Leverage Dynamic Process Simulation

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Dynamic simulations are able to replicate actual plant behavior, making them valuable for plant design, operation, optimization, and training.

Chemical process simulation enables engineers to identify the stable and reproducible operating conditions that help attain acceptable product purities, reaction yields, and cycle times. These simulations give companies and facilities the insight needed to comply with safety and environmental regulations and estimate process economics.

While continuous processes are usually studied with steady-state simulation, batch and semi-batch processes require dynamic simulation. Steady-state simulations can be adapted to predict dynamic behavior by carrying out a series of runs, sensitivity studies, and optimizations, but they do not allow a detailed study of all interactions. Dynamic simulations based on real-time or accelerated-time principles can represent actual plant behavior.

This article reviews the benefits and potential of dynamic process simulation in plant design, operation, optimization, and training.

Dynamic simulation overview

In addition to all of the basic steady-state features of a process, a dynamic simulator includes dynamic unit operations, such as dead time and capacity characteristics, and enables properties and components to be manipulated with respect to time.

Dynamic simulations may be real-time or accelerated and are based on process characteristics. The calculation step time depends on the process dynamics. For example, a relief valve's discharge behavior may require a run time on the order of minutes and a step size of seconds, whereas a batch reactor's discharge behavior may require a run time of hours and a step size of minutes.

Dynamic simulations are often used to model process routing, sequential operations in a batch process, material transfers in a pipe network, and emergency relief and blowdown systems, as well as to assess the risks of an equipment failure and identify hazardous conditions.

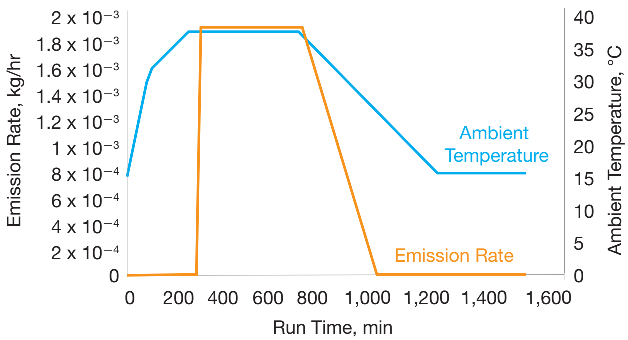
A dynamic model of a continuous process can indicate the impact of varying throughput, startup and shutdown, feed and composition changes, troubleshooting, control loop tuning, and real-time optimization. A dynamic simulation of a batch process can be used to study reaction kinetics and thermal performance of a stirred-tank reactor, the effect of batch distillation cut decisions and control strategies, and the suitability of emergency relief systems.

Process equipment such as vessels, columns, stirred-tank reactors, pumps, controllers, and control valves can all be simulated. A full and accurate dynamic model requires detailed information, but a model that provides some valuable insights can still be built with only basic knowledge of control system technology.

Dynamic simulations may also be used to simulate:

• vessel geometry and orientation in various thermal modes

- packed-bed and plate column geometries in various modes
- stirred-tank reactor geometry with jacket and coil configurations in various modes



▲ **Figure 1.** A dynamic simulation can predict emissions from storage tanks due to ambient temperature changes, referred to as diurnal breathing.

- variable-speed pumps and performance curves
- complex pipe network behavior, including two-phase and slurry flows
- controllers manipulating control valves
- control valves of different sizes, ranges, or operation characteristics, as well as connections to a controller.

Most process and equipment parameters in a model can be adjusted and monitored by connecting the model to Microsoft Excel or a supervisory control and data acquisition (SCADA) system.

