Using digital process twin technology to drive Operational Excellence

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A practical approach to creating value for chemicals, petrochemicals & refining operating companies

Digitalisation of process operations is not something new. Rather, it represents the combination and increasingly widespread adoption of several technologies that have matured over the last two decades – sensor technologies for generating large quantities of data, IT developments that provide the means to transmit information rapidly across the organisation, continual increase in computational power, and the maturing of analytical technologies such as modelling and numerical solution technology.

Digital replicas of operating assets that combine deep process knowledge in the form of high-fidelity process models with live plant data are now bringing a new level of decision support to operations in refineries and petrochemicals plants. The combination of plant data and predictive model is enormously powerful, turning raw data into highly useful information that can be used to generate value in many different ways.

Analysts McKinsey state that by collecting and interpreting (or applying analytical methods to) the enormous amounts of plant data now available “it is possible to achieve higher yields and throughput, lower energy consumption and more effective maintenance”. They maintain that, using such techniques to promote “functional excellence in manufacturing operations”, it is possible to achieve a 3 to 5 percent return in production operations, and that for many companies these are potentially easy wins that can be achieved using existing IT and process control systems.

But how are these substantial benefits achieved in practical terms? The specifics are often quite vague. This paper defines a set of technologies and methodologies that can be applied to virtually any large process plant, using an ethylene plant as an example.

A. The Digital Process Twin: combining deep process knowledge and plant data

One of the key ways is to create digital process twins that couple deep process knowledge in the form of predictive process models with the enormous amount of data generated by most chemical plants. These are then used to derive new, high-value information that can be used in a variety of ways to support better-informed and faster decisions on a range of operational aspects, in a way that cannot be achieved using plant data alone. The process is shown schematically in Figure 1.

Digital Process Twins

![Digital Process Twin applications and the relationship between model and data](image)

Digital process twins: key characteristics

The term digital twin typically refers to a digital replica of physical assets, processes and systems that can be used for various purposes, for example to optimise the operation and maintenance of the asset or system.

A digital process twin has several important characteristics. Those relevant to this discussion are:

1. It embodies a core of deep process knowledge in the form of detailed physics and chemistry relationships describing the process.
2. It continuously updates itself (or is updated) in real-time to ensure that it reflects current plant operation and status as closely as possible.
3. It typically applies software analytics with real-time data to turn data into useful information that can be acted upon by operations and maintenance personnel to increase value.
4. It integrates information from a variety of sources – not just plant data, but business systems that provide data such as current product prices and feedstock costs, or plant maintenance and scheduling information.
5. It typically fulfils a single purpose – for example, the applications listed in section B.
6. It typically operates in an automated or semi-automated fashion within the appropriate plant information system – for example, the automation system or management information layer (though certain applications may be available for execution on demand).

In creating a viable digital process twin, two key requirements are a high-fidelity predictive model of the process and a means to keep the model up-to-date to reflect current plant state.
1. Key requirement 1: the ability to predict

At the heart of the digital process twin concept is a predictive mathematical model of the asset. Where possible, this is typically a high-fidelity model based on chemical engineering first-principles relationships describing the process physics and chemistry, with empirical model parameters such as reaction kinetic constants validated against real-life data.

For example, a catalytic reactor model may contain detailed physics and chemistry models of the overall reactor heat and material balances, catalyst-filled tubes within the reactor shell, the catalyst beds within the tubes, down to the pellets in the beds, including such phenomena as reaction, multicomponent diffusion, heat transfer and so on. It may also contain a catalyst deactivation model in order to model the change in catalyst performance over time.

The model would typically be validated before use by fitting key empirical model parameters (for example, reaction kinetic parameters) to observed data in the form of laboratory or pilot plant data. Figure 3 shows the progress of a typical parameter estimation exercise. If performed diligently, this ensures that the model is predictive across a range of scales and operating scenarios. This is essential for effective functioning of the digital process twin.

The models developed in this way differ from statistical models that use machine-learning techniques to determine the relationship between process variables. Such models may reflect the patterns and scenarios similar to the ones on which they are trained reasonably well, but cannot be relied on to predict anything that is outside their experience. Nevertheless, where knowledge of physics and chemistry is unavailable, it is possible to augment the first-principles model with data driven models to create a hybrid model.

High-fidelity predictive models are now a well-established part of many chemical companies’ standard toolset. Often created for optimising the plant design, they can be readily transferred into the operational sphere.

