Model-based predictive control increases batch reactor production

Better dynamic control of the temperature in an exothermic chemical reactor allows increasing the injection of reactants

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After a feasibility study, Repsol YPF decided to apply a model-based predictive controller to a batch reactor producing polyols. The predictive controller for reactors (PCR) is a set of control modules that are designed to face most of the reactor configurations. The important increase of production is a consequence of the better handling of the reactor temperature. Here's a description of the unit and control objectives, methodology, project steps, results and the corresponding benefits.

Process description and specifications. The Chemicals Division of Repsol YPF operates a large petrochemical complex in Tarragona, Spain. Among the plants of the facility, a polyols reactor (Fig. 1) has been selected by the producer as a good candidate for a control technology able to significantly improve stability of the unit.

This reactor is operated in fed-batch; a first product is introduced into the tank and heated. Then, while several reactants are injected, the exothermic reaction requires efficient cooling to respect a temperature setpoint and avoid reaching a too-high limit.

The temperature setpoint value is defined by the following trade-offs:

• Highest possible value because that increases the reaction strength and, therefore, speeds the production

• Low enough to keep it far from the high limit because of the usual temperature fluctuations.

The product is heated by steam injected into a coil inside

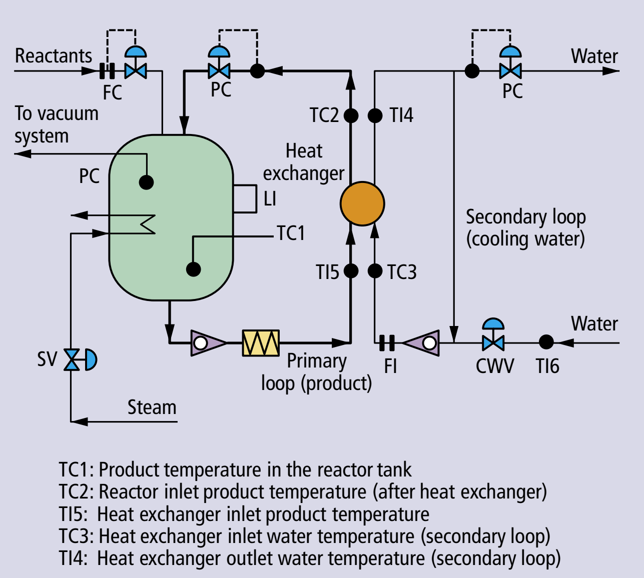


FIG. 1 Simplified process diagram.

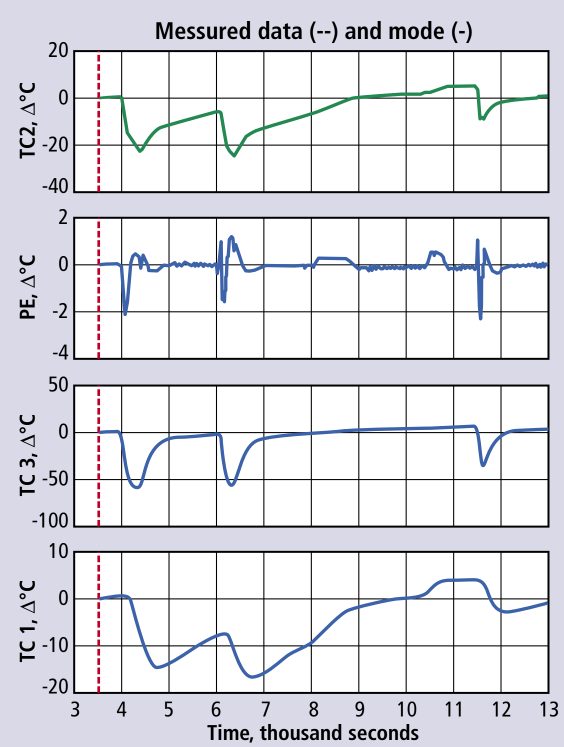


FIG. 2 Part of the identification results. TC2 is explained by TC1 and TC3. The error signal, PE, is reasonably small compared to the total TC2 moves.

Predictive controller for reactors model

The model, which is embedded in the controller, is a mathematical equation that computes a "model" output that is comparable to the process output *PV*. The model represents the relationship linking the process input(s) to the process output.