Dynamics without process control

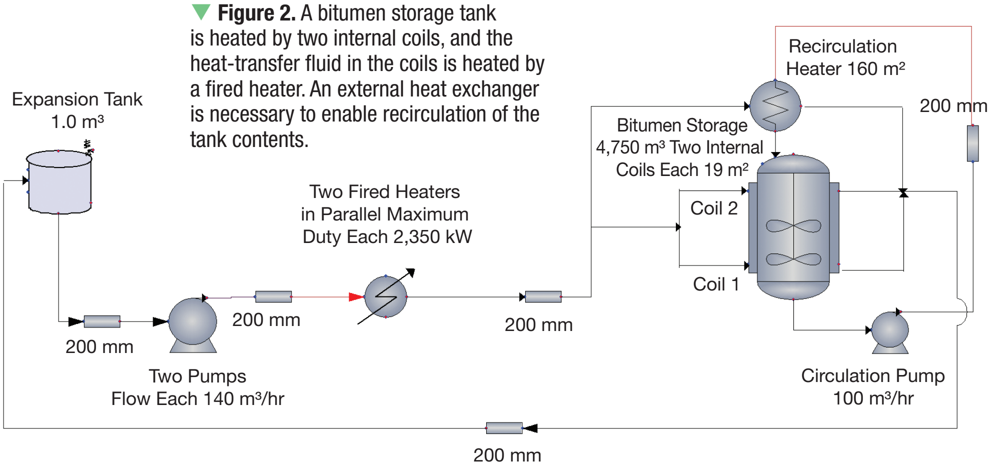
Dynamic simulation can model process behavior without the need to consider process control. Many plant operations that involve material transfer and safety considerations can be suitably studied and analyzed without simulating the control strategy.

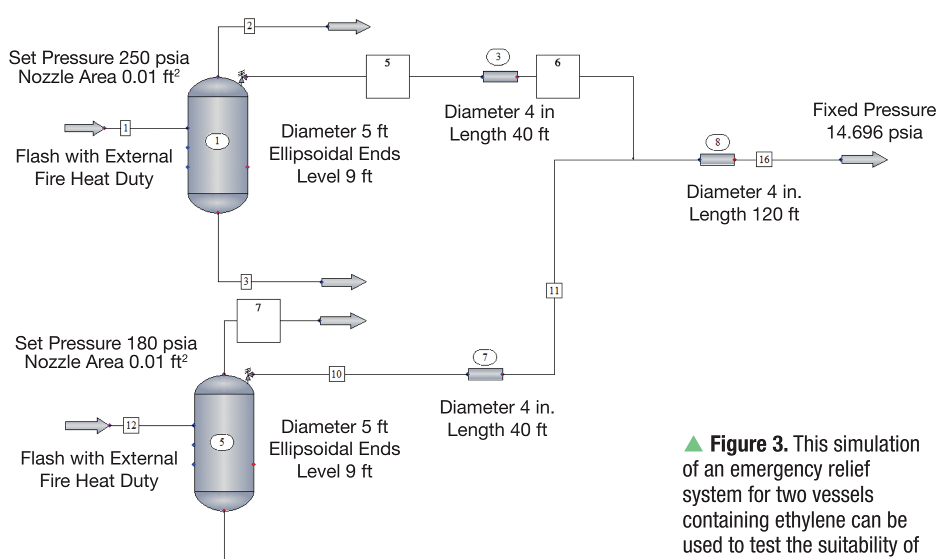
Tank farm operations and diurnal breathing. Tanker truck offloading, filling, and transfers are among the most frequent operations carried out in storage and process facilities. Dynamic simulation can inform the design and operation of associated pumps and pipes, estimate transfer times, balance tank levels, and sequence operations. Simulations may also describe the behavior of viscous fluids in heat-traced piping and two-phase flow regimes.

Tank farms and material transfers contribute to facility emissions. A dynamic simulation can predict volatile component material losses to the atmosphere and discharges to treatment facilities during material transfers or due to diurnal breathing (Figure 1).

Storage tank heating. Dynamic simulations can help engineers size tank coils, heat exchangers, and pipe networks, as well as assess system thermal performance. For example, consider a storage tank for bitumen that is fitted with two internal coils

▼ **Figure 2.** A bitumen storage tank is heated by two internal coils, and the heat-transfer fluid in the coils is heated by a fired heater. An external heat exchanger is necessary to enable recirculation of the tank contents.