2. Key requirement 2: keeping it real – aligning the model with the current plant state

While they provide unprecedented accuracy for design, such models do not necessarily describe day-to-day plant operation well. The performance of key items of equipment changes over time due to long-term degradation processes, such as deactivation of catalyst, accumulation of coke in cracking furnaces, drift in column tray efficiencies and so on. All of these have important effects on plant...
operation, and some of them can have a major effect on plant economics, for example due to the need to take cracking furnaces out of operation for cleaning.

Knowledge of the current state of the key plant equipment is an absolute pre-requisite for producing an accurate real-time view of what is happening within each unit at any particular time, especially with respect to ascertaining how close the plant is to violating important operational constraints – such as maximum tube metal temperature (TMT) in cracking furnaces, or flooding limits in distillation columns – and for predicting the future behaviour of the plant starting from its current state.

Establishing the current state of equipment is quite challenging for many plants. The information from the plant itself is also subject to many types or error – instrumentation may drift or otherwise be faulty, flow measurements are notoriously inaccurate, data may be missing, and so on.

A central part of the digital process twin approach is the use of long-term equipment monitoring techniques. These use advanced mathematical computations combining

- nonlinear dynamic models of the key plant units that incorporate sufficient physical understanding of the operation of these units, as described above
- all data made available from plant sensors and potentially other sources (e.g. offline analysis where available) with varying degrees of accuracy

to provide a reliable, continually updated estimate of the current state of equipment.

The long-term monitoring approach exploits the redundancy between the ‘perfect’ data generated by model predictions and the imperfect but up-to-date plant data, to determine selected quantities of particular importance for representing an accurate picture of current operation. Examples can range from parameters for catalyst deactivation or coking kinetic equations to instrument errors on specific instruments.

The above approach is very different to commonly used steady-state data reconciliation techniques. In particular, instead of relying only on current plant measurements, the underlying mathematical techniques process simultaneously plant data from transient plant operation over a finite time window without the need for the plant operation to settle to a near-steady state.

Such an approach also has the benefit of effectively being self-calibrating, by virtue of the fact that the twin continuously updates itself to maintain its accuracy as new data is received from the plant. This means that it also captures the effects of disturbances or changes in operation on the parameters in question – for example, the effect of ‘coke-inducing’ feed impurities on the current furnace coking rate.

**B. Applying digital process twins to create value**

The information from the long-term monitoring calculation can be useful in its own right for equipment and process health monitoring. For example, in a catalytic reactor, knowledge of the catalyst deactivation state provides valuable information to operations and maintenance personnel for planning of maintenance schedules; it is even possible to use the information to adjust the unit’s operation in order to meet required schedules.

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However, going beyond this, the up-to-date plant model resulting from the health monitoring twin can be applied in a range of other digital process twins to provide valuable information about the current process operation, or decision support information for future operations, each creating value in its own right. These typically involve generating:

- predictions of maintenance requirements for various operating scenarios, based on e.g. accurate run length prediction
- information about the current plant state that cannot easily be determined by other means – for example, soft-sensed measurements of important but hard-to-measure quantities, or conditions internal to a unit or equipment
- predictions of future operation, for example, look-ahead what-if scenarios, for operations decision support
- optimal set points for current or envisaged operation, or optimal trajectories for feedstock or grade change scenarios, to maximise plant economic performance.

Some typical applications are described below.

1. Prediction of long-term performance – e.g. run length prediction

Many chemical and petrochemical process run for a limited time before cleaning, regeneration and/or replenishment activities are required. For example, it is typically necessary to regenerate or replace catalyst periodically in catalytic reactors, or to de-coke furnace coils every 1-3 months, or clean fouled heat exchanger tubes every year or two. Long-term performance prediction is particularly applicable to equipment that is subject to such gradual degradation, especially when this requires the equipment to be taken off-line for maintenance.

A digital process twin for run length prediction can estimate the remaining run time as accurately as possible, based on current equipment state as determined by long-term health monitoring and taking into account the anticipated operation. This provides decision support information on the economic impact of undertaking maintenance or not, and also allows operations to investigate the impact on long-term performance of different operating scenarios.