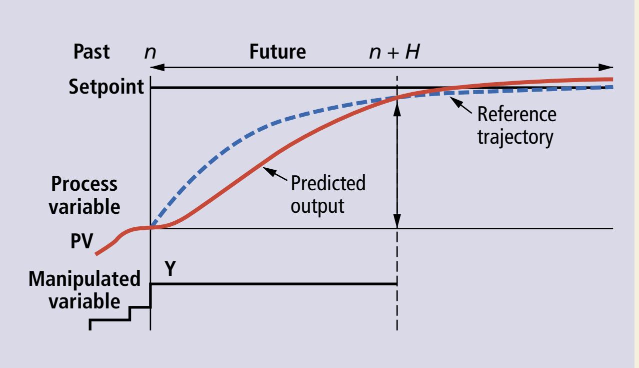
This model must be identified: the model parameters are estimated by an identification algorithm that exploits data collected during a specific experiment. The model is used to predict the process output and compute the control action to satisfy a given target specified on the *PV*.

In the case of PCR, the model is built in such a way that its structure is very close to the architecture of the process equipment (jacket, heat exchangers, steam injection, mixers, varying tank level, etc.). This model structure is very helpful for the control design phase.

Future desired trajectory. At present, n, the process output *PV* is PV_n and the setpoint value is SP_n. The future desired trajectory (so-called reference trajectory) is the desired behavior of the process output to move from its present value PV_n to SP_n in the future.

The reference trajectory is computed by a first-order system (see figure) and the time response of this trajectory is the closed-loop time response: the *PV* will respond to a setpoint step change with the time response given by the user. The closed-loop time response is here a specification. An intermediate target is selected along that trajectory at a future time, $n + H$, where H is called the prediction horizon.

Solver. The solver is the part of the controller that computes the control action to be applied in such a way that the predicted output at time, $n + H$, is equal to the reference trajectory at the same future instant. The computed control action takes into account the constraints that limit the input moves (high and low limits and rate of change).



Reference trajectory is computed by a first-order system.

Self-compensation. Some nonmeasured variables may disturb the process and have an effect that cannot be predicted by the model (because the disturbance is not accessible to the controller). A bias could be the result of that situation, mainly in case of integrative processes. The self-compensation, installed in the controller, is a procedure that avoids such a bias.

Control blocks. The PCR control blocks are designed to fit with most of the process equipment that can be seen around chemical reactors. These blocks include very useful procedures to solve the classical problems usually met on such units such as the oscillating split-range or the actuator saturations that are not transferred to the upstream controllers of a cascaded control or the tracking error when following the specified temperature profile. The control equations embedded into the PCR control blocks are such that these aspects are explicitly taken into account. **HP**

the reactor tank. Product cooling is obtained through a heat exchanger that circulates cooling water. The actuators (steam and water cooling valves) have very different dynamic effects on the reactor temperature. Once the product is heated in the tank, the reactant is injected into it and produces an exothermic reaction. The reactor temperature must be controlled at a constant setpoint during that injection. In case the temperature gets too high, the injection flowrate must be decreased.

The specified objective is to improve temperature control performance. Difficulty in controlling the temperature is due to:

- Link between the actuators and the temperatures is integrative with time delays.
- Heating and cooling actions affect reactor temperature with very different dynamics, which limits performances of the usual split-range control.
- Nonlinearities in the manipulated variable require a specific controller.

The consequences of improving the temperature control are usually:

- Improved quality by better temperature stability
- Shorter batch duration by better temperature profile tracking
- Higher unit availability by longer lifetime of the valves (less activated)
- Decrease of marginal costs through smaller consumption of utilities.

Model-based predictive controller technology and tools. The proposed technique, PCR, is a model-based predictive controller. The methodology relies on a dynamic model of the process to be controlled. The estimated model, describing the relationships between the manipulated variables (actions) and the temperatures to be controlled, makes possible predicting behavior of these temperatures and computing the actions to be applied to the unit.

PCR is a set of control modules. Some are specific to chemical reactors such as temperature profile tracking.