▲ **Figure 3.** This simulation of an emergency relief system for two vessels containing ethylene can be used to test the suitability of the vent header size.

that maintain a temperature of 175°C at ambient conditions as low as –10°C (Figure 2). A fired heater supplies a heat-transfer fluid to the coils at 240°C, with a return temperature of 225°C. An external heat exchanger enables recirculation of the tank contents to provide additional heating capacity in the event of a low-temperature shipment. The time between offloading a shipment and loading to a road tanker needs to be minimized. The simulation can predict this time, considering varying shipment offload temperatures, bitumen type, and ambient temperature. The simulation in Figure 2 determined that each coil should have an area of 19 m^2 and the tank a volume of 4,750 m^3.

Dynamic charts and graphs produced by a simulation can present component physical properties (*e.g.,* viscosity), design data (*e.g.,* heat-transfer coefficients), and equipment parameters (*e.g.,* storage vessel temperature).

Emergency relief. While emergency systems are designed in accordance with industry standards and regulations, it is advantageous to ensure their functionality before they are tested during operation. The simulation shown in Figure 3 investigates the dynamic relieving behavior of two identical vessels containing the single component ethylene when subjected to a coincident external fire, with the heat input based on API 520/521 *(1, 2)*. The model tests the suitability of the vent header under coincident relieving conditions, and can also be used to check the impact of two-phase flow, line pressure drops, and variable backpressure. The simulation is based on a relief valve with a specified area and vessel and vent flow in accordance with homogeneous equilibrium models *(3)*.

The suitability of the header design is determined by ensuring that the pressures at the relief valve exits do not exceed the calculated critical flow backpressure. This critical backpressure depends on design relief pressure, composition, relief valve type, and pressure at the discharge point. The simulation results show that under all dynamic conditions of two-phase flow, the coincident pressures at the relief valve exits do not exceed the critical backpressure for the system (Figure 4).

Batch distillation (4). Batch distillation dynamic simulations can be run in various operating modes, with cuts controlled based on time or component composition specification in the distillate or receiver. Batch distillation may be operated at reduced pressure to help achieve the desired separation, reduce the operating temperature to reduce costs, or process temperature-sensitive materials. Other typical batch distillation modes include:

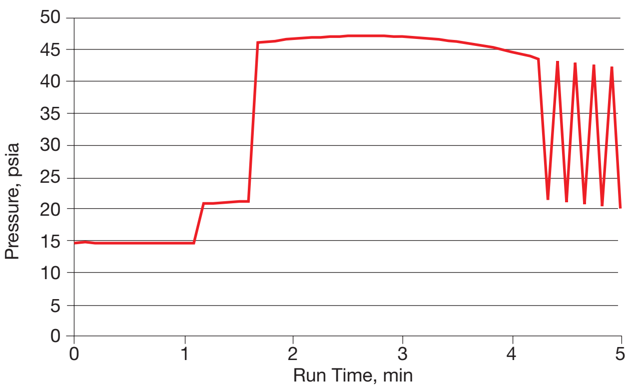
• Constant-reflux-ratio operation provides varying overhead composition. Distillation continues until the desired composition is achieved in the still or the distillate receiver.

• Constant-overhead-composition operation is achieved by varying the reflux ratio. As the distillation proceeds, the still is depleted of the lighter component and the reflux ratio continually increases. The stage is terminated upon reaching a maximum economic reflux ratio or the desired still composition. This technique can be extended to a multicomponent mixture.