Long-term performance prediction is normally carried out under a user-specified operating scenario involving:

1. a time schedule of planned actions (e.g. gradual decreases to the COT set point in a cracking furnace)
2. a time profile of disturbances that may affect the system (e.g. normal feed flowrate over the next week, followed by 2 weeks of reduced feed availability, with the feed flowrate being restored to normal thereafter)
3. a set of criteria that may be used to decide the end of run, such as minimum conversion in a catalytic reactor, or maximum tube metal temperature (TMT) in a cracking furnace.
Such run length prediction can be executed by operations or maintenance personnel as required, at any time, and can be used to investigate the effect of different operational scenarios on catalyst regeneration, catalyst replenishment or de-coking schedule. Multiple operating scenarios may be proposed by the user, thereby allowing comparisons to be made among them with respect both to performance (e.g. total amounts of products generated over the remaining run-length) and to maintenance considerations (e.g. ensuring that maintenance of units may be staggered to ensure availability).

Long-term performance prediction requires a model of the unit that incorporates the slow dynamics associated with equipment degradation (e.g. catalyst deactivation, formation of coke, etc.). This is usually identical to the model used for long-term equipment monitoring.

The evaluation of each scenario involves performing a dynamic simulation starting from the current state of equipment degradation and making use of the up-to-date estimates of the degradation kinetic parameters; all of this information is automatically produced by the corresponding long-term monitoring application. The simulation progresses until one or more of the end-of-run criteria are met.

2. Real-time soft sensing

The aim of soft sensing applied to key equipment items is to produce real-time (typically minute-by-minute) estimates of KPIs such as yields and conversions, as well as key information about the internal state of the unit. For example, in a catalytic reactor it might be possible to provide real-time information on yields of impurities that cannot easily be measured, or temperature profiles through the bed. Soft sensors typically execute on a continuous 24/7 basis, making use of all plant measurements that are readily available in real-time.

This is achieved by using the digital twin model in combination with real-time plant data. The current state of the equipment (e.g. coking profile in steam furnaces, catalyst activity in acetylene converters, tray efficiencies in distillation columns) has already been estimated by the long-term monitoring application, and updated values for the parameters describing long-term degradation phenomena provided to the soft sensor.

Depending on the time constants of the equipment and the frequency of soft sensing, the underlying model may be steady-state or dynamic. In dynamic models, the soft sensor maintains an up-to-date best estimate of the dynamic state of the unit, for example the variables describing the material and energy holdups on each distillation column tray. This is particularly important in forecasting applications such as those involved in what-if studies described below. Indeed, because providing soft-sensed values involves solving the model, in reality all model variables are determined by the soft sensor and may be made visible to the user, providing a wealth of information about the operation.

Once it has been established that the model is predicting reliable values for the quantities of interest, by observing and verifying in open loop over a period of weeks to months, these variables can then be used in control – for example, conversion control for furnaces.

3. Operations decision support

What-if studies allow plant operation personnel to investigate the consequences of their proposed actions – for example, a change in reactor feed composition, or an increase in the hydrocarbon-steam ratio for a cracking furnace – and/or the implications of external disturbances affecting the unit under consideration – for example, a change in feedstock costs or product price, or reduced availability of cooling water. For units with very fast dynamics (e.g. cracking furnaces), the what-if analysis involves steady-state simulations with user-specified inputs.
On the other hand, the analysis of units with slow dynamics (e.g. distillation columns) requires a dynamic simulation starting with the current system state, i.e. the material and energy holdups determined by the soft-sensor. In such cases, the user may provide time profiles (rather than just instantaneous values) for any subset of the inputs affecting the unit. Such dynamic simulations are normally carried out for a relatively short period of operation – typically of a few hours or until steady-state is reached.

What-if calculations are typically executed mainly on demand. The underlying mathematical models are generally identical to those used for soft sensing.

4. Real-time optimisation

Ultimately much of the gain from applying digital process twin technology arises from *optimising the economics* of operation. This is done by executing a formal mathematical optimisation calculation to maximise an economic profit objective by varying multiple decision variables, while respecting equipment, product quality and other relevant constraints.

The up-to-date model incorporating the parameters determined by long-term monitoring can be executed continually to provide the operator with (a) a set of optimised set points for the key control variables in the process and (b) an indication of the economic benefit that can be realised by implementing the optimal set points. The operator can choose at any time to accept the optimal set points, which are then implemented on the plant. Once the operations team has built up confidence in the predictions, the loop can be closed.

C. Example: digital process twins applied to ethylene plant operations

Several of the applications listed above are illustrated for an ethylene plant using a series of digital process twins implemented in PSE’s gPROMS Olefins technology.

Each of the above elements deploys an appropriate high-fidelity model of the relevant part (e.g. furnace or furnace section) of the olefins plant. The overall gPROMS Olefins solution architecture is shown schematically in Figure 5.