These control modules can be used profitably on this reactor since the performance of traditional PID controllers is not good enough. This is generally the case if the process is integrative, if there are some measured disturbances and the dead-time is

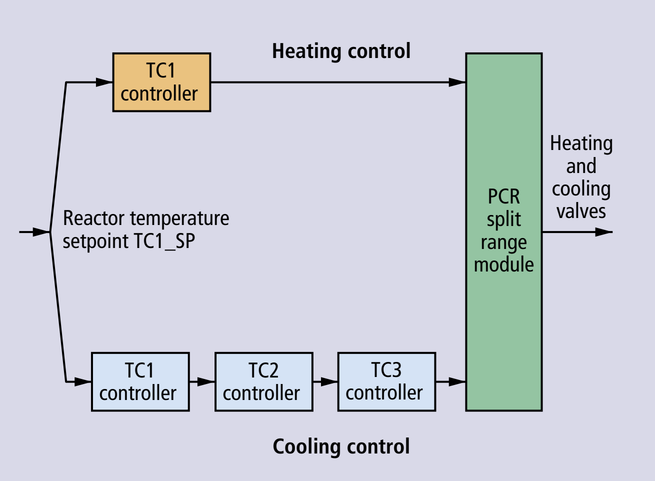


FIG. 3 Control architecture. The reactor temperature is controlled through cascaded PCR controllers according to the process architecture.

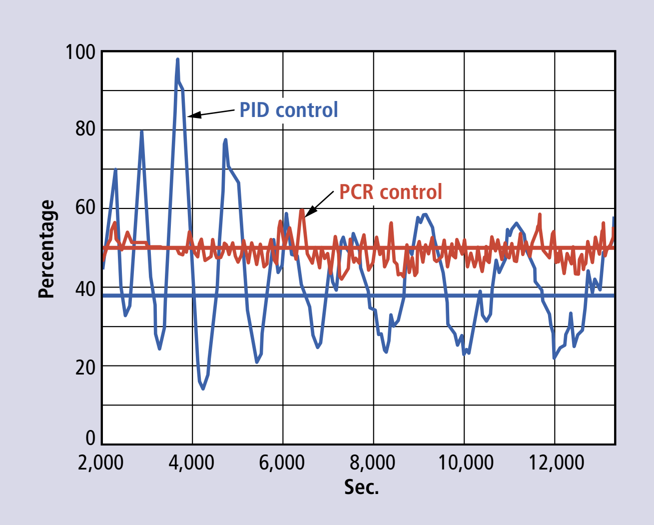


FIG. 4 Improvement in the reactor temperature control is significant.

important.

The PCR modules are designed and programmed in such a way they can be easily embedded into PLCs or DCS boards.

Project steps. The first project step is to establish the model structure corresponding to the architecture of the equipment of the unit: jacket, heat exchangers, mixers, heat device, etc.

The model parameter values are then estimated from data recorded during specific plant tests: voluntary moves applied to the heating and to cooling actuators when the reactor tank contains dead load (see example Fig. 2). When the reactant feed rate is measured (which is the case in the present project), it is considered a feed-forward variable and its effect is also identified from collected data during regular batch runs.

The controller is then designed (Fig. 3) and applied on a simulation of the process based on the identified dynamic model. Simulated closed-loop and robustness tests are performed to ensure that the controller keeps on running with acceptable accuracy even in case of process-model mismatch.

After its integration into the control system, the designed controller is validated. Then the global controller is applied progressively to the real reactor.

Results. The improvement in the reactor temperature control is significant (Fig. 4).

The fluctuations were reduced at least by half. That makes it possible for the producer to increase the temperature setpoint closer to the high constraint.

This improvement has an effect on several aspects: less valve movement (longer process availability) and no further competitive actions between heating and cooling (energy saving).

Although these items have a nonnegligible impact on savings, the most significant benefit clearly comes from the fact that the producer could push the process to its limits thanks to PCR control performance.

Total batch duration is reduced due to the increase of the injection flowrate of reactants. Such an increase is now possible because the temperature deviations have been reduced. Thus, a higher mean temperature is achievable thanks to the PCR controller giving more flexibility to the cold valve to deliver the necessary cooling.

Depending on the recipe, production increase coming from the upward shift of the temperature setpoint is estimated between 17% and 20%.

Another consequence of better unit handling is the capability to perform reproducible operating conditions for the different batches and, therefore, to obtain a more uniform product quality. **HP**

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Jacques Papon is a senior control engineer for Sherpa Engineering Corp., Nanterre, France. His duties include feasibility studies and advanced control projects for industrial applications of multivariable predictive control techniques. He performed technology transfers to control systems manufacturers and to several engineering companies in the world. Mr. Papon has prior experience at Adersa, where these techniques were developed 30 years ago.