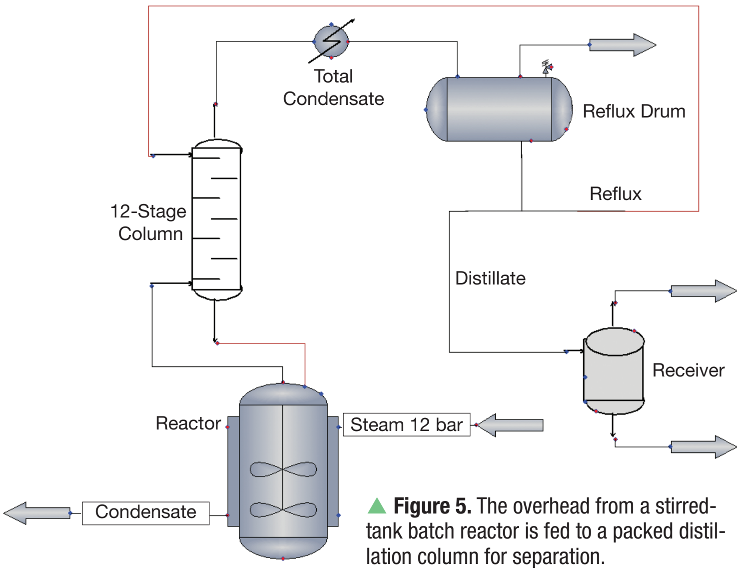
• Repetitive-total-reflux operation requires that the unit operate at total reflux until equilibrium. Once equilibrium is achieved, distillate is withdrawn for a short period of time before returning to total reflux. This technique is useful when separating trace components with low boiling points.

• Minimum-time operation also involves varying the reflux ratio. It is the most cost-effective mode of operation that can achieve the desired separation.

The simulation in Figure 5 shows a typical batch distillation arrangement that includes a jacketed stirred-tank batch reactor, packed column, overhead condenser, and a single



▲ **Figure 4.** This plot depicts the pressure at the exit of the relief device on Vessel 1 in Figure 3 during emergency relief of the two tanks at about 1.2 min and 1.7 min.



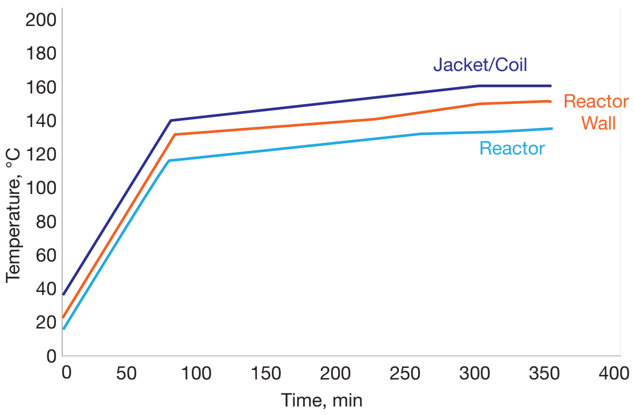
▲ **Figure 5.** The overhead from a stirred-tank batch reactor is fed to a packed distillation column for separation.

accumulator (receiver). This format replicates actual plant operations by considering equipment specifications, utility conditions, and variable parameters such as heat-transfer area. Plotting the resulting component compositions and key parameters allows for study and optimization.

The boil-up rate achievable with jacketed stirred-tank reactors depends on many factors, including the operational temperature difference, jacket heating media, and heat-transfer considerations *(5)*. Consider the distillation of a mixture of methanol (MeOH), ethyl acetate (EtAc), and water at 10 bar(a) pressure using 11 bar(g) steam on the jacket. The distillation is carried out at a constant reflux ratio of 5.7. Residue curve plots indicate two azeotropes:

- EtAc/H_2O, 85.1/14.9 wt% at 150.1°C
- MeOH/EtAc, 74.4/25.6 wt% at 136.1°C.

Plotting the reboiler temperature, bottoms composition, and heat-transfer area enables analysis of cycle times and separation characteristics. The temperature chart in Figure 6 shows the heat-up time and control system behavior. A key consideration is the temperature difference driving force, as this determines the rate of heat transfer. The driving force is the difference between the temperature of the vessel contents and the utility stream maximum temperature. The wall temperature can also be important for sensitive materials.



