GOOD PRACTICE IN PYGAS HYDROGENATION OPERATIONS THROUGH ADVANCED PROCESS CONTROL

Advanced Process Control (APC) offers a solution to systematize the implementation of best practices to generate substantial benefits.

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In addition to producing the many basic chemical building blocks for the polymer industry, steam-cracking yields significant amounts of aromatic-rich gasoline (pygas), especially when naphtha is fed to cracking furnaces.

Before the pygas can be routed to downstream units, (aromatics extraction...) it is necessary to remove unstable compounds such as diolefins and styrenics. Olefins and sulfur must also be eliminated to ensure that final products will meet their specifications. This pygas treatment is achieved through hydrogenation steps.

However, if the pygas treatment operation is not optimized; there may be hydrogen flaring, reactor channelling, poor use of the second beds or other issues.

Advanced Process Control offers a solution to systematize the implementation of best practices, avoiding misoperation and generating substantial benefits.

This article describes the operational improvements and the steps necessary for the implementation of APC. A case study using real plant data demonstrates and quantifies the benefits that can be obtained from APC implementation.

Process

The discussion that follows describes the industrial results obtained with the two-stage pygas hydrogenation process (PGH or Pygas) depicted in Figure 2.

Table 1 shows typical pygas yield and composition and confirms that pygas is a large contributor to benzene production capacities.

Table 1 Typical naphtha cracker Pygas (C5-200°C) yield and composition

<table>
<thead>
<tr>
<th>Composition, wt%</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Paraffins + Naphthenes</td>
<td>11.8</td>
</tr>
<tr>
<td>Olefins</td>
<td>5.5</td>
</tr>
<tr>
<td>Diolefins</td>
<td>18.1</td>
</tr>
<tr>
<td>Benzene</td>
<td>28</td>
</tr>
<tr>
<td>Toluene</td>
<td>13.9</td>
</tr>
<tr>
<td>Xylenes</td>
<td>7.2</td>
</tr>
<tr>
<td>Styrene</td>
<td>3</td>
</tr>
<tr>
<td>C\text{+} Aromatics</td>
<td>12.5</td>
</tr>
<tr>
<td>Total Aromatics</td>
<td>64.6</td>
</tr>
</tbody>
</table>
One concern that cannot be ignored is that other processes are also hydrogen users, such as selective hydrogenation of C2, C3 and C4 streams.

In a situation of low hydrogen availability, these processes have priority.

As a consequence, pygas can reach a situation where the first stage is temporarily operated with insufficient hydrogen, which has negative consequences for the process performance and catalyst life.

When excess hydrogen is available it is important to reduce wasteful hydrogen flaring and to improve pygas operation by utilizing all the available hydrogen.

Efficient pygas operation can ensure that the best use is made of available hydrogen.

**Possible Operating Improvements**

There are four key areas which have the potential to deliver operational improvements. We will examine each in turn, describing the areas for improvement. These areas are: improving first stage product quality, reducing the risk of channeling, maximizing second bed usage and optimizing global hydrogen usage.

- **Improving first stage product quality to increase second stage stability**
  
  The product entering the second stage must be hydrogenated to the correct level, to prevent polymerization of any remaining diolefins or alkenyl-aromatics in the second stage reactor which is operated at higher temperature and in the vapor phase.

  If hydrogenation is not sufficient due to lack of hydrogen or a low temperature profile, there will be a high tendency to form gums at the inlet of the second stage reactor, generating unacceptable pressure drop and performance reduction.

  A good indicator of the hydrogenation of diolefins or alkenyl-aromatics is the styrene content of the first stage reactor product. Normally the styrene specification is set at 1500 ppm, for efficient protection of the second stage catalyst, coupled with reasonable catalyst cycles.

  Figure 4 presents a statistical distribution of the styrene content at the outlet of the first stage reactor on a plant without APC. The histogram is characterized by a small number of off specification values that could have damaged the second stage catalyst.
We can also observe the large proportion of product that is well below the required specification. This overquality is translated as a cost or give-away due to the unnecessarily high reactor temperature in the first stage that would have reduced the catalyst cycle.

**Figure 4** Typical Styrene statistical distribution in first stage reactor outlet (ppm wt from on-line analyzer)

If the diluent flow is too low, the hydraulic load of the catalytic bed may become too small, ending up with possible channeling problems.

