current-to-pneumatic transducers, or positioners) with small flow coefficients.

The dead time from dead band is often significant and is calculated by dividing the dead band by the rate of change of controller output. It is simulated by the use of a backlash functional block. Control valves with excessive friction, breakaway torque, or dynamic unbalance can exhibit stick-and-slip action. This is simulated by use of a stroke quantizer block.

The dead times of chromatographs and digital transmitters and the dead times caused by the scan, cycle, and update times of digital controllers are simulated by delay blocks. The dead times from transportation delays for plug flow, conveyors, pipelines, and sampling lines are also simulated by use of delay blocks, but their delay times are a function of the throughput. A decrease in time delay can be handled bumplessly, but an increase does pose some computational difficulties. Most users pick a conservative fixed delay time.

The damping settings of sensors and transmitters are simulated by the addition of filters. For temperature and pH sensors, the time constant is variable. It depends upon such operating conditions as fluid velocity and process coatings, and the direction and magnitude of the change. Filter time constants can be bumplessly updated.

**Simulation Languages**

The Advanced Continuous Simulation Language (ACSL) will sort the equations in the dynamic section for integration and will identify any algebraic loops. It has many different integration methods and functional blocks. There are no blocks for unit operations, so users must develop their own library of macros and FORTRAN subroutines for process models. Also, the user must construct an extensive steady-state section for a starting point.

**REAL-TIME SIMULATION**

Real-time simulation connects a simulation of the process to the actual control system. Consequently, the control strategies, proportional–integral–derivative (PID) algorithms, filter time constants, and update, cycle, and scan times do not need to be simulated. It would be difficult to get enough information on proprietary PID algorithms with antireset windup protection and integral tracking options to do a good job of simulating their action. Thus, the use of the actual control system considerably reduces the simulation burden.

The wiring (documentation and installation) of a large simulation system to a control system can take as much time as the construction of the simulation. Most new systems use a high-speed serial communication link from the computer, which directs the simulation and the controller. Here the computer functionally replaces the input and output (I/O) wiring to the field, as shown in Figure 2.16e.

In other words, the same I/O channel assignments are used and the configurations are unaltered so that it is transparent to the controller whether it is connected to the actual plant or to a simulation. This setup as depicted for a combined DCS and PLC system is best from a standpoint of checking the entire control system as it will be used in actual operation.
The use of the DCS data highway for the serial link is not advised because the data flow rate for fast loops will bog down the highway.

When the purpose of real-time simulations is to train operators, the emphasis is more on process rather than on familiarity with the control system. One can then emulate the control system to eliminate the need for communication links and control system hardware.

Real-time integration uses a fixed step size equal to the cycle time of the simulation. Consequently, the step size is too large to simulate fast pressure dynamics or use momentum balances. The gas volumes are increased or calculations similar to those for liquid pressure dynamics are used to achieve numerical stability. Compressor surge is simulated by following the negative slope and jumping over the positive slope portions of the characteristic curve and by the use of a filter to break the algebraic loop between compressor flow and discharge pressure.

The simulation is speeded up or slowed down by the multiplication of the derivative by a gain factor adjustable by the user. The filling and emptying of tanks are often speeded up to test batch operations. Also, the subroutine for integration can be set up to detect a change between the present and last accumulation that is larger than what is possible, and will substitute this as the new desired operating point. This gives the user the ability to make step changes in the operating point. This is particularly useful for batch operations where it is desired to change tank levels to start or retry sequences.

The running of a simulation connected to a control system other than real time will not show the true response of a control loop unless the PID algorithm speed is adjusted and the same ratio is maintained between loop dead time and time constant. This means that all delay times and time constants need to be scaled to simulation speed.

**FUTURE TRENDS**

The management of change and the desire for increased automation and design efficiency will be the impetus for integration of simulation, computer-aided design (CAD), and DCS or PLC configurations. The goal will be to enter a minimal amount of data (eventually this will be done graphically) and have an integrated system generate the documentation, simulations, control strategy, and interlock configurations required for implementation.

For example, a CAD drawing of the process flow diagram (PFD) with input streams might generate a steady-state simulation of the process that would fill in missing operating conditions and output stream compositions on the PFD. The PFD would in turn generate the skeleton for the piping and instrument diagrams (P&ID). The steady-state simulation would initialize a dynamic simulation whose controlled and manipulated variables would be set by instrumentation added to the P&ID.

The dynamic simulation would consist of two parts, the field and the control strategy. The field data source would be the P&ID, and the control strategy and the safety interlock system data source would be a graphical representation of the DCS or PLC configurations. The dynamic simulation of the strategy and interlocks would migrate to the actual configuration of the DCS or PLC used for real-time control. The dynamic simulation of the field would be designed to prove that the DCS or PLC configuration is wrong rather than to prove that it is right.

Specifically, the control system configuration would not generate the field portion of the dynamic simulation. Toward this end and to reduce common mode failures and to prevent frequent changes to the configuration from affecting the field simulation, the sources of the two parts of the simulations would be kept separate. Similarly, the interlock and control strategy configurations would be separated. These separations would be done by software rather than hardware because the continual increase in reliability and power of computers and the need for fast coordination will push the trend toward integration within a single computer for an operating unit.

Thus, the control strategy and interlock documentation, dynamic simulation, and configuration before and after commissioning would be generated by graphical entry of the configuration. The dynamic simulation would be run faster than real time for control system studies and for accelerated control system testing or operator training. The flow of information for integration is shown in Figure 2.16f.

It is possible that neural networks (Section 2.18) will be used in conjunction with first-principle dynamic models to efficiently predict complex nonlinear effects and that rules and fuzzy logic will be used for more qualitative relationships. Equations from chaos theory may generate data that are not possible to obtain from a deterministic approach. These simulations would run online faster than real time to project future failures and violations of operating
constraints that will facilitate global online optimization of processes.\textsuperscript{20}

**VIRTUAL PLANT**

Virtual plants are the models and the seamless extension of the actual process and control system design. The dynamic process model must be the steady-state model used to design the process with just volumes and valves added, and the control system must be the actual configuration running in the DCS. The configuration from the DCS can be downloaded into the virtual plant and vice versa. This concept ensures maximum fidelity and eliminates errors from duplication, emulation, and simplification.

The virtual plant becomes a dynamic warehouse of process and control system knowledge. This knowledge can be used for fast prototyping and opportunity assessment in addition to the conventional uses of configuration checkout and operator training.\textsuperscript{21} The virtual plant can be operated under conditions that might be considered hazardous for the actual plant. This provides an opportunity to explore new operating regions and methods for model predictive control and real-time optimization.\textsuperscript{22}

**References**


**Bibliography**