▲ **Figure 6.** The temperature difference driving force is the difference between the utility stream maximum temperature and the temperature of the vessel contents. In this case it is approximately 20°C, which enables sufficient heat transfer to the vessel contents.

A bottoms composition chart shows the component separations and cycle time for the set reboiler duty and reflux ratio. To test the material handling strategy, consider the continuous or intermittent addition of feed material to the reboiler or at some point in the column.

Charts that show the varying heat-transfer area enable the analysis of the impact of composition changes on heat-transfer behavior in the reboiler. The simulation also allows for the detailed study of thermal behavior and component physical property data.

If component physical property data and thermodynamics are known with confidence, dynamic simulations of batch distillation can save time and money related to laboratory analysis, while also providing scale-up data for equipment selection.

Dynamics with process control

Engineers need only a basic understanding of process control fundamentals to implement and study dynamics with process control.

All processes contain the dynamic elements dead time and capacity. Dead time is the interval, after the application of an action, during which no response is observed. Capacity is a location where mass or energy can be stored. These dynamic elements determine the ease of control, the control strategy, and control loop behavior in terms of speed of response and stability. Simple feedback control loops can be configured, tuned, and tested to obtain optimal stable performance, as well as to identify interactions within the process.

Conventional process controllers have three tuning parameters, which are used to minimize or eliminate error between the setpoint and the measured value and achieve stable control:

- proportional band (P, %), controller gain is 100/P — increasing P reduces the controller output change in response to error
- integral action (I, min) — increasing I eliminates error but reduces the speed of the controller output change
- derivative action (D, min) responds to the rate of change of the measurement.

Table 1. Recommended control parameters for different process characteristics.

Property	Flow Liquid Pressure	Gas Pressure	Liquid Level	Temperature Vapor Pressure	Composition
Dead time	No	No	No	Variable	Constant
Capacity	Multiple	Single	Single	Multiple	Single
Period	1–10 sec	Zero	1–10 sec	Min to hr	Min to hr
Linearity	Square (Orifice)	Linear	Linear	Non-linear	Either
Noise	Always	None	Always	None	Often
Controller Parameters					
Proportional	50–250%	0.5–5%	5–50%	10–100%	100–500%
Integral	Essential	Not Required	Yes	Yes	Essential
Derivative	Never	Not Required	Never	Yes	If Possible
Valve	Linear	Equal %	Linear	Equal %	Linear

Table 1 summarizes the process characteristics and the control parameter settings and provides a useful starting point for selecting controller parameters *(6).*

Control valve sizing and characteristic selection are critical for stable and effective control. Incorrectly sized valves can cause model convergence problems and unstable conditions. Dynamic simulation can help ensure suitable valve specifications. Valve rangeability is based on the ratio of the maximum to minimum controllable flows, with typical values being 50 for valves with equal-percentage characteristics and 33 for valves with linear characteristics. Most simulators have control valve sizing options, which should be verified against the manufacturer's sizing software.

The control valve can be operated in various modes (fail open, fail closed, split range) to allow a simulation to drive the valve to the desired condition. Control valve positions can be set manually or automatically from the assigned controller.

Advanced control loops involving cascade control, ratio control, and override techniques can all be simulated. In cascade control, the output of one controller, called the primary or master, manipulates the setpoint of another controller, called the secondary or slave. Each controller has a separate measurement, and the secondary controller manipulates the controlled device. Ratio control is frequently used in ingredient formulation, where any number of streams can be set in ratio to one independent stream whose flow is set according to production requirements. Auto-select (override) control is used in situations where two or more variables must not exceed limits specified based on economics, efficiency, or safety considerations.

Control systems should not be used to overcome shortcomings in plant design. If a processing unit takes a long time to achieve stable and optimal operating conditions, surge tanks can help hold feed streams constant.