Coking state is monitored on a daily basis using the gPROMS Olefins Coking Monitor. The coking state (i.e. thickness) and rate of coking information is then used for several further digital process twin applications to provide

- run length prediction for planning of operations and maintenance scheduling
- soft-sensed information for KPI monitoring and use in control
- real-time optimisation of the furnace section.
Digital process twin 0: Long-term furnace health monitoring

A gPROMS Olefins Coking Monitor installed on each furnace or cell (whichever is appropriate) performs long-term health monitoring. This uses a combination of live plant data and historical run data to determine the current state of coking and the rate of coke build-up, typically on a daily basis. The coking information – for example the thickness profile of coke in each coil – can be reported to the operations team for equipment health monitoring.

The coking calculation is self-adapting, being updated by plant data daily, and thus takes into account the effects of disturbances or changes in operation on coking rate. This means that it can also alert operators to events such as a sudden increase in the rate of coking.

This coking information is an essential pre-requisite information for the digital process twin applications for accurate furnace section optimisation and run length prediction. The daily-updated coking parameters are therefore implemented within the various digital process twin models performing the tasks described below.

Digital process twin 1: Run length prediction

Being able to predict when a furnace will need to be taken out of service for de-cokeing provides valuable information for Operations and Maintenance.
The Run Length Predictor predicts the end-of-run (EOR) for each furnace based on typical EOR criteria such as maximum pressure drop or maximum tube metal temperature (TMT), taking into account the current state of coking and anticipated operational profile between the current time and EOR.

Run length prediction can be executed by operations or maintenance personnel as required, at any time, and can be used to investigate the effect of different operational scenarios on de-coking schedule. It is possible either to maximise run length, minimise de-coking times, or to adjust operation in order to hit a certain EOR date to ensure two furnaces are not out at the same time.

Figure 7 shows an example of run length prediction applied to a cracking furnace cell. The prediction is performed at day 10 of the current run, and three different future operating scenarios are being considered, corresponding to conversion being held constant at 61% (red line), 60% (blue line) and 59% (green line) respectively. The actual run-length of the furnace is determined by when the tube metal temperature approaches the end-of-run criterion (1100 °C). More elaborate scenarios (e.g. involving gradual reduction in conversion over the remainder of the run) can easily be simulated.

**Digital process twin 2: Real-time soft-sensing and improved control**

The Cracking Monitor performs a minute-by-minute soft-sensing of key furnace variables such as product yield and conversion, and provides reliable real-time value for tube metal temperatures. The availability of reliable conversion information makes it possible to run the furnaces on closed-loop conversion control rather than traditional semi-manual coil outlet temperature control.

Figure 8 shows typical results obtained from a soft sensor applied to a cracking furnace. The predictions of the sensor are shown as red lines while actual plant measurements are shown as black points. The ethylene and propylene yield measurements shown in the top diagrams were not made available to the soft sensor; therefore, the results presented confirm the ability of the sensor to accurately estimate important KPIs that are not normally measured directly. For comparison, the grey lines show what a soft sensor would predict for a bare-metal (i.e. coking-free) tube. This emphasises the importance of coupling the soft sensor with a long-term equipment monitoring application that tracks the degree of coking.

Indications from large-scale plant applications show that through tighter conversion control it is possible to generate $5-15m per year in additional profit. This also provides for smoother operation, with less variation in ethylene and propylene yields in the cracked gas streams, helping to stabilise plant operation.
Digital process twin 3: Operations decision support

It is possible to use the up-to-date furnace models to perform what-if studies. These can be used to analyse the effects on the product value or other KPIs of proposed operator actions, external changes, disturbances or upsets – for example:

- change in reactor feed composition
- increase in the hydrocarbon-steam ratio for a cracking furnace
- change in feedstock costs or product price
- reduced availability of cooling water

What-if calculations are typically executed mainly on demand, from custom-configured screens that allow easy input of data and visualisation of results. The underlying mathematical models are generally identical to those used for soft sensing.

Digital process twin 4: Furnace section optimisation

The Furnace Optimiser digital process twin performs an economic optimisation of the furnace section by determining optimal values for decision variables such as conversion/severity in each furnace, as well as feed allocation between furnaces if required, taking into account the current operational demands, equipment availability, product pricing and demands and equipment and/or process constraints.