- Reducing risk of channeling by appropriate diluent flow
  In the first stage reactor, the flow entering the reactor is mainly in liquid phase, and is constituted of fresh pygas feed, diluent cooled and recycled from first stage reactor outlet and hydrogen make-up (Figure 5).

**Figure 5** Diluent flow adjustment in first stage reactor

If the diluent flow is too high, the velocity in the reactor might be excessive, but more importantly, it will lower the average bed temperature, thus requiring a higher inlet temperature to maintain performance. This will negatively impact the stability of the catalyst.

The total flow to the first stage reactor (fresh feed + diluent), also called “Liquid Load” has to be adjusted to an optimal target value close to the design value, which produces the most continuous temperature profile. This is illustrated in Figure 6: with inappropriate Liquid Load, the irregular temperature profile reveals the occurrence of channeling.

**Figure 6** Improving from bumpy to smooth temperature profile with APC

Maximizing second bed usage by appropriate quench flow
In both pygas reactors (first and second stage) there is usually a quench injection, between the first and second bed, in order to control the reactor temperature profile.

Quench flow is often kept too high by panel operators in order to prevent temperature runaways.

In the first stage reactor, as illustrated in Figure 7, the consequences of excess quench flow are a lower bed Delta_T, resulting in lower hydrogenation levels in the second bed. This leads to increased styrene content in the product and to compensate, the first bed temperature is frequently increased which is detrimental to catalyst life cycles.
In reality, the hydrogen network pressure-control strategy implemented in the DCS can be much more complex than presented in Figure 8.

Using in-depth knowledge of DCS capabilities, Axens has developed a method to minimize hydrogen loss and further increase the hydrogen make-up to the pygas unit without affecting the network pressure.

This approach uses pressure controller parameters (setpoint, process value, valve opening, etc...) and dynamic models derived from step test data.

The benefits of this method are to deliver more hydrogen to the pygas unit and thus improve the hydrogenation performance.

**APC Strategy**

Axens has developed and implemented a successful APC strategy to optimize industrial pygas process operations. It incorporates the following points to improve the control of the process:

- **Feed flow maximization**
  Common practice is to place an intermediate product tank between the steam cracker and the pygas unit. The volume of this tank can usually absorb one day’s production of pygas. The inventory of this tank has to be minimized to reduce the risk of polymerization of the unsaturated components present in the raw pygas, until downstream constraints have been saturated.

- **Usage of all available hydrogen**
  Optimization of global hydrogen management, see description in previous section.

- **1st stage reactor**
  The first target is to perform ultra deep hydrogenation of diolefins and alkenyl aromatics, by controlling the styrene content, measured by an on-line analyzer, in the first stage product.

  The next step is to stabilize reactor operation, by controlling the reactor liquid load at a target optimized to avoid channeling.

  Hydrogen partial pressure is maximized, to promote hydrogenation by increasing the reactor pressure, to maximize the dissolved hydrogen fraction in the liquid phase, and to ensure a minimal gas purge flow, preventing concentration of inert species in the hydrogen recycle gas (applicable if the unit is equipped with a recycle gas compressor).
Temperature profile is optimized, using both reactor inlet temperature, diluent and quench flow to prevent temperature run-away, to balance reactor Delta_T between the two beds, and to maximize catalyst cycle length.

- **Fractionation:**
  APC needs to identify the right compromise between the quality of the separation and energy savings.

- **2nd stage reactor**
  The first target is to perform complete hydrogenation of olefins and sulfur removal, by controlling the bromine index and sulfur content of the reactor effluent.

  The next step is to minimize hydrogenation of aromatics, by avoiding operation at unnecessarily high temperatures.

  Finally, stable reactor operation will be achieved by the control of reactor Delta_T and by the control of hydrogen recycle gas density.

**Pygas Inference and Optimizer**

The pygas inferential model proposed for APC, schematized in Figure 9, is based on highly evolved kinetic models developed by Axens that enable on-line styrene content and bromine-index estimation, and consequently, reactor optimization.

Laboratory analyses of the first stage effluent are used to estimate the first stage feed quality (styrene content, bromine number and density).

The first stage reactor model integrates the estimated feed quality and measured reactor operating conditions, continuously inferring the first stage product quality: styrene, diolefins and bromine number.