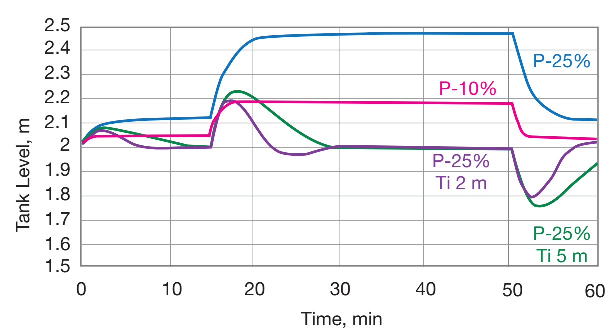
Control loop tuning. Dynamic simulation can elucidate control system behavior, and can be used to train operators on controller tuning. Trainers can develop application-specific simulations to demonstrate process control behavior of continuous processes, such as heat exchanger networks and distillation units, and batch processes involving reactions and distillations.

Consider the tuning of a level controller on a surge tank (Figure 7). The surge tank's liquid level is controlled by manipulating the outlet flowrate when the tank is subjected to a rapid increase in the inlet flow, followed by a rapid decrease. A simulation of this scenario can be adapted to evaluate variations in process surges, retention times, and control valve sizing.

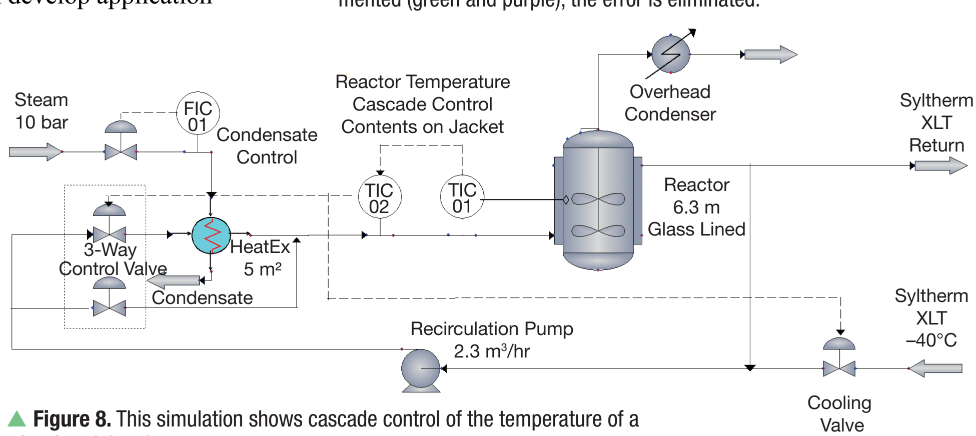
Batch reactors. Simulation can be used to establish process cycle times that are limited by heat-up and cool-down characteristics. The thermal stability of exothermic reactions can be tested based on known reaction kinetics, the transient physical properties of the reaction mix, and heat removal considerations such as mixing and heat exchanger performance.

The simulation shown in Figure 8 features a stirred-tank reactor using indirect heating with a heat exchanger and direct cooling on the jacket. The jacket recirculation system uses a heat-transfer fluid that floats on the return line, allowing for thermal expansion and contraction.

To eliminate thermal lag, the control system uses cascade control. The reactor contents temperature controller (TIC01) output sets the reactor jacket inlet temperature controller (TIC02) setpoint, which manipulates the three-way control valve and cooling valve in split range to represent a three-way valve. The heat exchanger has a constant steam supply pressure of 10 bar(a) to ensure that condensate return is



▲ **Figure 7.** The flowrate to a tank is variable and the flow from the tank is controlled by level control. The controller's tank level setpoint is 2 m, and the inlet flow increases at 15 min and decreases at 50 min. With only proportional control (blue and pink lines), there is no error control and the tank level does not reach 2 m. When proportional-integral control is implemented (green and purple), the error is eliminated.