Because it is based on the current state of coking in each furnace (as determined by the Coking Monitor), the optimisation calculation is highly accurate and can be executed continually. This contrasts with existing approaches, where ‘optimisation’ calculations provide sub-optimal results because they do not take into account the current coking state, or it is necessary to wait for an approximate steady state (perform a steady-state detection) before executing the optimisation.

Figure 8 – Typical results from soft sensor applied to cracking furnaces

Figure 9 – gPROMS Olefins Furnace Optimiser running within a Siemens SIMATIC PCS 7 distributed control system
Furnace section optimisation is typically performed on a time scale of hours, or on-demand, with the optimiser returning optimal set points and potential gain in economic value. By default the optimiser is in open loop ‘advisory’ mode; the operator has a choice of whether to accept and apply the optimal set points or not. The optimiser can also be used as required to provide a ‘rapid response’ capability to ensure a rapid return to optimal operation follow a disturbance or equipment outage.

Again, by ensuring optimal severity / conversion profiles through the furnace section and optimal allocation of feedstock, the application of a digital process twin can result in millions of dollars in additional profit annually for a large ethylene plant.

D. Further essential ingredients and practical considerations

The McKinsey analysis says that “for many companies these are potentially easy wins that can be achieved using existing IT and process control systems”. While recent advances on modelling, computing and information technology mean that it may be relatively straightforward to access the benefits of digital operations, the following are essential ingredients.

1. Numerical solution power

The applications described above involve complex repeated calculations involving simultaneous solution of tens or hundreds or thousands of equations. It is essential to have a set of underlying calculation technologies that supports this, in order to perform complex calculations rapidly and robustly. In particular it is necessary to have:

- a robust equation-oriented solution engine capable of solving complex process models rapidly, including those involving multiple recycles. The sequential modular solution approaches found in many traditional process simulators are simply not up to the job.
- the ability to perform parameter estimation and state estimation calculations on large, complex models rapidly and robustly, for long-term monitoring and soft sensing
- a powerful, multi-variable optimiser to search for the optimal values of multiple decision variables simultaneously
- robust steady-state and dynamic simulation
- high-performance computing (HPC) capabilities that allows the parallelisation of calculations, and the ability to perform calculations on multiple cores or clusters, or in the cloud.

Modern solution engines such as PSE’s gPROMS platform have all of these capabilities as standard.

2. Robust online implementation

An essential requirement for online implementation and execution of models is a robust framework for importing and processing plant data, executing calculations and transferring calculation values back to the plant automation system, to other calculation modules, or to other information systems.

The gPROMS Digital Applications Platform (gDAP) shown schematically in Figure 10 provides an integrated software framework for the development and deployment of complex decision support systems for process operations such as the gPROMS Olefins suite functionality described above. It incorporates a number of separate software components, including:

- an External Data Manager that manages communication with the external data servers
- an Execution Schedule Manager that manages the timing of the execution of the various calculations and recovery from failure (for whatever reason) of any component
• Data Validation Modules that apply extensive validation to all data exchanged between the decision support system and the external data servers, and handle any cases of missing or invalid data.

• Computational Modules (CMs) corresponding to the different types of calculation required for the applications described in the section above (for example, parameter estimation, dynamic simulation, optimisation, and so on).

![Diagram of gPROMS Digital Applications Platform](image)

**Figure 10 – gPROMS Digital Applications Platform – schematic overview**

3. **Mechanisms for data transfer and delivery across the organisation**

It is essential that information is delivered to operations and maintenance teams, or across the plant networks to other applications or users. The information can be delivered at many levels:

1. The **plant automation system** or DCS, and associated Operations dashboards. For example, the optimal set points calculated by a real-time optimisation will be delivered to the operator screens for analysis or, in closed loop optimisation, may be implemented directly. Likewise, soft-sensed values may be delivered to the DCS for display and/or use in control.

2. The **Management information layer**, for plant KPIs and other operational data

3. The **Executive information layer**, for monitoring of overall (perhaps multi-site) KPIs.

In many cases information handling uses the facilities of the plant automation system or management systems. However in certain cases it is useful to have bespoke dashboards that gather together all relevant data in one place.

**Conclusions**

The application of Digital Process Twins that combine high-fidelity process models and plant data open up a wealth of new possibilities for creating new value for a typical plant operation with little or no capital expenditure. The advances in sensors, IT, modelling and solution technology mean that such applications are all achievable now, and are increasingly being adopted as part of Operational Excellence initiatives by the most competitive operators.