Figure 10 illustrates the prediction of the styrene compared with on-line analyzer measurement.

![Figure 10 Styrene estimation in first stage effluent by first stage reactor model](image)

The second stage reactor model integrates estimated feed quality and measured reactor operating conditions, continuously inferring the second stage product quality.

![Figure 11 Bromine Index estimation in second stage effluent by second stage reactor model](image)

Using spot detailed analyses and collection of operating conditions, the user of Axens APC generates the best tuning parameters to fit the current operation, thus allowing “real-time” control moves to improve performance.

**Recommended APC Architecture**

All APC components are embedded in an APC Server connected to the DCS architecture, as depicted in Figure 12. The control and optimization application consists of the following modules:

- MVAC module: State Space Multivariable Predictive Controller
- Pygas Inference
- First Stage Optimizer
The application provides one-minute cycles for MVAC (the MVPC) and sixty-minute cycles for the optimizer. Controller execution time was determined by the process dynamics.

**Example of APC performance**

Here is a simple example of APC potential, illustrated by the application to a real pygas unit optimization.

The control matrix components are presented in Figure 13.

**Figure 13** Simplified APC variables used for simulation example

The inputs, or Manipulated Variables are:
- **Feed Flow**, to be maximized when available to reduce tank inventory;
- **H2 Flow**, used as long as available, to prevent flaring,
- **Reactor Inlet Temperature**, used to control styrene content, but minimized when possible to lengthen catalyst cycles
- **Quench Flow**, used to control styrene content.

The outputs, or Controlled Variables are:
- **Styrene in product**, which should stay below the maximum limit and

**Figure 14**: 8 hours closed loop APC simulation example

- **Styrene in Product** 1300 → 1500 ppm
- **Reactor 2nd Bed ∆T** 65 → 73 °C
- Reactor Second Bed Delta_T, which should stay below the maximum limit.

When APC is turned ON, the styrene analyzer is at 1300 ppm, below its 1500 ppm maximum limit and Reactor 2nd Bed Delta_T is at 65°C, below its 73°C maximum limit.

As far as the operation is concerned, Quench Flow is too high; resulting in excessive cooling of the second bed and reactor inlet temperature is too high, generating give-away on styrene specification.

More feed is available, the intermediate tank is not empty and additional hydrogen is available, but it is currently flared.

APC actions on the process, plotted in Figure 14, can be summarized as making use of all available hydrogen to reduce the styrene at the first stage reactor outlet and reducing Quench Flow as far as the Second Bed Delta_T allows: this will also reduce Styrene Content. Simultaneously, Reactor Inlet Temperature is reduced and Feed Flow is maximized within the constraints of the maximum Styrene Content limits.

By better operation of the second bed, and by the using the 10% additional hydrogen available, Axens’ APC was able to increase the production by 10%, while decreasing reactor inlet temperature by 4°C.

Conclusion
Advanced process control with inferential modeling has been successfully applied to operations in pygas hydrogenation units. The overall benefits observed from Axens’ APC installation are summarized as follows:

- On-specification product without give-away
- Ability to treat more feed +10%
- Reduction of first stage reactor inlet temp. - 4 °C
- Catalyst run length maximization
  months/current + 4
- Reduction of aromatics hydrogenation -10%
- Reduction of H2 waste to flare -10%
- Energy savings 5%

The lengthening of the catalyst run length limits downtime for both the pygas unit and upstream units such as the steam cracker.

An additional benefit observed by the operating staff was that, with the ease in setting targets and confidence that Axens’ APC system would meet these targets, they were free to concentrate on other plant activities.

Bibliography


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Gildas Rolland is Deputy Product Line Manager - Hydroprocessing & Olefins. He started his career in 1998 at IFP Energies nouvelles as a Process Engineer in the R&D department. In 1999 he joined the Process Design department of our North American office in Princeton and in 2001 moved back to Axens head-office where he served successively as Start-up and Tech Service advisor, specialist in Olefins Technologies including R&D activities related to technology and catalyst improvement. Gildas was appointed to his current position in 2010. Gildas is a graduate of the Ecole Centrale de Lille (E.C.Lille) and holds a Master's Degree in Refining and Petrochemicals from the IFP School.