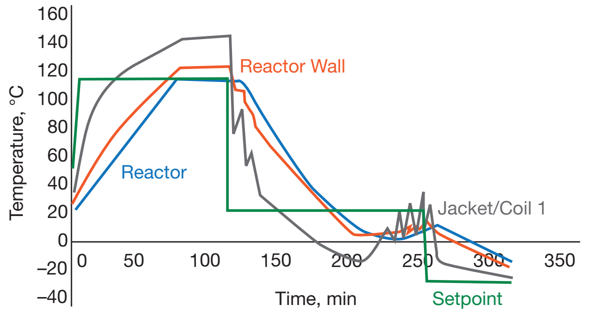


▲ **Figure 8.** This simulation shows cascade control of the temperature of a stirred-tank batch reactor.

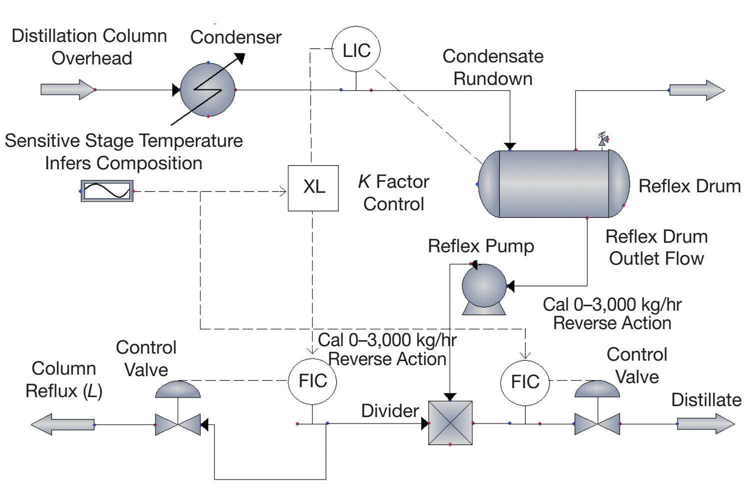
maintained under all load conditions.

Figure 9 shows the reactor temperature controller (TIC01) setpoint profile, which has a maximum temperature during the heat-up and reaction phases followed by two cool-down phases, alongside the reactor contents, reactor wall, and jacket inlet temperatures for the same period of time. The charts depict the heat-up rate based on maximum heat input, but on approach to the setpoint, the controller avoids any temperature overshoot. The hold period is followed by a cool-down period. This simulation allows for accurate prediction of the cycle time and demonstrates acceptable thermal stability.

Distillation column overhead feed-forward control (2). Feed-forward control balances the material and energy supplied to the process against the demands of the load by predicting process lags and manipulating flowrates. Feed-forward control is often applied to balance the firing rate of fuel to a boiler with the steam demand.



▲ **Figure 9.** The controller setpoint reaches a maximum (110°C) during heat-up and reaction, and then decreases for two periods of cooling. The cascade control scheme effectively maintains the reactor temperature, which never overshoots the maximum setpoint temperature.



▲ **Figure 10.** The composition of the overheads from this distillation column are controlled by a feed-forward control scheme in which output of the level controller and the distillate flowrate determine the reflux flowrate.

During processing, some material and energy are stored within the process, due to capacity effects of retention time and heat retention by equipment metal, which change as the throughput changes. Ultimately, feedback control is required to trim the feed-forward model parameters and maintain the required output specification.

The distillation column overhead control system in Figure 10 improves distillate composition control response characteristics by introducing lead-lag features to the reflux flow control. These are introduced by using the reflux drum's level controller output in the reflux flow calculation.

The distillate flow is set directly by the composition controller output. The simulation is linked to Excel, enabling exchange of parameters and calculation of the reflux flow (L) from the distillate flow (D) and the reflux drum level controller (LC) output m using the equation: $L = m - KD$. The coefficient K sets the lead-lag ratio, while the lag time varies with the retention time of the reflux drum and the level controller tuning parameters. Figure 11 illustrates the relationship between the K value and the reflux flow.

Online process simulation. Process optimization with online simulators is now recognized as a useful management tool to achieve optimal asset utilization and performance. This technique has been applied successfully to continuous process plants using steady-state simulators in a pseudo-dynamic mode, where process data is sampled on a timed interval basis and compared to the steady-state simulation results. Dynamic process simulators can replicate equipment performance and process behavior under real plant conditions, and can be used to provide powerful process optimization capabilities.

For online optimization to be a success, the simulation must be calibrated to represent the real process, and it must be operationally robust. Once a process simulation has been calibrated, the potential for improving plant performance and operational efficiency is significant. The simulation can help the engineer to proactively identify process and equipment problems.

The user interface is based on a SCADA system, which provides a graphical user interface (GUI) of the process plant together with typical controller faceplates and process parameter displays. This setup provides access to the process and equipment parameters in the model, allowing detailed dynamic study for optimization of design and control system performance.

System integration involves the automated data exchange of plant process and equipment parameters between SCADA and the process models.

This technique enables:

• optimization of process yield and control system performance

• prediction of unmeasurable parameters, including fluid physical properties

• data reconciliation, troubleshooting, and instrument fault diagnosis

• condition monitoring of equipment (*e.g.,* ensuring optimum operation of rotating machinery and detection of fouling in heat exchangers)

• calculation of economics to reduce manufacturing costs and save energy

• environmental auditing and reporting.

Training simulator. Digital twins or virtual plants developed through dynamic simulations can be used to reproduce normal or abnormal plant operations in a training environment. The simulation can be adapted to emulate startup, shutdown, and process control system functions. The twin can be used to study process responses, interactions, and effects of control loop tuning parameters to improve plant safety and operational performance, as well as reduce costs.

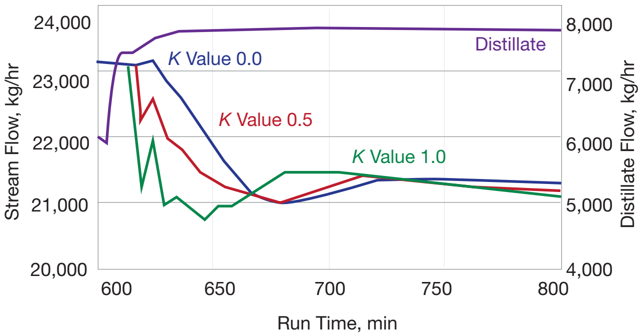
Instructors can generate process changes and upsets in the advanced training simulator and the trainee can respond to these changes on a remote workstation. The simulation can be linked to a simple GUI, using simulator connection features or a SCADA, set up to replicate the operating plant. Depending on the simulation, trainees can practice stopping and starting pumps, driving valves open and closed, tuning controllers, selecting control valve sizes and characteristics, and introducing power failure conditions.

Closing thoughts

Dynamic simulations can help users better understand transient behavior of batch and continuous processes to save time and money during plant design, commissioning, operation, and training, as well as ensure safe operation. Batch distillation procedures can be optimized to increase yields and reduce cycle times, and exothermic reaction behavior can be studied to gain insights into thermal stability and emergency relief behavior. Transient conditions during continuous processes, such as feed changes and utility upsets, can be better understood and managed. Process control system configurations can be tested and optimized to provide stability and increase yields.

Safety is a critical concern for processing facilities, and hazard and operability (HAZOP) studies are frequently used to identify unsafe scenarios. These studies are based on discussion and experience, whereas dynamic simulation provides a more rigorous technique for determining maloperation, equipment failure impacts, and proposed actions. Training based on dynamic simulations can also help test operator responses to process changes and equipment behavior or failure and help them to understand process control.

Dynamic simulation has not been universally accepted due to the perceived difficulty in its application and the investment in engineering time to develop the models. Fortunately, a detailed knowledge of process control technology is not required to obtain significant benefits from optimizing the design and operating procedures. CEP



▲ **Figure 11.** When the *K* value is 0, the reflux flow is determined only by the level controller. It experiences a significant lag and slow rate of change. The larger the *K* value, the larger the effect changes in the distillate flow have on the reflux flow.

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